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Carbon nanotubes and fullerites in high-energy and X-ray physics

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It is demonstrated that the unique structures of carbon nanotubes and single-crystals of C₆₀ fullerenes may have applications to X-ray, neutron and high-energy particle physics, based on channeling, Bragg diffraction and coherent radiation. These are reviewed, pointing out the peculiarities and advantages of nanocrystals compared to ordinary crystals. New applications are explored: X-rays and neutron channeling, undulator radiation in periodically bent nanotubes, "channeled" transition radiation. Quantum and classical channeling, channeling in bent nanocrystals, Bragg scattering of X-rays and neutrons, channeling radiation, coherent bremsstrahlung, parametric X-ray and nanotube undulator radiation are particularly studied using both analytical and Monte-Carlo methods. Continuous potentials, electron densities, transverse energy levels, and spectra of various types of coherent radiation are calculated. Large dechanneling lengths of positive particles, bending efficiencies, reflecting coefficients of soft X-rays and PXR yields are predicted. Principles of particle detectors using photo- and secondary electron emissions are discussed.

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1. Introduction

Fullerenes and *nanotubes*, recently discovered, are the building blocks of a new class of ordered materials [1,2]: spherical fullerene C_{60} molecules can assemble in fcc crystals called *fullerites* and single-wall nanotubes can gather in *ropes*, the cross section of which makes an hexagonal lattice. These structures, called *nanocrystals* differ from ordinary crystals in many points. In particular, they have spatial periods of the order of 1 nm, which is much larger than those of ordinary crystals (typically 0.2 nm). In addition, they are very inhomogeneous in density, being made of almost empty “cages” the walls of which are dense nets of carbon atoms. The above two features are advantageous for various applications in X-ray, neutron and high-energy particle physics, which are based on Bragg diffraction, channeling and coherent radiation. These phenomena, which also exist in ordinary crystals, are recalled below:

Bragg diffraction, channeling and coherent radiation: At first sight, a particle (electron, proton, photon, neutron, etc.) of sufficiently high energy penetrating a sample of condensed matter might be thought to “ignore” any microscopic ordered architecture of the latter. For instance, an electron having an energy much above the typical chemical binding energies (a few electron-volts) would undergo roughly the same processes in a crystal and in an amorphous solid or liquid: essentially random multiple scattering on target electrons and nuclei, energy loss by ionization and bremsstrahlung. This naive thinking has been refuted almost one century ago by the Laue- and Bragg-diffraction of X-rays in crystals [3] and later by the corresponding phenomenon for electrons [4] and neutrons. Another surprise was the discovery of charged particle channeling in crystals [5] which is the guiding of fast particles along atomic strings or atomic planes by many correlated small-angle scattering.

Whereas Bragg diffraction depends on the wave behavior of the particle, channeling is originally considered as an essentially classical phenomenon. Later, when electrons and positrons with relatively low (~ 10 MeV) energy were considered, it appeared that their motion transverse to main crystal axes or planes is quantized. This is the intermediate region where the motion may be considered either as multi-wave diffraction or quantum channeling.

There is no need to recall the numerous applications of Bragg diffraction in many branches of physics, industry and biology. The not so widely known phenomenon of channeling has found applications in solid state physics (impurity localization or ion implantation in crystals) and in high-energy particle physics (deflection of proton beams by bent crystals, measurement of the magnetic moments of short-living particles).

The electromagnetic radiation from ultra-relativistic electrons and positrons in condensed media has also many unusual features. At first sight, in hard X-ray and γ region there could not be interference between the radiations produced in particle collisions with different atoms. However, Landau and Pomeranchuk and then Ter-Mikhaelyan showed that the characteristic length for radiation in this case is much longer than the wavelength and the coherence may exist. In amorphous media the coherence is always destructive and leads to the suppression of bremsstrahlung described by usual Bethe–Heitler theory. On the contrary, as shown by Ferretti, Uberall and Ter-Mikhaelyan, in crystals the coherence can be constructive giving rise to the *coherent bremsstrahlung* (CB) the spectral density of which can be a decimal order higher than in amorphous media. Channeling effects restrict the catastrophic growth of CB at relatively small angles between the particle velocity and a crystallographic axis, nevertheless on channeling conditions, electrons or positrons emit X- and γ -rays with a larger intensity than bremsstrahlung in amorphous matter as well. Coherence mechanism can be used as a source of high-energy photons for particle physics or to enhance the efficiency of positron sources. Another specific kind of radiations emitted by electrons and positrons

in crystals is parametric X-rays (PXR). It may be considered as a consequence of Bragg diffraction of the proper electromagnetic field of the charged particle. The useful quasi-monochromatic spectra and linear polarizations of both CB and PXR come from constructive interferences between the radiation fields generated by successive, periodically spaced, atomic planes or rows. More detailed information about channeling of high-energy particles in crystals and associated phenomena can be found in review articles [6–9].

The advantages of nanocrystals: All the phenomena described above are expected to occur in fullerites and nanotube ropes as well, since these have a crystalline structure, but with the following important particularities and advantages:

- The large spatial periods allows to extend Bragg reflection of X-rays and thermal neutrons down to the nanometer wavelength domain, which is not possible with ordinary crystals.
- In fullerites and nanotube ropes the modulation depth of the atomic and electron densities is large while the X-ray absorption is relatively low. This is a condition for having a good Bragg reflectivity, a large yield of PXR and of coherent bremsstrahlung. It is not fulfilled by ordinary macromolecule crystals with comparable periods.
- The channeling potentials wells of nanotubes are sufficiently deep and broad to allow an efficient capture of positive particle beam in channeling states. Moreover, for nanotube ropes, the low electron and atomic density inside the channels makes their channeling more stable than in ordinary crystals, due to a much smaller number of incoherent scatterings on substance electrons and thermal vibrations of atoms.

In addition, nanotube tips may be used as cathodes for electron emitting devices (e.g. electron guns for accelerators) thanks to their very sharp ends which favors field emission. Good photo-emission and secondary electron emission yields can be also used for new photon and charged particle detectors.

2. Structure, electric potentials and electron density of nanocrystals

2.1. Continuum potentials and electron density of nanotubes

2.1.1. Geometrical structure of a nanotube

A carbon nanotube can be regarded as one gigantic carbon molecule (fullerene) which is obtained by folding graphite planes into a cylinder whose diameter is measured in nanometers and whose length can reach macroscopic dimensions [2]. This linear structure determines the extremely high mechanical strength of nanotubes [10] whereas their electrical conductivity depends strongly on the diameter and the helicity which is the angle between the most highly packed chains of atoms and the axis of the cylinder [11]. There exist nanotubes whose walls contain a single layer of atoms (*single-wall nanotubes*, or SWNT) [12] and nanotubes with walls consisting of several concentric or onion-like layers (*multi-wall nanotubes*, or MWNT) [13]. A remarkable feature of some single-layer nanotubes is their capability, as they grow from a plasma, to unite into a “rope” whose transverse cross section is a two-dimensional hexagonal superlattice [14]. Since the discovery of nanotubes in 1991 by Iijima [13], a large number of papers have appeared on the problems of synthesizing nanotubes, on their physical properties and on possible applications in nanoelectronics [15], catalysis [16] and other fields. It is also noteworthy that,

Fig. 1. Structure of an unrolled nanotube wall (left) and of the cross section of a nanotube rope (right).

besides carbon nanotube ropes, ropes of “inorganic” nanotubes made of boron nitride [28] and tungsten disulfide [29] have been discovered. In this report we restrict ourselves to carbon nanotubes.

Let $\mathbf{a}$ and $\mathbf{b}$ denote the basis vectors of a planar lattice of graphite, whose unit cell (dashed rhombus in Fig. 1a) contains two carbon atoms of coordinates $(\mathbf{a} + \mathbf{b})/3$ and $2(\mathbf{a} + \mathbf{b})/3$, respectively. Taking account of the fact that the angle between the vectors $\mathbf{a}$ and $\mathbf{b}$ is $\pi/3$ and the vectors have the same modulus ($a = b$) and denoting by l the length of the bond between the carbon atoms (which is usually 0.14 nm), we obtain $a = b = l\sqrt{3}$. The roll-up vector $\mathbf{r}_0$ is determined as a linear combination $\mathbf{r}_0 = n\mathbf{a} + m\mathbf{b}$ of the basis vectors, where the pair (n, m) of integers is called *the indices* of the nanotube. The nanotube may be considered as a strip of width r_0 , marked up by dashed lines in Fig. 1a, cut out of the graphite carbon plane perpendicularly to $\mathbf{r}_0$, rolled-up in a cylinder and closed at either end with caps containing carbon pentagons in a manner that conserves bonding length. The angle ϑ between $\mathbf{r}_0$ and the lattice vector $\mathbf{a}$ defines the corkscrew symmetry of the nanotube and is called *helicity* or *chiral angle*. The helicity is also equal to the angle under which the most closely packed chains of carbon atoms are wound on the cylindrical surface of the tube. As follows from simple geometry, the nanotube indices (n, m) uniquely define the nanotube diameter d and helicity ϑ

$$d = \left(l\sqrt{3}/\pi \right) \sqrt{n^2 + nm + m^2}, \quad (2.1)$$

$$\vartheta = \arctan \left[\sqrt{3}m/(m + 2n) \right]. \quad (2.2)$$

Since the basis vectors $\mathbf{a}$ and $\mathbf{b}$ are equivalent, it can be assumed with no loss of generality that $n \geq m$ and therefore the helicity lies in the range $0 \leq \vartheta \leq \pi/6$. SWNTs with $m = 0$ ($\vartheta = 0^\circ$) are labeled as *zigzag*, tubes with $m = n$ ($\vartheta = 30^\circ$) are labeled as *armchair*, all other tubes (between $\vartheta = 0^\circ$ and 30°) are *chiral*. The structures of the different SWNTs are presented in Fig. 2. The concentric nanotubes of a MWNT are necessarily arranged in an incommensurate manner as they have different diameters and different helicities.

Fig. 2. Structure of (10, 10) armchair, (20, 0) zigzag and (16, 5) chiral nanotube.

It is easy to show [17] that the spatial symmetry of a SWNT along its axis is determined by the following translational vector:

$$\mathbf{t} = q^{-1}[(2m + n)\mathbf{a} - (2n + m)\mathbf{b}] , \quad (2.3)$$

which occurs to be orthogonal to $\mathbf{r}_0$ (indeed, $\mathbf{t} \cdot \mathbf{r}_0 = 0$) and thus directed along the nanotube axis z . The integer $q = \text{gcd}(2m + n, 2n + m)$ denotes the greatest common divisor of its arguments, therefore the modulus t of vector $\mathbf{t}$ represents the main spatial period of a nanotube along z . Thus in physics terms an isolated nanotube can be treated not only as a giant carbon molecule, but also as a one-dimensional single crystal of a period t and with $4(n^2 + nm + m^2)/q$ atoms in the unit cell. SWNTs can be either metallic or semiconducting, depending on their structure. In particular, calculations of electronic band structures show that all armchair nanotubes ($n = m$) and zigzag or chiral nanotubes with integer $(n - m)/3$ are metallic. In other cases nanotubes are semiconducting with an energy gap near 0.5 eV.

2.1.2. The nanotube continuum potential

It is noteworthy that channeling was primarily discovered as a result of computer simulations of ion beam propagation along atomic rows in a crystal, based on binary collisions of ions with atoms [18]. After the experimental evidence of channeling effect [19] Lindhard [20] gave a simple theoretical explanation of it. He showed that if a fast charged particle enters a single crystal at small enough angle θ_0 with respect to an atomic row, it is governed by the *continuum potential*, i.e. the actual periodic potential of the rows averaged over the direction parallel to the rows. For the case of an isolated atomic row the continuum potential $V_R(\rho)$ can be written as

$$V_R(\rho) = (1/d_R) \int_{-\infty}^{\infty} u \left(\sqrt{\rho^2 + z^2} \right) dz ,$$

where $u(r_a)$ is the atomic potential, r_a is the distance from the atomic nuclei, ρ is the distance from the row, z the coordinate along the row and d_R the average distance of neighboring atoms along the row. Due to the thermal vibrations of the crystal the atoms have small displacements from the z -axis. The velocity of channeled particles is usually so high that the interaction times with individual atoms are much shorter than the thermal vibration periods. Thus, the particles interacts with atoms at effectively stationary positions and the continuum potential experienced by the particles should be averaged over the thermal displacements of the atoms as well.

Erginsoy [21] went further and in the case of a small enough angle with respect to a family of atomic planes (but far from directions of main crystallographic axes) he introduced the continuum potential of the planes. For the case of an isolated atomic plane the planar continuum potential can be presented as

$$V_p(x) = (1/S) \int \int u \left(\sqrt{x^2 + \rho^2} \right) d^2 \rho ,$$

where x is the distance from the plane, $\rho = \{y, z\}$ are the coordinates along the plane and S is the average area of the plane occupied by one atom. Similar to the case of the row the additional averaging over the thermal displacements of the atoms from the plane is needed.

The concept of continuous potential can be applied to a particle entering a nanotube rope at small angle to the tube axes. For this case, it is important to note that a nanotube with indices (n, m) can always be represented as a collection of $2N$ atomic rows parallel to the axis of the nanotube and arranged in a definite manner along the perimeter of the cylinder. It is interesting to note that the total number of rows $2N$ (sometimes overlapping) coincides with the number of carbon atoms in the unit cell of a nanotube (Appendix A). Thus the exact continuous potential is of the axial type, and not of the planar type as suggested by the simple picture of a rolled graphite plane. Accordingly, the continuum potential of a nanotube can be written as

$$U(\mathbf{r}) = \frac{1}{d_R} \int_{-\infty}^{\infty} \sum_{i=1}^{2N} u(\mathbf{r} - \mathbf{r}_i, z - z_i) dz , \quad (2.4)$$

where $u(\mathbf{r} - \mathbf{r}_i, z - z_i)$ is the potential of a carbon atom number i with coordinates $(\mathbf{r}_i, z_i)$ in the nanotube unit cell. In general, the distance d_R between the neighboring atoms within such a row coincides with the modulus of the translational vector $\mathbf{t}$ and is given by

$$d_R = (3l/q)(n^2 + nm + m^2)^{1/2} . \quad (2.5)$$

Let us take into account the fact that the unit cell of a graphite plane shown in Fig. 1a contains two carbon atoms and the surface density σ of atoms on the plane is $\sigma = 3^{-3/2}4l^{-2}$. The pair of the unit cell atoms generates two sequences of atomic rows parallel to the axis of the nanotube. In each of the sequences the rows are equally spaced around the cylinder. We choose a cylindrical coordinate system (r, φ, z) in which the radial coordinate r is measured from the axis of the tube, and we denote by $\varphi_k^{(\mu)}$ the azimuthal angle of the k th row ($k = 0, 1, 2, \dots, N - 1$) in the corresponding sequence of rows ($\mu = 1, 2$). Thus each sequence contains exactly

$$N = (2/q)(n^2 + nm + m^2) \quad (2.6)$$

atomic rows, whose azimuthal coordinates are determined by the relations

$$\begin{aligned} \varphi_k^{(1)} &= k\delta\varphi, \quad \delta\varphi = \pi q / (n^2 + nm + m^2) , \\ \varphi_k^{(2)} &= \varphi_k^{(1)} + \Delta\varphi, \quad \Delta\varphi = \pi(n + m) / (n^2 + nm + m^2) . \end{aligned} \quad (2.7)$$

We note two limiting values of the helicity $\theta = 0$ and $\pi/6$ where the atomic rows, parallel to the axis of the nanotube, have the largest linear density and therefore the number of the rows is relatively small. The first case corresponds to zigzag nanotubes $(n, 0)$; here, $q = n$, $N = 2n$, $d_R = 3l$, $\delta\varphi = \Delta\varphi = \pi/n$,

and the two row sequences overlap, i.e. there are actually $2n$ rows with a doubled linear atomic density $2/d_R$. This overlap does not occur with zigzag nanotubes exclusively, but is found, for instance, in chiral nanotubes with $n = 2m$. The other case corresponds to armchair nanotubes (n, n) ; here $q = 3n$, $N = 2n$, $d_R = l\sqrt{3}$, $\delta\varphi = \pi/n$, $\Delta\varphi = 2\pi/(3n)$, i.e., there are $4n$ rows arranged in pairs.

From the regular distribution of the rows around the nanotube, it appears that the continuum potential, written as a function of the polar coordinates (r, φ) is a periodic function of the azimuth φ , of period $2\pi/N$. To perform the summation in (2.4) it is useful to expand first the continuum potential of an individual atomic row in Fourier series of azimuthal harmonics

$$V_R = \sum_{v=-\infty}^{\infty} V_v(r) e^{iv\varphi} . \quad (2.8)$$

Here r is the distance from the axis of the nanotube and φ is the azimuthal angle around this axis which is counted from one of the atomic rows. Using the above expansion we may represent the continuum potential of a nanotube with arbitrary indices (n, m) as [17]

$$U(r, \varphi) = 2N \left\{ V_0(r) + 2 \sum_{s=1}^{\infty} V_{sN}(r) \cos[\pi s(n+m)/q] \cos[sN\varphi - \pi s(n+m)/q] \right\} . \quad (2.9)$$

(Note that the azimuthal period is no more 2π but $2\pi/N$.) Thus, the task is reduced to the standard calculation of the continuum potential of a row, however the latter must be presented as a function of the distance r from the nanotube axis.

To derive the expansion coefficients $V_v(r)$ in (2.9) it is convenient to choose an appropriate analytical approximation to the atomic potential $u(r_a)$ or its Fourier transform $f(\mathbf{k})$. In a first approximation we may neglect the influence of the covalent bindings between the neighbors on the distribution of valence electrons which are responsible for the nuclear charge screening at relatively large distances from the nuclei, in other words, we may consider carbon atoms as isolated. Under this assumption analytical calculations of the nanotube potential (2.9) become possible at least in two commonly used forms of atomic potential $u(r_a)$. The first one corresponds to the Moliere approximation [22]

$$u(r_a) = \frac{Ze}{r_a} \sum_{j=1}^3 \tilde{a}_j \exp\left(-\frac{\tilde{b}_j r_a}{a_{TF}}\right) . \quad (2.10)$$

Here $\{\tilde{a}_j\} = \{0.35, 0.55, 0.1\}$ and $\{\tilde{b}_j\} = \{0.3, 1.2, 6.0\}$ are three pairs of universal empirical constants, $a_{TF} = 0.529 Z^{-1/3} \text{ \AA}$ is the Thomas–Fermi atomic radius, Ze is the non-rationalized nuclear charge and r_a is the distance from the nucleus. Calculations of the expansion coefficients (2.8) using (2.10) give us the following result [17]:

$$\begin{aligned} V_v(r) &= (2Ze^2/d_R) \sum_{j=1}^3 \tilde{a}_j I_v(\tilde{b}_j r/a_{TF}) K_v(\tilde{b}_j R/a_{TF}) \quad \text{at } r \leq R , \\ V_v(r) &= (2Ze^2/d_R) \sum_{j=1}^3 \tilde{a}_j K_v(\tilde{b}_j r/a_{TF}) I_v(\tilde{b}_j R/a_{TF}) \quad \text{at } r \geq R , \end{aligned} \quad (2.11)$$

where $R = d/2$ is the nanotube radius, d_R is determined by (2.5), K_v and I_v are the modified Bessel functions. Since the Moliere approximation is based on the Thomas–Fermi model, it may be not enough accurate in the case of light atoms like carbon, however Cox and Bonham [23] improved the accuracy using a form of atomic potential similar to (2.10): a_{TF} is removed, more pairs of empirical parameters are used which for carbon have the following values:

$$\begin{aligned}\tilde{a}_j &= \{1.5022, 0.1591, 1.8307, 1.8309, -2.4146, -1.5629\}, \\ \tilde{b}_j &= a_0^{-1} \{1.4662, 12.7644, 3.8463, 6.2618, 3.0492, 5.3504\},\end{aligned}$$

where $a_0 = 0.529 \text{ \AA}$ is the Bohr radius. Another approximation, accurate enough and convenient for the further analytical calculations of continuum potentials, is based on the expression for the Fourier-transformed potential $f(\mathbf{k})$ given by Doyle and Turner [24]:

$$f(\mathbf{k}) = 4\pi Ze \sum_{j=1}^{j=4} a_j \exp[-\mathbf{k}^2/(4b_j^2)] . \quad (2.12)$$

Here

$$\begin{aligned}a_j &= \{3.222, 5.270, 2.012, 0.5499\} \times 10^{-4} \text{ nm}^2, \\ b_j &= \{10.330, 18.694, 37.456, 106.88\} \text{ nm}^{-1}\end{aligned}$$

are dimensional parameters which were determined from the condition of the best fit of (2.12) to the most accurate calculations of $f(\mathbf{k})$ based on the Hartree–Fock method. The discrepancy of (2.12) with the tabulated values of $f(\mathbf{k})$ [25] is not larger than 0.6% up to $k = k_{\max} = 126 \text{ nm}^{-1}$ which corresponds to a distance from the nuclei shorter than the thermal vibration amplitude of atoms in the rows (see below). Using (2.12) we find the expansion coefficients of (2.9) in the form

$$V_v(r) = (4Ze^2/d_R) \sum_{j=1}^4 a_j b_j^2 \exp[-b_j^2(r^2 + R^2)] I_v(2b_j^2 Rr) . \quad (2.13)$$

The zero azimuthal harmonic ($s = 0$) in expansion (2.9) corresponds to the continuum potential of a nanotube averaged over the azimuthal angle [47,50]. The remaining harmonics lead to an azimuthal modulation of the potential. As the number of atomic rows forming the walls of a nanotube increases, the modulation frequency increases and the amplitude of the modulation decreases. The distance between the neighboring rows (in each of the two sequences) is determined by $\delta = 3^{1/2} 2^{-1} q l (n^2 + nm + m^2)^{-1/2}$. If δ is much less than the range of the atomic potential, then the analysis of (2.9) shows that the higher order azimuthal harmonics ($s \geq 1$) are negligibly small and we obtain the following axially symmetrical potential of a nanotube:

$$U(r, \varphi) = 3^{-3/2} 32\pi Ze^2 l^{-2} R \sum_{j=1}^4 a_j b_j^2 \exp[-b_j^2(r^2 + R^2)] I_0(2b_j^2 Rr) \quad (2.14)$$

for the Doyle–Turner approximation (2.12) and

$$U(r, \varphi) = 3^{-3/2} 16\pi Ze^2 l^{-2} R \sum_{j=1}^4 \tilde{a}_j K_0(\tilde{b}_j R/a_{TF}) I_0(\tilde{b}_j r/a_{TF}) \quad (r \leq R) \quad (2.15)$$

Fig. 3. Azimuthal profile of the potential barrier $U(R, \varphi)$ of nanotubes with various indices (n, m) . The curves correspond to different indices: curve 1—(10, 10), 2—(17, 0), 3—(12, 8). The horizontal straight line 4 corresponds to nanotubes with intermediate helicity, for example, (11, 9).

for the Moliere approximation (in outside region $r \gg R$ we should permute I_0 and K_0). In the general case the azimuthal dependence of the height of the potential barrier $U(R, \varphi)$ of nanotubes with different indices (n, m) , based on (2.9) and (2.13), is illustrated in Fig. 3. The curves correspond to different indices of the nanotube: curve 1 to indices (10,10); 2—(17,0); 3—(12,8). The horizontal straight line 4 (azimuthal symmetrical case) corresponds to nanotubes with parameter q defined in (2.3) which is much less than N , for example (11,9).

According to Fig. 3, in armchair and zigzag nanotubes the continuum potential should be treated as the sum of the corresponding row potentials while in chiral nanotubes with intermediate helicity it is close to the continuum potential of the (rolled-up) graphite plane. This is similar to the transition from axial to planar channeling in ordinary crystals.

Expressions (2.11) and (2.13) describe continuum potential of a static atomic row. Small displacements of the atoms of a nanotube relative to their equilibrium positions in an ideal lattice can be due to thermal vibrations (what we call “thermal vibrations” is in fact the sum of purely thermal vibrations and the quantum zero-point vibrations of the lattice) as well as other factors (for example, structural defects). In general, thermal vibrations of atoms in nanotubes are anisotropic and can be taken into account by introducing an additional factor (the Debye–Waller factor) of the form e^{-W} in the Fourier transformed atomic potential (2.12). The exponent is given by

$$W = (1/2)(k_r^2 u_r^2 + k_\tau^2 u_\tau^2 + k_z^2 u_z^2) ,$$

where u_r^2, u_τ^2, u_z^2 are the mean-square deviations of the atoms in the different directions: normal to the circumference of the cylinder (r), tangential (τ), and along the axis of the cylinder (z). Accounting for the thermal vibrations, the expansion coefficients (2.8) take a form more complicated

than (2.13):

$$V_v(r) = \frac{4Ze^2}{d_R} \sum_{j=1}^4 \frac{a_j}{\sqrt{\beta_j^{(r)} \beta_j^{(\tau)}}} \exp \left[-\frac{R^2}{\beta_j^{(r)}} - \frac{r^2}{2} \left(\frac{1}{\beta_j^{(r)}} + \frac{1}{\beta_j^{(\tau)}} \right) \right] \sum_{\mu=-\infty}^{\infty} I_{\mu}(\gamma_j) I_{v-2\mu}(\alpha_j), \quad (2.16)$$

where $\alpha_j = 2Rr/\beta_j^{(r)}$, $\gamma_j = (1/\beta_j^{(\tau)} - 1/\beta_j^{(r)})r^2/2$, $\beta_j^{(r)} = b_j^{-2} + 2u_r^2$, $\beta_j^{(\tau)} = b_j^{-2} + 2u_{\tau}^2$. To estimate the effect of thermal vibrations on the continuum potential of the nanotube it is necessary to know the temperature dependence of the radial and tangential vibrational amplitudes (due to the averaging along z longitudinal vibrations is not important for the continuum potential). In absence of the experimental values of u_r^2 and u_{τ}^2 it may be reasonable to assume that they are close to the corresponding values $u_{\perp} = 8.5 \times 10^{-3}$ nm and $u_{\parallel} = 3.8 \times 10^{-3}$ nm in graphite (at room temperature) [26]. As numerical calculations showed [17], the influence of thermal vibrations on the continuum potential happens to be relatively small. An other effect of thermal vibrations is the fluctuations of the actual potential around the continuum potential which cause incoherent scattering of channeled particles. The channeling theory beyond the limits of the continuum potential approximation will be considered in Section 5.

2.1.3. Longitudinally averaged electron density in a nanotube

X-rays are scattered primarily by the electrons of the material. The recoil may be taken by individual electrons (Compton), individual atoms (Raleigh) or by the crystal as a whole (Bragg). In the latter case, the “scattering potential” is roughly proportional to the time-averaged local electron density. The spatial distribution of the electron gas also determines the importance of the incoherent scattering of channeled particles on these electrons; this will be discussed in Section 5. The Fourier component of the electron density in a carbon atom can be approximated [25] to an adequate degree of accuracy by an expression

$$f^{(e)}(\mathbf{k}) = Z \sum_{j=1}^5 a_j^{(e)} \exp[-k^2/(2b_j^{(e)})^2], \quad (2.17)$$

similar to (2.12), but where

$$a_j^{(e)} = \{0.3499, 0.3014, 0.2103, 0.0946, 0.0438\},$$

$$b_j^{(e)} = \{17.300, 11.400, 75.501, 155.24, 7.596\} \text{ nm}^{-1}$$

are five pairs of fitting parameters which are determined to obtain the best fit of (2.17) to the corresponding values calculated by the Hartree–Fock method and the experimental values of X-ray scattering amplitude. With help of (2.17) the electron density averaged over the z -coordinate is found quite similarly to what was done in the case of electric potential.

2.1.4. Ion channeling

Let us now consider ion channeling. The potential energy of a point particle in the field of an atom is just the product of the atomic potential and the electric charge of the particle. In the case of ion channeling the situation may be much complicated due to the screening of the nucleus of the ion by the remaining electrons. Nevertheless, it is possible to obtain an analytical expression for the effective potential of ion–atom interaction, if we assume, as is usually done in the theory of ion channeling [5], that: the velocity of the ion is small compared to the velocities of electrons on outer orbits; the electron energy

levels of the ion and carbon atoms considered as a function of ion–atom separation do not intersect at any impact parameters. Under the above conditions we may neglect the processes of electron loss or charge exchange between the colliding particles. Let us represent the electron distribution in an ion with nuclear charge $Z_1 e$ as

$$f^{(x)}(\mathbf{k}) = Z_1 \sum_{m=1}^{N_1} a_m^{(x)} \exp(-k^2/4b_m^{(x)2}) ,$$

where N_1 is the number of pairs of fitting parameters needed for a good approximation and the sum of $a_m^{(x)}$ equals the number of electrons of the ion (or atom) divided by Z_1 . Then, assuming that the ion cloud does not deform in the nanotube field, the effective potential for carbon + ion scattering may be given, in Fourier space, by

$$f_{\text{ion}}(\mathbf{k}) = 4\pi Z Z_1 e \sum_{j=1}^{N(1+N_1)} A_j \exp(-k^2/4B_j^2) . \quad (2.18)$$

Parameters A_j, B_j are connected with the known parameters for the scattering form factors of electrons (2.12) and X-rays through the following relations $A_j = a_j, B_j = b_j$ for $j \leq N$, $A_j = -a_i a_m^{(x)}, B_j^2 = b_i^2 b_m^{(x)2} / (b_i^2 + b_m^{(x)2})$ for $N < j \leq N(1 + N_1)$, where i and m run from 1 to N or N_1 , respectively, N is determined as number of pairs of the parameters in (2.12). The case of the bare nucleus corresponds to $a_m^{(x)} = 0$ for all m . Since (2.18) conserves the functional form of (2.12) it enables to calculate the continuum potentials for ion channeling in a manner quite similar to the one used above for point particles using fitting parameters from [25].

From a formal viewpoint, the continuum potential of a nanotube is the zero term of the expansion of the actual potential in Fourier series along the nanotube axis z (Appendix A). The other terms are generally speaking not small in amplitudes, but according to (2.3) they oscillate with periods t/v , where $t = |q^{-1}[(2m + n)\mathbf{a} - (2n + m)\mathbf{b}]|$ and v is the integer. The oscillation periods of the actual potential occur to be much shorter than periods of channeled particle oscillation inside a nanotube and thus the periodic part of the potential causes only small perturbations of the smooth motion in the continuum potential. However, if the ion is channeling along a nanotube with velocity v_z such that vv_z/t coincides with a transition frequency between the electronic (nuclear) states of the ion, the periodic part of nanotube potential may cause resonant transitions between the states. This effect was first considered by Okorokov [27] for ordinary crystals. In nanotubes, the conditions for resonant atomic transitions may be more easily satisfied, because the periods t are relatively large (except for zigzag and armchair) and ions can have relatively long paths along the nanotube.

2.1.5. Continuum potentials of nanotube ropes

Up to this point we have been considering an isolated carbon nanotube, but, as noted above, nanotubes may unite in ropes. The two-dimensional superlattice of a nanotube rope (see Fig. 1b) has the hexagonal symmetry determined by the pair of the basis vectors $\mathbf{A}$ and $\mathbf{B}$, whose modulus is the period L of the superlattice. Nanotubes in a superlattice are kept in the position of equilibrium by van der Waals forces. The gap between the walls of neighboring nanotubes is usually about 3.15 Å which is close to the

inter-planar separation in graphite. For example, a superlattice with period $L \simeq 16.95 \text{ \AA}$, consisting of (10,10) nanotubes with diameter $d \simeq 13.8 \text{ \AA}$, has been observed by Thess et al. [14].

To obtain the continuum potential of a nanotube rope inside the superlattice unit cell (shown as hexagons in Fig. 1b) it is necessary to add the continuum potentials of a sufficient number of neighboring nanotubes. The continuum potentials of the ropes of (10, 10) armchair, (20, 0) zigzag and (16, 5) chiral nanotubes are illustrated in Figs. 4a, b and c, respectively. For positive particles there are relatively deep potential wells inside nanotubes, about 15.9 eV for (10, 10), 24 eV for (20, 0) and 60 eV for (16, 5), and very shallow (about 1 eV deep for all of the ropes) potential well between the nanotubes. It can be seen that chiral nanotubes have the deepest potential well. Analytical expressions for the Fourier transform of these potentials will be given in Section 3.1.

2.2. Continuum potentials of fullerenes

Fullerenes are molecular cages consisting of carbon atoms. The arrangement of the atoms is almost exclusively in the form of hexagons and pentagons. Nanotubes discussed in the previous subsection may be considered as a kind of fullerenes. Twelve pentagons and twenty hexagons make the famous C_{60} cage shown in Fig. 5. The C_{60} molecule contains a carbon at each vertex of the “truncated icosahedron”, C = C double bonds along the lines separating hexagons, C–C single bonds along the hexagon–pentagon boundaries, and has a diameter of roughly $7.1 \text{ \AA}$.

This cage was first identified experimentally by Kroto et al. [30]. These researchers were awarded the Nobel prize in Chemistry for their discovery in 1996. This structure might indeed impart unusual stability to the C_{60} cluster because all valences are satisfied. The proposed molecule was dubbed buckminsterfullerene because its shape is reminiscent of the geodesic domes popularized by Richard Buckminster Fuller (1895–1983), American architect and visionary. Bulk solid C_{60} is sometimes referred to as “fullerite” in analogy to graphite, and X-ray powder diffraction has shown [31] that fullerite adopts the face-centered cubic (fcc) structure with a relatively small van der Waals cohesive energy and a lattice constant $a = 14.17 \text{ \AA}$. Pure fullerite is a semiconductor with a band gap of about 1.6 eV. Fullerite does not appear to melt, but rather sublimates at low pressure. In addition, the molecules in fullerite freely rotate for temperatures above $\approx 257 \text{ K}$. At lower temperatures, they begin to “stick” at certain orientations and eventually, below $\approx 90 \text{ K}$ (the precise value depends on how fast the system is cooled), they become completely stuck. Besides, the low-temperature structure is no longer fcc but simple cubic. These cooling and phase transition processes has not been understood yet quite well.

Another interesting feature of fullerite is the ability of the C_{60} units to polymerize at high pressure (30–80 kbar) and high temperature (600–1000 K) [32] or under intense exposure to visible or UV light. The origin of this polymerization is the formation of covalent bonds between molecules. As temperature is increased, a continuous transformation occurs from fcc fullerite to an orthorhombic phase of polymerized C_{60} chains that, in turn, can polymerize to two-dimensional C_{60} polymers. Three-dimensional polymerization can lead to ultra-hard material, material which is harder than diamond [33]. The density of C_{60} formed as a fcc crystal at 298 K is 1.65 g cm^{-3} while the density of a new solid formed by 3D polymerization is 2.6 g cm^{-3} . Besides fullerenes consisting of C_{60} fullerenes, there exist similar molecular crystals consisting of “non-spheroidal” C_{70} molecules [34]. The fullerene derivatives (fullerides), such as compounds of fullerenes with alkaline metals, may also have a crystalline structure [35]. From the practical point of view, fullerites have still the evident advantage of being presently grown in single crystals of macroscopic dimensions, while existing nanotube ropes are available only as microscopic objects as

Fig. 4. Continuum potentials of the ropes of (10, 10) armchair (a), (20, 0) zigzag (b) and (16, 5) chiral (c) nanotubes.

Fig. 5. Schematic view of C–C bonds in C_{60} fullerene.

yet. The specific features of continuum potentials and channeling in C_{60} fullerites were first considered in [36,37]. Below we follow the results of these papers.

In the case of nanotube ropes discussed in the previous subsection the existence of a regular ordering between nanotubes is not necessary, at least for the channeling along the ropes. By contrast, for the channeling in 3D crystals, particularly in fullerites, the existence of perfect enough crystalline structure is crucial. There are 360 electrons in the C_{60} molecule, half of which are involved in typical covalent bonding between the atoms of the molecule. In a first approximation, neglecting the influence of the bonding on the spatial distribution of the valence electrons, we may calculate the total potential of C_{60} fullerene as a sum of atomic potentials centered at the vertices of the truncated icosahedron. In the following calculations we use the Doyle–Turner model (2.12) which gives the representation of atomic potential in real space

$$\varphi(r_a) = \frac{4Ze}{\sqrt{\pi}} \sum_{j=1}^4 a_j b_j^3 \exp(-b_j^2 r_a^2) . \quad (2.19)$$

We consider a normal fullerite crystal at room temperature in which fullerenes are not stuck at certain orientations or polymerized, but weakly bound with van der Waals forces, and can rotate freely. When a fast charged particle travels along a fullerene row in a fullerite it collides with randomly oriented molecules and in the first approximation it is reasonable to average the potential of a fullerene row not only over the longitudinal direction, but also over all angular coordinates of carbon atoms. As a result of the averaging over the random orientations we find the fullerene potential (for a positron)

in the form

$$U_1(r) = 60 \frac{Ze^2}{\sqrt{\pi}rR} \sum_{j=1}^4 a_j b_j [\exp(-b_j^2(r-R)^2) - \exp(-b_j^2(r+R)^2)] . \quad (2.20)$$

Here r is the distance from the center of the fullerene and $R = 3.53 \text{ \AA}$ is the fullerene radius. Further averaging (2.20) along the row gives the continuum potential of the fullerene row

$$U_R(\rho) = 60 \frac{2Ze^2}{Rd_R} \sum_{j=1}^4 a_j \int_0^\infty \exp(-k_\perp^2 b_j^{-2}/4) J_0(k_\perp \rho) \sin(k_\perp R) dk_\perp , \quad (2.21)$$

where d_R is the distance between the centers of two neighboring fullerenes in the row, ρ is the distance from the row, J_0 is the Bessel function and the channeling particle considered has charge $+e$. The effective potential $U(\mathbf{r})$ acting on an axially channeled particle is the sum of potentials of the form (2.21) of all rows parallel to the given crystallographic direction:

$$U(\mathbf{r}) = \sum_n U_R(|\mathbf{r} - \boldsymbol{\rho}_n|) . \quad (2.22)$$

Here $\mathbf{r}$ denotes the vector coordinate in the plane normal to the rows, and $\boldsymbol{\rho}_n$ is the vector coordinate of the n th row.

Expression (2.21) corresponds to a static fullerene row and a rigid arrangement of carbon atoms in the fullerenes. One has to take into account two kind of thermal vibrations: (a) of the carbon atoms about their equilibrium positions in the molecule, (b) of the molecules in the fcc lattice. Vibrations of atoms tangential to fullerene sphere obviously do not affect the averaged potential (2.20) due to the averaging over the molecular rotations while the vibrations normal to the sphere can be formally taken into account by introducing the Debye–Waller factor e^{-W} in the integrand of (2.21), where $W = k_\perp^2 u_\perp^2/2$ and $u_\perp^2$ is the mean square amplitude of thermal vibrations. Vibrations of the molecules along the row is not important due to the corresponding averaging. Vibrations in the plane transverse to the rows can be taken into account through e^{-W_f} which must also be introduced in the integrand of (2.21). Assuming that transverse thermal vibrations of fullerenes are isotropic in the transverse plane, we may write the Debye–Waller exponent as $W_f = k_\perp^2 u_1^2/2$, where

$$u_1^2 = \frac{3\hbar^2 N_A}{k_B A T_D} \left[\left(\frac{T}{T_D} \right)^2 \int_0^{T_D/T} \frac{\xi d\xi}{\exp(\xi) - 1} + \frac{1}{4} \right] \quad (2.23)$$

denotes the mean square amplitude of fullerene vibrations, N_A is the Avogadro number, A the atomic number, k_B the Boltzmann constant, T_D the Debye temperature. The latter corresponding to these vibrations was measured to be 55.4 K [38], which gives the value $u_1 = 1.39 \times 10^{-2} \text{ nm}$ at room temperature. In absence of experimental values for $u_\perp$, we may use the graphite value $u_\perp = 8.5 \times 10^{-3} \text{ nm}$ at room temperature [26] as a rough estimate of atomic vibrations in a fullerite. The calculated continuum potential of a fullerite at room temperature for positron channeling along the $[100]$ direction is presented in Fig. 6. Cartesian coordinates x, y are in the plane normal to the rows and measured in units of fullerene radius R while the z -coordinate represents the values of the continuum potential of a fullerite measured in eV. The potential wells inside the rows have almost axial symmetry and are about 7 eV deep. Other

Fig. 6. Continuum potential of a fullerite at room temperature for positron channeling along the $[1\ 0\ 0]$ direction.

wells about 14 eV deep are located between the rows. The wells are separated by a relatively thin potential barrier. We come to the conclusion that two kinds of channeling of positive particles may exist in fullerites, one corresponding to the motion between the rows (like in the ordinary crystals), the other one corresponding to the motion inside the rows (impossible in the ordinary crystals). For negative particles (electrons) the sign of the potential must be changed to negative, the wells transform to the barriers and vice versa and as a result there are practically no potential wells for the channeling of electrons along the $[1\ 0\ 0]$ direction. However, more favourable conditions for electron channeling exist in the $[1\ 1\ 0]$ direction. The corresponding continuum potential for electrons is shown in Fig. 7. There are wide and deep enough (about 40 eV) potential wells separated by relatively thick barriers. The interesting feature is the existence of the central bump inside the wells. On the contrary, for positrons in the $[1\ 1\ 0]$ direction the central well is narrower and much shallower than in the $[1\ 0\ 0]$ direction.

3. Channeling of positively and negatively charged particles in nanocrystals

Classical channeling and channeling radiation in a nanotube was first considered by Klimov and Letokhov [48]. However their calculations were based on quite unrealistic model for the continuum potential which lead the authors to some erroneous conclusions. Then Gevorgian and Ispirian [47,49] made estimates of channeling properties of nanotubes using more realistic continuum potential. Their works stimulated more systematic theoretical investigations of channeling and associated phenomena in nanocrystals based on the most accurate continuum potential [46] discussed above.

Fig. 7. Continuum potential of a fullerite at room temperature for electron channeling along the $[1\ 1\ 0]$ direction.

3.1. Quantum channeling of low-energy electrons and positrons

In channeling the characteristic quantum parameter is the de Broglie wavelength of the particle $\lambda_D = \hbar/mv\gamma$ divided by $\sin \theta_0$ where θ_0 is the incidence angle. The typical value of θ_0 is the Lindhard angle $\theta_L = (2U_0/E)^{1/2} \ll 1$, where U_0 is the potential well depth for the transverse motion. Here m , E , v , γ are the mass, total energy, velocity and Lorentz factor of the particle, respectively. The typical *transverse de Broglie wavelength* $\lambda_\perp = \lambda_D/\theta_L$ is proportional to $E^{-1/2}$ and can be comparable to the width of the channels d_w up to relatively high energies $E \sim 10^2$ MeV of electrons and positrons. Hence, the transverse motion of particles in the channels may be considered either as classical or quantum-mechanical, depending on the ratio $d_w/\lambda_\perp$. This is analogous to case of Bragg diffraction, which depends on the ratio between $\lambda_D/\sin \theta_0$ and the interplane spacing. For the particles heavier than electrons this ratio is always high and the transverse motion may be considered in terms of classical trajectories. However, for electrons and positrons in the MeV energy range, numerical estimates show that quantum effects are important. In order of magnitude the ratio $(d_w/\lambda_\perp)^2$ represents the number of quantum bound states of the transverse motion in the two-dimensional well. Due to quantum tunneling through the potential barrier separating neighboring channels, there are energy bands rather than discrete energy levels. Besides, incoherent scattering of channeled particles on the electrons of the crystal and on atomic vibrations give rise to an additional broadening of the transverse energy levels. To neglect quantum tunneling through the potential barrier we must additionally assume that $\lambda_\perp$ is small compared to the wall thickness. This may be the more severe condition for the applicability of the classical approach to channeled positrons (especially moving close to the top of the wall). Quantum channeling is a well-known phenomenon in ordinary crystals [7,9]

where in the axial case it is noticeable up to electron energies of 50 MeV [39]. In nanocrystals the situation may be different due to the larger width of the potential. In this section we consider the peculiarities of quantum channeling of electrons and positrons in nanotubes and fullerites.

The wave-functions of a channeling relativistic electron or positron may be presented as a product of the plane-wave $\exp(ip_z z)$, corresponding to the uniform motion in the axial direction, and the transverse wave-function $\psi(\mathbf{r})$ describing the particle motion across the axial channel in the continuum potential and satisfying the following equation:

$$[\Delta_r + p_\perp^2(\mathbf{r})]\psi(\mathbf{r}) = 0. \quad (3.1)$$

Here Δ_r is the Laplacian in the plane of the transverse coordinates $\mathbf{r}$, $p_\perp^2(\mathbf{r}) = 2E[\varepsilon - U(\mathbf{r})]$, E is the total energy of the relativistic particle, $\varepsilon = E - \sqrt{p_z^2 + 1}$ is the so-called transverse energy, $U(\mathbf{r})$ is the continuum potential. To simplify the formulae we use here and below $\hbar = m = c = 1$ as units. Eq. (3.1) looks like the Schroedinger equation, however E plays the role of the “relativistic mass” of the particle. Eq. (3.1) implies that spin effects are negligible. As shown in [40] and Appendix B, it follows from the exact Dirac equation under the assumption that the transverse energy ε is small compared to the total energy E (i.e. the Lindhard angle θ_L is small compared to unity).

Let us assume first that the potential of a single nanotube is independent of its azimuthal orientation, which is a good approximation for chiral nanotubes. Then the continuum potential $U(\mathbf{r})$ of a nanotube rope is a periodic function of the transverse coordinates, and we may represent $\psi(\mathbf{r})$ in the Bloch form

$$\psi(\mathbf{r}) = \exp(i\mathbf{\kappa}\mathbf{r})\phi(\mathbf{r}), \quad (3.2)$$

where $\phi(\mathbf{r})$ is a periodic function of the transverse coordinates and $\mathbf{\kappa}$ denotes the transverse quasi-momentum which, without loss of the generality, can be limited to the first Brillouin zone. Expanding $U(\mathbf{r})$ and $\phi(\mathbf{r})$ in the Fourier series

$$U(\mathbf{r}) = \sum_{\mathbf{H}} U_{\mathbf{H}} e^{i\mathbf{H}\mathbf{r}}, \quad (3.3)$$

$$\phi(\mathbf{r}) = \sum_{\mathbf{G}} \phi_{\mathbf{G}} e^{i\mathbf{G}\mathbf{r}}, \quad (3.4)$$

where $\mathbf{H}$ and $\mathbf{G}$ are reciprocal lattice vectors orthogonal to the axis, we come to the following infinite system of homogeneous algebraic equations for the amplitudes $\phi_{\mathbf{G}}$ of the Bloch-waves:

$$\left[\frac{1}{2E} (\mathbf{\kappa} + \mathbf{G})^2 - \varepsilon \right] \phi_{\mathbf{G}} + \sum_{\mathbf{H}} \phi_{\mathbf{G}-\mathbf{H}} U_{\mathbf{H}} = 0, \quad (3.5)$$

Eq. (3.5) is the two-dimensional analogue of the system of equations used in electron diffraction [4]. System (3.5) has non-trivial solutions if its determinant is zero and the allowed transverse energy zones $\varepsilon = \varepsilon_i(\mathbf{\kappa})$ are determined by this condition. The transition from the axial to the more simple planar channeling along the planes of the superlattice formally reduces to taking account in (3.5) of only those reciprocal lattice vectors $\mathbf{H}$ which are orthogonal to the corresponding planes.

The transverse unit cell can be chosen so that it contains a single nanotube (see Fig. 1b). The two-dimensional superlattice has the hexagonal symmetry determined by the pair of basis vectors $\mathbf{A}$ and $\mathbf{B}$, whose modulus is the period L of the superlattice. The reciprocal-lattice vectors $\mathbf{H} = n_1 \mathbf{h}_1 + n_2 \mathbf{h}_2$ are

represented as a superposition of basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ (orthogonal to the corresponding vectors $\mathbf{A}$ and $\mathbf{B}$ of the direct superlattice) with integer coefficients n_1 and n_2 . The moduli of the vectors are determined by the relations $h = 4\pi/L\sqrt{3}$, $H = h(n_1^2 + n_2^2 + n_1 n_2)^{1/2}$. As a result, the expansion coefficients in (3.3) are expressed by

$$U_{\mathbf{H}} = \frac{1}{S} \int_S U(\mathbf{r}) e^{-i\mathbf{H}\mathbf{r}} d^2r, \quad (3.6)$$

where $U(\mathbf{r})$ is determined by Eq. (2.22). This equation involves the addition of the potentials of all the nanotubes given by (2.14) or (2.15). The integration in Eq. (3.6) extends over the area of a unit cell $S = L^2\sqrt{3}/2$ shown in Fig. 1b as the hexagon. Equivalently, one can consider only the potential of the nanotube which is in S , but extend the integration in Eq. (3.6) over the entire transverse plane. Substitution of expression (2.14) into Eq. (3.6) and the subsequent integration gives [41]

$$U_{\mathbf{H}} = \frac{N}{S} \frac{8\pi Z e^2}{d_R} \sum_{j=1}^4 a_j \exp\left(-\frac{H^2}{(2b_j)^2}\right) J_0(RH). \quad (3.7)$$

These coefficients can be rewritten in the form

$$\begin{aligned} U_0 &= K Z e^2 R / L^2, \quad U_{\mathbf{H}} = U_0 \mathfrak{F}(\mathbf{H}), \\ \mathfrak{F}(\mathbf{H}) &= s^{-1} \sum_{j=1}^4 a_j \exp\left(-\frac{H^2}{4b_j^2}\right) J_0(RH), \\ s &= \sum_{j=1}^4 a_j \simeq 1.105 \times 10^{-3} \text{ nm}^2, \quad K = 16\pi^2 3^{-1/2} \sigma s \simeq 3.848 \end{aligned} \quad (3.8)$$

where s and K have the same numerical values for all nanotube indices. Other notations used here are the nanotube structure factor $\mathfrak{F}(\mathbf{H})$, normalized by the condition $\mathfrak{F}(\mathbf{0}) = 1$, and the van der Waals gap $g = L - 2R$ (about 3.15 Å). Small imperfections of the nanotube superlattice can be taken into account by the substitution of b_j^{-2} in (3.8) by $\beta_j = b_j^{-2} + 2u_s^2$, where u_s^2 denotes the mean-square deviation of the superlattice sites from their equilibrium positions in a perfect structure.

In a multiwall nanotube consisting of concentric SWNTs the latter have different radii R_i and consequently different indices (helicity). The inter-wall interaction is very similar to the inter-fullerene interaction in fullerite, particularly, the inner tubes rotate about (or slide along) the tube axis. For multiwall nanotubes consisting of n of concentric cylinders

$$U_{\mathbf{H}} = \frac{K Z e^2}{s L^2} \sum_{j=1}^4 a_j \exp\left(-\frac{H^2}{4b_j^2}\right) \sum_{i=1}^n R_i J_0(R_i H). \quad (3.8')$$

The van der Waals gap $g \simeq L - 2R_n$, where R_n is the external radius of a MWNT, between the neighboring MWNTs is supposed to be the same as for a SWNT rope. Moreover, since it is also the gap between the neighboring walls, the internal radius R_1 and the external radius of a MWNT are connected by relation $R_n = R_1 + (n - 1)g$.

Let us now consider the case where the continuum potential of a single nanotube substantially depends on the azimuthal angle (e.g. in the case of zigzag and armchair nanotubes). Nanotubes gather in the rope in

a highly incommensurate arrangement, i.e. the azimuth orientation of the nanotubes is random, therefore the continuum potential of the nanotube rope *is not periodical* any more with the period of the superlattice and expansion (3.3) ceases to be valid. To be more precise, the potential of the rope has a periodic part coming from the azimuthally homogeneous term of $U(r, \varphi)$ (first term of 2.9) and a random part coming from the $s > 0$ terms of (2.9) with random origin of the φ variable. It is this random part which we have neglected in the case of chiral nanotubes. Besides chiral nanotubes, another case where the azimuthal asymmetry is not important is planar channeling. Here we average the potentials of many nanotubes with random axial orientations laying in the same crystallographic plane of the nanotube superlattice (rope) and, from the beginning, we can discard $s \gg 1$ terms of (2.9). A similar situation exists for axial (or planar) channeling in fullerites with randomly oriented fullerenes (see below).

Similarly to (3.6), in the case of a fullerite single crystal $\mathbf{H}$ and $\mathbf{G}$ mean the reciprocal lattice vectors normal to the fullerene rows and

$$U_{\mathbf{H}} = \frac{1}{S} \int_S U(\mathbf{r}) e^{-i\mathbf{H}\mathbf{r}} d^2r, \quad (3.9)$$

where $U(\mathbf{r})$ is the periodic continuum potential of the fullerene rows (2.22). Substituting for $U(\mathbf{r})$ the sum of single-row potentials coming from the rows of the unit cell only, we can expand the integration in (3.9) over the entire plane and, using the form (2.21), obtain the following analytical representation of the expansion coefficients for the fullerite continuum potential [42]:

$$U_{\mathbf{H}} = 60 \frac{16\pi Z e^2}{V} \sum_{j=1}^4 a_j \exp[-H^2(\beta_j/4)] \frac{\sin HR}{HR} S(\mathbf{H}). \quad (3.10)$$

Here $V = d^3$ is the volume of the fcc unit-cell of the fullerite, $\beta_j = b_j^{-2} + 2u_1^2$, u_1^2 is the mean square amplitude of fullerene thermal vibrations and $S(\mathbf{H})$ is the geometrical structure factor which depends on the specific choice of the two-dimensional unit cell ($S(\mathbf{H}) \equiv 1$ if the unit cell with a single row is chosen).

3.1.1. Numerical results for nanotubes

The equation system (3.5) may be solved numerically keeping only a finite number of Bloch waves $\phi_{\mathbf{G}}$ and then increasing this number step by step, until the calculated transverse-energy eigenvalues no longer vary appreciably. Figs. 8 and 9 show the transverse-energy bands computed in [41] for the planar channel (1, 0) of the two-dimensional superlattice formed by (10, 10) nanotubes, for positrons and electrons, respectively, with various energies (1, 3, and 9 MeV). About 440 Bloch waves were used in the calculations. The transverse quasi-momentum in units of the Brillouin zone width $\delta = 2\pi/d_p$ (where d_p is the inter-planar space) is marked in abscissa. In the same figures are also plotted the planar potentials for positrons and electrons. The number of allowed transverse-energy bands within the potential well increases with the total energy of the particles, and this number is greater for positrons than for electrons (with the same total energy E). For 1 and 3 MeV there are also relatively wide above-barrier bands, which high above the barrier transforms into the continuous (parabolic) energy spectrum, corresponding to almost free particles. Concerning similar results for the axial channeling along nanotubes, the number of bands in this case is much larger than in the corresponding planar cases. For example 1 MeV positrons have several tens of bands below the barrier and this number increases approximately linearly with the total energy of the particles.

Fig. 8. Potential well (a) and transverse-energy bands of positrons, within the first Brillouin zone, with energy: (b) 1 MeV, (c) 3 MeV, (d) 9 MeV in a planar channel (1, 0) of a superlattice of (10, 10) nanotubes.

3.1.2. Numerical results for fullerenes

In the axial channels of a fullerite the number of the transverse-energy bands is much less and they can be easily distinguished. The results in the case of 1 MeV positrons moving along the [1 0 0] direction of a fullerite are illustrated in Fig. 10. The corresponding axial potential is shown in Fig. 6. The transverse energy is plotted as a function of the absolute value κ of the two-dimensional quasi-momentum vector κ for two directions of κ in the reciprocal space: (a) along the line from the center Γ of the first Brillouin zone to the nearest point L of the boundary and (b) from the center to the corner W of the Brillouin zone. The deepest bands are very narrow, i.e. practically independent of the quasi-momentum, while the upper bands (close to the top of the potential barrier) significantly depend on both the absolute value and the direction of κ . Some bands are strongly degenerated and look as a single band. It should be noted that in all cases the number of quantum states inside the potential well is large compared to that in ordinary crystals. This is quite expectable since the well in nanocrystals is broader and of comparable depth.

The probability distribution of channeled positrons in the transverse plane is illustrated in Fig. 11 by the contour plots of the squared wave-function for the specific states labeled 1, 2 and 3 in Fig. 10. These

Fig. 9. Potential well (a) and transverse-energy bands of electrons in nanotubes, within the first Brillouin zone, with energy: (b) 1 MeV, (c) 3 MeV, (d) 9 MeV in a planar channel (1, 0) of a superlattice of (10, 10) nanotubes.

states are strongly localized and practically independent of κ . The transverse coordinates are measured in units of fullerene radius. One can see that the lowest state 1 relates to the channeling between the fullerene rows, state 2 to the channeling inside the fullerene rows, and state 3 refers to positrons which can penetrate through the potential barrier separating neighboring channels.

The analogous results [42] for 1 MeV electrons channeling along the [110] direction are shown in Figs. 12 and 13. As compared to the above case of positrons, the total number of transverse-energy bands is higher, but zones are narrower and their positions do not depend significantly on the direction of the quasi-momentum. These differences are probably due to the thicker potential barriers and the more symmetrical form of the potential of the [110] channel for electrons (Fig. 7). Typical probability distributions of electrons are illustrated in Fig. 13. State 1 corresponds to the channeling between the main potential barrier and the central bump. The transverse energy of state 2 is above the central bump and it corresponds to the channeling in the full width of the well.

When channeled particles leave a crystal the angular distribution of the beam is determined by the quantum-mechanical densities in the transverse momentum space corresponding to the different states, as well as the relative populations of these states. If the number of occupied states is not too high, maxima in the angular distribution corresponding to the different states can be detected [43–45]. Another more precise identification of the quantum states of the transverse motion is provided by spontaneous radiative transitions between the states. We will return to this question in Section 6.1.

Fig. 10. Transverse energy bands of positrons channeling along $[1\ 0\ 0]$ direction as functions of the quasi-momentum modulus κ for the two directions of vector $\mathbf{\kappa}$ in the reciprocal lattice space (shown in the upper-right corner) for fullerite.

It should be noted that in the axial case the periodicity of the potential in the transverse plane is not crucial for the existence of the tightly bound states inside the well as it may be seen from the above calculations with Bloch waves. Moreover, as a starting point, these states can be more rapidly calculated using the continuum potential of an isolated nanotube. On the contrary, the possibility of planar channeling requires the alignment of the nanotubes in the transverse plane.

3.2. Classical channeling of ultra-relativistic electrons and positrons and of ions in straight nanocrystals

As shown in the previous subsection devoted to the quantum channeling, the number of transverse states in the axial potential wells grows approximately linearly with the particle energy E and for electron (positron) energies about 10 MeV it becomes possible to use classical mechanics for the description of the transverse motion. As noted above, heavy particles, like π -mesons and protons, can be treated as classical irrespective of their kinetic energy. Let us first consider the case of classical motion of high-energy particles in a straight nanotube rope or a non-deformed fullerite. Since the continuum potential $U(\mathbf{r})$ of the axial channels does not depend on time and on the longitudinal (with respect to the channels) coordinate z , there are two integrals of motion: the total energy of the particle E and the relativistic longitudinal momentum $p_{\parallel}$:

$$\begin{aligned} E &= U(\mathbf{r}) + (1 - v_{\parallel}^2 - v_{\perp}^2)^{-1/2}, \\ p_{\parallel} &= v_{\parallel}(1 - v_{\parallel}^2 - v_{\perp}^2)^{-1/2}. \end{aligned} \quad (3.11)$$

Fig. 11. Probability density in the transverse plane for different quantum states (states 1, 2, 3 of Fig. 10) of a positron channeled along the axis $[1\ 0\ 0]$ of a fullerite crystal.

Here $v_{\parallel}$ denotes the longitudinal velocity, $\mathbf{v}_{\perp} = d\mathbf{r}/dt$ is the 2D vector of the transverse velocity, the system of units $\hbar = m = c = 1$ is used to simplify the expressions. The so-called transverse energy ε is defined as the following difference $\varepsilon = E - (1 + p_{\parallel}^2)^{1/2}$ which is an integral of motion too. On channeling or close to channeling conditions the inequality $\varepsilon \ll E$ is always satisfied, then using the definition of ε

Fig. 12. Transverse energy bands of electrons channeling along $[1\ 1\ 0]$ direction as functions of the quasi-momentum modulus κ for the two directions of vector κ in the reciprocal lattice space shown in the upper-right corner.

and (3.11) we may rewrite it as

$$\varepsilon = \frac{E\mathbf{v}_{\perp}^2}{2} + U(\mathbf{r}) .$$

Using the Hamilton function $H = (1 + p_{\parallel}^2 + \mathbf{p}_{\perp}^2)^{1/2} + U(\mathbf{r})$, where $\mathbf{p}_{\perp} = E\mathbf{v}_{\perp}$ is the transverse momentum, and taking into account that $U \ll E$, we find the following equations of motion in the transverse plane

$$\begin{aligned} d\mathbf{p}_{\perp}/dt &= -\nabla U(\mathbf{r}) , \\ d\mathbf{r}/dt &= \mathbf{p}_{\perp}/E \end{aligned} \tag{3.12}$$

from which follows

$$\frac{d^2\mathbf{r}}{dt^2} = -\frac{1}{E} \nabla U(\mathbf{r}) . \tag{3.13}$$

The latter equation can be recognized as the Newton equation for non-relativistic transverse motion of a particle with “relativistic mass” E and potential energy $U(\mathbf{r})$. It is in full agreement with the corresponding quantum analogue (3.1).

Fig. 13. Probability density in the transverse plane for different quantum states (states 1 and 2 of Fig. 12) of an electron channeled along the axis $[1\ 1\ 0]$ of a fullerite crystal.

As regards the longitudinal velocity, it has the simple expression in the ultrarelativistic limit $E \gg 1$:

$$v_{\parallel} = 1 - \left(\frac{1}{2}\right) (E^{-2} + v_{\perp}^2) . \quad (3.14)$$

This one is close to the light speed but not constant due to the presence of the time-dependent term $v_{\perp}^2$ in (3.14). This may be of importance in calculations of the electromagnetic radiation from ultra-relativistic electrons and positrons since the Doppler shift depends strongly on the small difference $1 - v_{\parallel}$ between the light speed and the longitudinal velocity. However, we may neglect this term in calculations of channeled particle propagation in nanocrystals.

The continuum potential $U(\mathbf{r})$ is too complicated to make any analytical calculations of particle trajectories. However, in the case of the motion *inside* a chiral nanotube or a fullerene row, the potential well $U(\mathbf{r})$ is almost axially symmetrical at any $\rho \equiv |\mathbf{r}|$. Then it is convenient to describe the particle

Fig. 14. Typical trajectories of a channeled positive particle with the transverse energy $\varepsilon = 25$ eV (a) and a negative particle with the transverse energy $\varepsilon = -15$ eV (b) in a (10, 0) nanotube.

trajectory in terms of the cylinder coordinates $\rho(t)$, $\varphi(t)$ and we have a second integral of motion which is the angular momentum about the tube axis

$$l = |\mathbf{r} \times \mathbf{p}_\perp| = E\rho^2 \frac{d\varphi}{dt} .$$

In the ascending part ($d\rho/dt > 0$) of the trajectory (which is symmetrical around the radial turning points) the cylinder coordinates are calculated by the well-known formulae

$$t = E \int \{2E[\varepsilon - U(\rho)] - l^2/\rho^2\}^{-1/2} d\rho, \quad \varphi(t) = (l/E) \int \rho^{-2}(t) dt . \quad (3.15)$$

It should be noted that even in armchair and zigzag nanotubes like (10, 10) and (20, 0) (Figs. 4a and b) there is a region of ρ far enough from the wall where the continuum potential with good accuracy can be considered as axially symmetric. The transverse energy ε and the angular momentum l are fixed at the entrance to the nanotube and may be written as $\varepsilon = U(\rho_0) + E\theta_0^2/2$, $l = E\rho_0\theta_0 \sin(\Phi_0 - \varphi_0)$, where θ_0 , Φ_0 are the polar and the azimuth angle of the velocity vector at the entrance point to the channel, respectively, while φ_0 is the azimuth of the entrance position. Since the real beams are much wider than a single channel, the initial position $\mathbf{r}_0$ should be considered as random. In particular, positive and negative values of l are equally probable.

Typical transverse trajectories (3.15) of channeled positively (a) and negatively (b) charged particles in an axially symmetrical nanotube field are presented in Fig. 14, respectively. It can be seen that the motion of positively and negatively charged particles have quite different characters. Positive particles are processing around the tube axis while moving inside the nanotube. Negative particles nutate near

the nanotube surface. The frequency ω_ρ of the radial oscillations and the frequency of the precession (nutation) Ω are determined by the formulae

$$\omega_\rho = 2\pi/T_\rho, \quad T_\rho = 2E \int_{\rho_{\min}}^{\rho_{\max}} \{2E[\varepsilon - U(\rho)] - l^2/\rho^2\}^{-1/2} d\rho, \quad (3.16)$$

$$\Omega = \Delta\varphi/T_\rho, \quad \Delta\varphi = 2 \int_{\rho_{\min}}^{\rho_{\max}} (l/\rho^2) \{2E[\varepsilon - U(\rho)] - l^2/\rho^2\}^{-1/2} d\rho. \quad (3.17)$$

Here $\rho_{\min}$, $\rho_{\max}$ are the perihelion and aphelion of the orbit and $\Delta\varphi$ is the precession (nutation) angle. Further analytical calculations, giving a qualitative picture of channeling, are possible with simplified expression for $U(\rho)$ [46,47]. It is important to note that the electric field of a nanotube is strong enough only in the vicinity of the wall, the bottom of the potential well for a positive particle being nearly flat (Fig. 4). Therefore, the trajectory is practically rectilinear inside the tube. A polynomial fit of $U(\rho)$ should begin with ρ^n with n very large. The Doyle–Turner parameterization of the atomic potential of a chiral nanotube leads to $U(\rho) \approx 60(2\rho/d)^{17}$ eV [46], which is much steeper than $\sim r^{-6}$ suggested in [47] as a result of the Moliere parameterization. The parabolic potential used in [48] seems quite unrealistic.

Let us now discuss the more complicated case where the nanotube potential cannot be considered as axially symmetric and therefore the orbital momentum l is no longer an integral of motion. It happens when the charged particles can cross the cylinder surface or approach close to it. The absence of the second integral of motion leaves the door open to the phenomenon of the dynamic chaos when, together with the regular radial oscillations described above, some part of the particles can be involved in extremely irregular transverse motions as first pointed out in [51]. The manifestation of the dynamic chaos in channeling is illustrated in Fig. 15. A typical trajectory of a positive particle with transverse energy $\varepsilon = 50$ eV close to the top of the potential barrier of a (10, 1) nanotube is represented in Fig. 15a. In this case the particle can reach the region where the second derivative of the potential is negative and its motion becomes chaotic, irrespective of the initial coordinates and momentum. The trajectory of a negative particle with $\varepsilon = -15$ eV is shown in Fig. 15b. It moves in the potential well near the nanotube surface where the potential is extremely axially asymmetric and its motion is predominantly chaotic.

3.3. Scattering of fast above barrier charged particles by nanotubes

Some particles may enter the nanotube rope between nanotubes or have their initial transverse energy sufficient to overcome the potential barrier of the walls shown in Fig. 4. The transverse motion of such particles is unconfined and can be treated as a succession of scatterings on individual nanotubes in the plane orthogonal to the rope axis, as schematically shown in Fig. 16.

Let us consider at first, following [52,53], scattering in an azimuthally homogeneous nanotube field (Fig. 4c). In classical theory the azimuthal scattering angle $\varphi(b)$ depends on the impact parameter b of the particle with the nanotube via the equation

$$\varphi(b) = \pi(b/|b|) - 2b \int_{\rho_{\min}}^{\infty} (1/\rho^2) \{[1 - U(\rho)/\varepsilon] - b^2/\rho^2\}^{-1/2} d\rho, \quad (3.18)$$

Fig. 15. Typical trajectories of a channeled positive particle with the transverse energy $\varepsilon = 50$ eV (a) and a negative particle with the transverse energy $\varepsilon = -15$ eV (b) in a (10, 1) nanotube.

Fig. 16. Schematic view of the scattering of a fast charged particle by a single nanotube.

where $\varphi(b)$ is usually called the *deflection function* [54,55]. It should be noted that the deflection function is odd in b and, generally speaking, different values of the impact parameters may give the same deflection angle. The total scattering angle ϑ_s of the particle by a single nanotube can be written as

$$\vartheta_s = 2\theta_0^{(s)} \sin(\varphi/2) , \quad (3.19)$$

Fig. 17. Deflection function (a) and transverse trajectories (b) of electrons scattered by (10, 1) nanotube. The curve in (a) corresponds to the incidence angle $\theta_0 = 0.3\theta_L$. Various trajectories in (b) are plotted for $\theta_0 = 0.6\theta_L$.

where $\theta_0^{(s)}$ is the angle between the tube axis and the velocity far from the tube (it may differ from the incidence angle θ_0 at the entrance to the rope, especially if $\mathbf{r}_0$ is close to the nanotube wall). The classical, differential over φ , scattering cross section can be written as

$$\frac{d\sigma_{cl}}{d\varphi} = L\theta_0^{(s)} \sum_n \left| \frac{d\varphi}{db} \right|_n^{-1}. \quad (3.20)$$

Here L is the total length of the nanotube and the summation index n corresponds to the different single-valued branches of the function $b(\varphi)$ which is inverse of the deflection function.

The calculated deflection function of a negative particle incident on nanotubes (10, 1) at small angle $\theta_0^{(s)}$ is illustrated in Fig. 17a for $\theta_0^{(s)} = 0.6\theta_L$. Such a behavior of the deflection function holds for any other value of $\theta_0^{(s)} < \theta_L$. It can be seen that at impact parameters somewhat larger than R , the deflection can be very strong. For example, the scattering angle $\varphi(b)$ can be of some radians while the total scattering angle θ_s is comparable to the Lindhard angle. The case where $\varphi(b)$ exceeds π is called *orbiting scattering*. The vertical asymptote corresponds to a particle which makes many turns while “hesitating” a very long time on the secondary maximum of the effective radial potential. The orbiting scattering from nanotubes (10, 1) can be seen more clearly in Fig. 17b where trajectories of electrons entering at $\theta_0^{(s)} = 0.6\theta_L$ are shown for various impact parameters.

The corresponding results for a positive particle are presented in Fig. 18, however in this case the scattering strongly depends on the ratio between the incidence angle $\theta_0^{(s)}$ on the tube and the Lindhard angle θ_L . At $\theta_0^{(s)} \leq \theta_L$ a positive particle cannot overcome the potential barrier and penetrate inside the nanotube and, as a result, the inverse deflection function in Fig. 18a is single-valued and monotonic. In the opposite case $\theta_0^{(s)} > \theta_L$ the penetration becomes possible and the inverse deflection function is multi-valued, like for negative particles.

The curves in Figs. 17a and 18a representing the deflection function may have a distinct maximum (near $b = 0.8R$) where the classical differential cross section (3.20) diverges. It is known that the so-called *rainbow scattering* takes place near such a point, like in the scattering of light by water drops. However, this divergence is replaced by a peak of finite height and width in quantum theory. An accurate enough treatment is based on the WKB theory. The quantum scattering cross section can be

Fig. 18. Deflection function (a) and transverse trajectories (b) of positively charged particles scattered by (10, 1) nanotube. Curve 1 in (a) corresponds to the incidence angle $\theta_0 = \theta_L$, 2— $\theta_0 = 1.5\theta_L$, 3— $\theta_0 = 2.0\theta_L$, 4— $\theta_0 = 3.0\theta_L$. Various trajectories in (b) are plotted for $\theta_0 = 1.5\theta_L$.

presented as [55]

$$\frac{d\sigma}{d\varphi} = \frac{L}{2\pi E} \left| \sum_{l=-\infty}^{\infty} e^{il\varphi} (\exp 2i\eta_l - 1) \right|^2, \quad (3.21)$$

where η_l are the *scattering phase shifts*. In the semi-classical WKB approximation η_l can be expressed in terms of classical trajectories:

$$\eta_l = \lim_{\rho_{\max} \rightarrow \infty} \left[\int_{\rho_{\min}}^{\rho_{\max}} \{2E[\varepsilon - U(\rho)] - l^2/\rho^2\}^{1/2} d\rho - \int_b^{\rho_{\max}} (2E\varepsilon - l^2/\rho^2)^{1/2} d\rho \right], \quad (3.22)$$

where the angular momentum l (in units of $\hbar = 1$) is connected with the impact parameter b by the equality $l = -b(2E\varepsilon)^{1/2}$.

Calculated using (3.21) and (3.22), the scattering cross section is presented in Fig. 19 by the oscillating curves for 10 MeV and 1 GeV electrons and in Fig. 20 for 10 MeV positrons, all incident on (10, 1) nanotubes at various incidence angles $\theta_0^{(s)}$. Oscillations occur around the corresponding classical values (smooth curves). Mathematically, the origin of the oscillations is due to the following reason. In the WKB approximation, the sum over the integer values of the orbital momentum l can be replaced by an integration over the continuous variable l and the arising integral can be calculated using the stationary phase method. Forgetting the -1 term of (3.21), which only contributes at $\varphi = 0$, the phase of the integrand is just $\psi = l\varphi + 2\eta_l$. At a stationary phase point, one has $d\psi/dl = 0$, i.e., $\varphi = -2(d\eta/dl)$, from which one can recover the classical result (3.18). Since $b(\varphi)$ is generally a multi-valued function, several stationary phase points can exist for one definite scattering angle φ . For a given $\varphi = \varphi_\alpha$ somewhat below the rainbow scattering angle φ_r , there are at least two stationary phase points l_α and l_β , corresponding to impact parameters b_α and b_β located on either sides of the rainbow point b_r , such that $\varphi(l_\alpha) = \varphi(l_\beta) = \varphi_\alpha$. The phase difference between the corresponding amplitudes is: $\psi_\beta - \psi_\alpha$ which is $(2E\varepsilon)^{1/2}$ times the area between the curve $\varphi(b)$ and the horizontal line $\varphi = \varphi_\alpha$ in Fig. 17. The “slow” oscillations of Figs. 19b and 20b come from the interference between the contributions of stationary points α and β , whose phase difference $\psi_\beta - \psi_\alpha$ is mentioned above. If $b(\varphi)$ is a single-valued function, such oscillations are evidently absent (Fig. 18a, curve 1, and Fig. 20a where one sees only diffraction fringes). The purely classical

Fig. 19. Classical (smooth curve) and semi-classical (oscillating curve) differential cross sections of electron scattering by (10, 1) nanotube. Electrons have $E = 10$ MeV (a) or $E = 1$ GeV (b) total energy and $\theta_0 = 0.6\theta_L$ incidence angle. The cross section is measured in units of $La_{TF} \theta_0$.

Fig. 20. Similar to Fig. 19, but for 10 MeV positrons incident at the angle $\theta_0 = 0.6\theta_L$ (a) and $\theta_0 = 1.5\theta_L$ (b).

result (3.20) can be easily derived [55] on the assumption that the interference between the different contributions to the scattering amplitude is negligible.

For angles φ close enough to φ_r the stationary phase method is inapplicable. Instead of it we can use an alternative approach. If l is close to l_r , which is defined by the condition $d^2\eta/dl^2 = 0$, we expand the phase η_l in powers of $l - l_r$ (up to the third power) and express the scattering amplitude in terms of the Airy function [54,55]. According to the well-known properties of the Airy function the cross section as a function of φ oscillates below φ_r and rapidly decreases above φ_r . In addition, the equation $\varphi(b) = \varphi_\alpha$ has two other roots on the negative axis, b_γ and b_δ . These are on either sides of the sharp peak which is symmetric of the sharp dip of Fig. 17 about the origin, owing to the odd parity of $\varphi(b)$. Whereas the α, β interference gives the slow oscillations of Figs. 19b and 20b, the α, γ (for instance) interference contributes to the fast oscillations (and the most visible oscillations of Fig. 19a). As regards the two remaining stationary phase points b_γ and b_δ mentioned above, their contribution does not vanish in the classical limit at $\varphi > \varphi_r$. With increasing particle energy, the frequency of the quantum oscillations of

Fig. 21. Trajectories of positive particles with the transverse energy $\varepsilon = 75$ eV in the $(10, 0)$ nanotube.

Fig. 22. Trajectories of negative particles with the transverse energy $\varepsilon = 5$ eV in the $(10, 0)$ nanotube.

the cross section grows and, averaged over the oscillations, the cross section becomes more closer to its classical limit (Fig. 19).

Let us consider now, following [56], the particle scattering in an azimuthally inhomogeneous nanotube field (Figs. 4a and b). When studying the particle channeling phenomenon in nanotube, we saw that the azimuthal asymmetry of the potential leads to a rather complicated pattern of particle motion and that the phenomenon of dynamic chaos in channeling is possible in this case. A similar situation takes place also for above-barrier particles which are scattered by the nanotube. Typical transverse trajectories of positive particles with various impact parameters relative to the axis of a $(10, 0)$ nanotube are shown in Fig. 21. All trajectories were calculated for transverse energies slightly above the potential barrier U_s at saddle points between the neighboring atomic strings of the nanotube. It can be seen that in this case the character of particle motion strongly depends on the impact parameter. At some values of the parameter the particle can penetrate inside the nanotube and make a large number of oscillations before going out. Fig. 22 shows the same phenomenon with negative particles.

The dependence of $T_s(b)$, which is the time spent by the above-barrier particle inside the nanotube, on the impact parameter b is represented in Fig. 23. There are intervals of the impact parameter where

Fig. 23. Time (multiplied by the light speed) spent by a positive particle with the transverse energy $\varepsilon = 75$ eV (a) and negatively charged particle with $\varepsilon = 5$ eV (b) inside a (10, 0) nanotube as a function of the impact parameter b (in units of nanotube radius R).

Fig. 24. Typical trajectories of electrons and positrons in a rope of (10, 10) nanotubes. The trajectories are marked by the values of the transverse energy of the particles in electron-volts.

a small change of the latter leads to a considerable change of the particle trajectory. It is interesting to note that an increase of the resolution scale of b does not change the aspect of the $T_s(b)$ curve. Such a behavior can therefore be described as fractal [57,58]. For negative particles (Fig. 23b), contrary to positive particles (Fig. 23a), the fractal behavior of $T_s(b)$ exists for the majority of possible impact parameters. With increasing transverse energy the fractal behavior of $T_s(b)$ disappears. Thus, the axial asymmetry of the nanotube potential can considerably affect the character of particle motion.

The picture of particle motion in *nanotube ropes* can be even more complicated. Typical transverse trajectories of positive and negative particles in a rope of (10, 10) nanotubes for different values of the transverse energy (indicated in eV at the trajectories) are shown in Fig. 24. Depending on the transverse energy value, confined (channeling) or unconfined (above-barrier) motion of particles usually takes place. The channeling of positive particles happens to be possible either inside or between the nanotubes (in the latter case, however, the potential well is very shallow, as seen in Fig. 4a) while channeling of negative particles can take place only near the nanotube surface.

It is noteworthy that the problem of particle channeling in a nanotube rope is similar to the problem of axial channeling in ordinary crystals [5–9,55], however, as shown above, the nanotube case possesses some peculiarities coming from the specific arrangement of the atomic strings.

3.4. Classical channeling of ultra-relativistic electrons or positrons and of ions in bent nanocrystals

Let us now assume that due to a bending of the nanocrystal, the axis of the channel is curved in a certain plane with a constant radius of curvature R_b . We choose a cylindrical system of coordinates ρ, φ, Z with the Z -axis perpendicular to the plane of the bend and passing through the center of curvature O . The potential of the bent nanocrystal is independent of the azimuth angle φ . Thus, in addition to the total

energy E , the component M of the relativistic angular momentum of the particle on the Z -axis is also an integral of motion:

$$\begin{aligned} E &= U(\mathbf{r}) + (1 - \mathbf{v}_\perp^2 - v_\tau^2)^{-1/2}, \\ M &= \rho v_\tau (1 - \mathbf{v}_\perp^2 - v_\tau^2)^{-1/2}. \end{aligned} \quad (3.23)$$

Here, $v_\tau = \rho(d\varphi/dt)$ is the tangential component of the velocity, and $\mathbf{v}_\perp$ represents the two other orthogonal components while $\mathbf{r}$ denotes the coordinates of the particle in the transverse plane $\varphi = \text{const}$. The system of equations (3.23) leads to the following equation for the transverse component of the velocity of a particle in the bent crystal:

$$\mathbf{v}_\perp^2 = 1 - \frac{1 + M^2/\rho^2}{[E - U(\mathbf{r})]^2}. \quad (3.24)$$

Let us now define the transverse energy of a relativistic particle as the difference

$$\varepsilon \equiv E - (1 + M^2/R_b^2)^{1/2} \quad (3.25)$$

which is also an integral of motion in the bent crystal. The local Cartesian coordinate x of the particle relative to the crystallographic axis (one of the components of vector $\mathbf{r}$) is connected with the cylindrical coordinate ρ introduced above through the relation $x = \rho - R_b$. Since the radius of curvature in the cases of practical importance is larger than the size of the channel ($x \ll R_b$), we obtain from Eqs. (3.24) taking into account definition (3.25) and the condition $\varepsilon \ll E$ (which always holds for channeled particles) the following approximate equation for the transverse velocity component:

$$\mathbf{v}_\perp^2 = \frac{2}{E} [\varepsilon - U(\mathbf{r})] + \frac{2x}{R_b}. \quad (3.26)$$

Thus, the bending of the crystallographic axis with a constant radius of curvature R_b is taken into account in the analysis of the transverse motion by replacing the electrostatic potential $U(\mathbf{r})$ in Eqs. (3.12) and (3.13) by the effective potential

$$U_{\text{eff}}(\mathbf{r}) = U(\mathbf{r}) - \frac{Ex}{R_b}. \quad (3.27)$$

The concept of effective potential can also be applied to the quantum motion discussed in the previous subsection. This is shown in the end of Appendix B. We assume that the diameter of a nanotube rope (or the thickness of a fullerite single crystal) is small compared to R_b thus all axial channels are bent with almost the same radius of curvature; in this case Eq. (3.27) applies to the nanocrystal as a whole, $\mathbf{r}$ and x being measured from a common origin (e.g. the axis of the central nanotube).

The above analysis is completely in accordance with intuitive considerations presented in pioneering works by Tsyganov [59], devoted to the deflection of a high-energy particle beam by bent crystal planes. A particle which is initially in the middle of the channel and with zero transverse velocity can overcome the potential barrier if $U_{\text{eff}}(d/2, 0) < 0$, i.e., if the curvature radius is less than the *Tsyganov radius* $R_c = Ed/(2U_0)$ determining the tolerance of channeling to crystal bending. Remembering that the Lindhard critical angle is expressed by $\theta_L = (2U_0/E)^{1/2}$, we may rewrite the Tsyganov radius as $R_c = d/\theta_L^2$. Nanotubes bent with the Tsyganov radius deviate charged particles like a uniform magnetic field equal to $H_{\text{eff}} = 2U_0/ed$, where d is defined by (2.1). For example, (11, 9) chiral nanotubes can deflect a beam

of positively charged particles as strong as a bending magnet of 588 T field strength. It should be noted that, for bending radius approaching the Tsyganov value, the width of the effective potential well (3.27) can be significantly narrower than the width of $U(\mathbf{r})$. This circumstance may reduce the total number of quantum states inside bent nanotubes or the fraction of a beam which is captured in channels and thus can follow the bend.

If produced with enough length and cross section, nanotube ropes are expected to be flexible, like optical fibers. The Young's modulus ($\sim 10^{12}$ Pa) and maximum tensile strength ($\approx 3 \times 10^{10}$ Pa) of nanotubes are very high [61] simply due to the cylindrical geometry and the rigidity of the hexagonal lattice. As regards fullerites, they can be bent, like ordinary crystals, either mechanically or by passing a high-intensity ultrasonic wave through the crystal. The bending strength of a fullerite and its resistance to the action of ultrasound are apparently comparable to the values observed in ordinary crystals of the graphite and even diamond type (this statement is valid for polymerized fullerites).

In both methods of bending, the radius of curvature is not constant along the channel. It can be taken into account by introducing the non-constant centrifugal force $\mathbf{F} = -E\mathbf{n}/R_b$ into the equations for transverse motion or, for a quantum treatment, a varying centrifugal potential (see Eq. (B.6)). Here, $\mathbf{n}$ is the unit vector directed towards the center of curvature.

A positron beam channeled in an undulated nanotube rope is therefore equivalent to a magnetic undulator of very intense field and very small period. It will emit much more power and at much higher frequencies than ordinary undulators. Similarly, by screwing a nanotube rope, one obtains a bunch of spiral nanotubes which are equivalent to an helical undulator, from which circularly polarized X- or γ -rays are obtained. This possible application, as well as the possibility of amplification by stimulated emission, will be discussed in Section 6.4. Below we discuss some aspects of channeling motion in a nanotubes submitted to planar sinusoidal or spiral bending.

Let us describe by $\mathbf{a}(z)$ the transverse deformation of the nanotube axis due to periodical bending, the z -axis being along the mean direction of the tube. The bending angle is assumed to be small ($\mathbf{a}'(z) = d\mathbf{a}/dz \ll 1$) and the curvature radius $|\mathbf{a}''(z)|^{-1}$ larger than R_c . The effective potential is given by

$$U_{\text{eff}}(\mathbf{r}) = U(\mathbf{r}) + E\mathbf{a}''(z) \cdot \mathbf{r}, \quad (3.28)$$

where $\mathbf{r}$ is the transverse position vector relative to the local nanotube axis. Since $z \simeq t$ we can consider $E\mathbf{a}''(z) \cdot \mathbf{r}$ as a “time-dependent perturbation”.

Here we consider periodic bending of the general form

$$\mathbf{a}(z) = A\mathbf{n}_x \cos k_w z + B\mathbf{n}_y \sin k_w z \quad (3.29)$$

with $A = B$ for a helical bending, $B = 0$ for a planar sinusoidal bending. The spatial period of the deformation is $\lambda_w = 2\pi/k_w$.

Let us consider first the planar case ($B = 0$). The second term of (3.28) breaks the axial symmetry, therefore the angular momentum l about the local axis of the nanotube ceases to be an integral of motion. It also breaks the invariance upon translations in z , therefore p_z and the transverse energy ε are not conserved.

If λ_w is large enough compared to the period λ_{ch} of the classical channeling oscillations (or k_w small compared to the spacing $\Delta\varepsilon$ between two transverse quantum energy levels), one expects that the channeling motion (or the quantum channeling state) evolve adiabatically. Then ε just oscillates with period λ_w . If λ_w is not large, the channeling motion evolves non-adiabatically. The classical trajectories may

be divided into stable ones, where the transverse energy keeps bounded, and chaotic ones leading to dechanneling.

The helical case ($A = B$) is mathematically simpler. Indeed, the effective potential is invariant under the product of a “time translation” of Δz times a rotation of $\Delta\phi = k_w \Delta z$ about the local tube axis. Accordingly, the quantity

$$\tilde{\varepsilon} = \varepsilon - k_w l = \frac{E}{2} \mathbf{v}_\perp^2 + U(\mathbf{r}) + E \mathbf{a}''(z) \cdot \mathbf{r} - k_w l \quad (3.30)$$

is conserved. Let us analyze the channeling motion in the rotating transverse coordinate frame where the x -axis remains parallel to $\mathbf{a}(z)$. Replacing $\mathbf{v}_\perp$ by $\tilde{\mathbf{v}} + \mathbf{v}_d$ where $\mathbf{v}_d = k_w \mathbf{n}_z \times \mathbf{r}$ is the drag velocity, one obtains

$$\tilde{\varepsilon} = \frac{E}{2} \tilde{\mathbf{v}}^2 + U(\mathbf{r}) - \frac{E}{2} k_w^2 (2\mathbf{a} \cdot \mathbf{r} + \mathbf{r}^2) = \frac{E}{2} \tilde{\mathbf{v}}^2 + \tilde{U}(\mathbf{r}) . \quad (3.31)$$

For not too large values of A and k_w , the new effective potential $\tilde{U}$ has a minimum inside the tube, about which the particle can be permanently trapped (neglecting the leakage by quantum tunneling). This occurs at least when the nanotube curvature radius does not exceed the Tsyganov radius.

In the rotating frame, one has to take into account the Coriolis force $\mathbf{f}_C = -2k_w \mathbf{n}_z \times \mathbf{r}$. The Hamiltonian $\tilde{H}$ from which we may derive the classical equations of motion, or the Schrödinger equation of the transverse states, is obtained from expression (3.31) of $\tilde{\varepsilon}$ by the substitution $\tilde{\mathbf{v}} \rightarrow \tilde{\mathbf{p}}_\perp / E - \mathbf{v}_d$. Note the equality $\tilde{\mathbf{p}}_\perp = \mathbf{p}_\perp$ and the similarity with the dynamics of a particle submitted to an electric potential plus a magnetic field.

Let us point out that in straight nanotubes with approximate cylindrical symmetry, a particle can be “over-barrier” as regards the transverse energy ($\varepsilon > U_0$) but nevertheless permanently channeled. Such particles describe fast and nearly circular motions close to the nanotube wall, where a large derivative ∇U of the potential can compensate the centrifugal force El^2/r . In periodically bent nanotubes, these states evolve adiabatically under the influence of the perturbation $E \mathbf{a}''(z) \cdot \mathbf{r}$, because their intrinsic orbital and radial periods are much shorter than λ_w . Therefore, like truly below-barrier particles, they can remain trapped for a rather long time.

To summarize, channeling is not too much destroyed by periodical bending of the nanotube, provided that the bending radius and the spatial bending period are large enough compared to the Tsyganov radius and the periods of channeling oscillations, respectively. Due to the existence of a conserved quantity, the motions in helically bent nanotubes may be generally more stable than in nanotubes with planar sinusoidal bending. In any case the real transverse motion which causes the emission of radiation is the superposition of the local channeling motion and the transverse motion of a fictitious particle moving on the local tube axis at the same $\langle v_z \rangle$. The channeling motion generates channeling radiation while the fictitious particle motion, generally slower, generates the softer undulator radiation.

An interesting effect occurs in a spirally bent nanotube when λ_w is comparable to the typical azimuthal period of the channeling motion: the angular momentum l of a positron starts to increase, due to a resonance effect, so that a population of channeled positrons which has initially $\langle l \rangle = 0$ gets a non-zero value of $\langle l \rangle$ (positive for a clockwise spiral) after a few oscillations. Let us then consider a nanotube which is helically bent in its first part ($0 < z < z_b$), then straight in the second part ($z > z_b$). The positive value of $\langle l \rangle$ acquired in the first part is conserved in the straight part. In this part, the positrons should produce

circularly polarized channeling radiation, difficult to obtain otherwise in the γ -ray range. According to a numerical simulation [60], rather large values of $\langle l \rangle$ and of the circular polarization may be obtained.

4. Scattering of X-rays and neutrons by nanocrystals

Like in ordinary crystals scattering of X-rays and thermal neutrons in nanocrystals can be described by introducing the complex dielectric (or nuclear) susceptibility $\chi(\omega, \mathbf{r})$ depending on the particle energy $\hbar\omega$ and coordinates $\mathbf{r}$ through the local density of scatterers (absorbers). For example, if the frequency ω is high compared to the carbon K-edge ($\hbar\omega_K \approx 284$ eV), we may express the real part $\chi'(\omega, \mathbf{r})$ through the electron density of the medium $n_e(\mathbf{r})$ as

$$\chi'(\omega, \mathbf{r}) = -(4\pi e^2 / m\omega^2) n_e(\mathbf{r}) . \quad (4.1)$$

Thermal neutrons are scattered by nuclei. The elastic interaction of a slow neutron with one nucleus of the medium can be described as a strong short-range force characterized by a potential with a depth about 40 MeV and a size a few times 10^{-13} cm. Besides, neutrons possess a spin of $\hbar/2$ and a magnetic dipole moment of 1.91 nuclear magnetrons which can interact with the nucleus spin. The scattering of slow neutrons is predominantly in the s -wave, i.e. isotropic, independent of the details of the potential and determined by a single parameter named *scattering length*. In general, the latter depends on the relative orientation of the spins of the neutron and nucleus. Since we are interested in carbon nuclei which are unpolarized, it is necessary to average the spin-dependent scattering length over all possible spin orientations. The averaging over carbon isotopes is also needed. The result is a quantity known as the *coherent scattering length* a . Like in X-ray optics, the coherent propagation of a neutron wave with a medium can be described by an index of refraction $n = k_{\text{med}} / k_{\text{vac}} = \sqrt{1 + \chi'(\omega, \mathbf{r})}$. In this case the real part of the nuclear susceptibility is $\chi'(\omega, \mathbf{r}) = -\pi^{-1} \lambda^2 a n_a(\mathbf{r})$ which depends on the neutron wavelength λ , the coherent scattering length a and the local number density of nuclei $n_a(\mathbf{r})$.

The imaginary part $\chi''(\omega, \mathbf{r})$ of the susceptibility is proportional to the total cross section which is the sum of absorption, non-elastic and elastic scattering cross sections. However, for the wavelengths under the consideration the absorption cross section σ_a of X-rays or neutrons is dominant: $\chi''(\omega, \mathbf{r}) = n_a(\mathbf{r})(\lambda/2\pi)\sigma_a$. Absorption of relatively soft X-rays is connected to atomic ionization or, for harder X-rays, electron-positron pair production. As far as thermal neutrons, it is known that the cross section of their absorption by nuclei is inversely proportional to the neutron wavelength λ , thus $\chi''(\omega, \mathbf{r})$ occurs to be independent of λ (or neutron velocity).

The general approach to the scattering problem in nanocrystals is based on the multi-wave diffraction theory. The scattering of X-rays is more complicated than that of thermal neutrons due to the vector character of the electromagnetic field. We expand the electric field in a superlattice in series of Bloch waves

$$\mathbf{E}(\mathbf{r}, t) = (2\pi)^{-4} \sum_{\mathbf{K}} \int \mathbf{E}_{\mathbf{K}}(\mathbf{k}, \omega) e^{i(\mathbf{k}+\mathbf{K})\mathbf{r}-i\omega t} d^3k d\omega \quad (4.2)$$

and from Maxwell equations find [3] the following infinite system of algebraic equations for the expansion coefficients $\mathbf{E}_{\mathbf{K}}(\mathbf{k}, \omega)$:

$$(\mathbf{k} + \mathbf{K}) \times (\mathbf{k} + \mathbf{K}) \times \mathbf{E}_{\mathbf{K}}(\mathbf{k}, \omega) + \omega^2 \mathbf{E}_{\mathbf{K}}(\mathbf{k}, \omega) + \omega^2 \sum_{\mathbf{H}} \chi_{\mathbf{H}}(\omega) \mathbf{E}_{\mathbf{K}-\mathbf{H}}(\mathbf{k}, \omega) = \mathbf{0} . \quad (4.3)$$

Here $\mathbf{K}$ and $\mathbf{H}$ are arbitrary reciprocal lattice vectors,

$$\chi_{\mathbf{H}}(\omega) = \frac{1}{V} \int_V \chi(\mathbf{r}, \omega) e^{i\mathbf{H}\mathbf{r}} d^3r \quad (4.4)$$

are the Fourier coefficients of the periodic complex dielectric susceptibility $\chi(\omega, \mathbf{r})$, and V is the volume of the crystal unit cell.

In the fullerite case [37,42] the expansion coefficients of the real part of $\chi(\mathbf{r}, \omega)$ may be written using (4.1) as

$$\begin{aligned} \chi'_0(\omega) &= -\frac{r_e \lambda^2 n_e}{\pi}, \quad \chi'_{\mathbf{H}}(\omega) = \chi'_0(\omega) F(\mathbf{H}) S(\mathbf{H}) e^{-W}, \\ F(\mathbf{H}) &= \sum_{j=1}^5 a_j^{(e)} \exp[-H^2/4b_j^{(e)2}] \frac{\sin HR}{HR}. \end{aligned} \quad (4.5)$$

Here $r_e = e^2/mc^2$ is electron radius, $F(\mathbf{H})$ is the fullerite form factor, $R = 0.353$ nm is fullerene radius, n_e is the electron density averaged over the volume of the crystal, $a_j^{(e)}$, $b_j^{(e)}$ are determined in (2.17), $\exp(-W)$ is the Debye–Waller factor and $S(\mathbf{H})$ is the geometrical structure factor of the fullerite unit cell normalized to $S(\mathbf{0}) = 1$. The absorption of X-rays is due to photo-effect on the K-shell electrons having a relatively compact spatial distribution, therefore the expansion coefficients of the imaginary part of $\chi(\mathbf{r}, \omega)$ may be presented in the form

$$\chi''_0(\omega) = \frac{r_e \lambda^2 \rho_0}{\pi} f''(\omega), \quad \chi''_{\mathbf{H}}(\omega) \simeq \chi''_0(\omega) \frac{\sin HR}{HR} S(\mathbf{H}) e^{-W}, \quad (4.6)$$

where ρ_0 is the mean number density of carbon atoms (nuclei) of the medium and $f''(\omega)$ denotes the imaginary part of the carbon atomic scattering factor tabulated in [13] as a function of radiation frequency ω .

In the case of the hexagonal two-dimensional superlattice formed by single-wall nanotubes and shown in Fig. 1b the corresponding relations may be written [42] similarly to (3.8)

$$\begin{aligned} \chi'_0(\omega) &= -\frac{r_e \lambda^2 n_e}{\pi}, \quad \chi'_{\mathbf{H}}(\omega) = \chi'_0(\omega) F(\mathbf{H}) e^{-W}, \\ F(\mathbf{H}) &= \sum_{j=1}^5 a_j^{(e)} \exp(-H^2/4b_j^{(e)2}) J_0(RH), \\ \chi''_0(\omega) &= \frac{r_e \lambda^2 \rho_0}{\pi} f''(\omega), \quad \chi''_{\mathbf{H}}(\omega) \simeq \chi''_0(\omega) J_0(RH) e^{-W}, \end{aligned} \quad (4.7)$$

where $\mathbf{H}$ is a two-dimensional reciprocal lattice vector, R and u_1^2 are the nanotube radius and mean-squared thermal vibration amplitude of carbon atoms, respectively. Note that $S(\mathbf{H}) = 1$, since the unit cell contains only one nanotube. We ignore the periodic modulations of $\chi(\mathbf{r}, \omega)$ along nanotubes described in Appendix A.

As calculations show, for multiwall nanotubes consisting of n of concentric cylinders we should replace in (4.7) $J_0(RH)$ by sum from 1 to n of the ratio $R_i J_0(R_i H)/\mathfrak{R}$, where $\mathfrak{R} = \sum_{i=1}^n R_i$. In case where thermal

vibration of MWNT are taken into account for the validity of such a procedure a common Debye–Waller factor should be assumed for all SWNTs.

In the case of thermal neutron scattering the corresponding results are

$$\begin{aligned}\chi_{\mathbf{H}}(\omega) &= \chi_0(\omega) F(\mathbf{H}) S(\mathbf{H}) e^{-W} , \\ \chi'_0(\omega) &= -\lambda^2 a \rho_0 / \pi , \\ \chi''_0(\omega) &= n_a (\lambda / 2\pi) \sigma_a ,\end{aligned}\tag{4.8}$$

where $a = 6.2469 \times 10^{-13}$ cm is the coherent scattering length in carbon. One can use the relation $\lambda = 0.287 \times E_{\text{kin}}^{-1/2}$ between the neutron wavelength λ (Å) and its kinetic energy E_{kin} (eV). As mentioned above, $\chi''_0(\omega)$ is velocity-independent and therefore can be calculated using the particular value of $\sigma_a = 0.00351 \times 10^{-24}$ cm² for 2200 m s⁻¹ neutron velocity in carbon of natural abundance (98.9% of ¹²C and the rest of ¹³C). The normalized form factors for neutron scattering have the simple forms

$$\begin{aligned}F(\mathbf{H}) &= \frac{\sin HR}{HR} \quad \text{for } C_{60} \text{ fullerenes} , \\ F(\mathbf{H}) &= J_0(RH) \quad \text{for nanotubes}\end{aligned}$$

corresponding to an infinitely thin layer of nuclei on a sphere or a cylinder while the Debye–Waller factor in (4.8) takes into account the finite thickness of the layer due to the atomic or fullerene vibrations.

4.1. Bragg reflection from fullerites and nanotube ropes

Following [41,42], let us first consider the Bragg reflection of X-rays from nanocrystals. Since the lattice constant is large compared to that in ordinary crystals, we expect that X-rays with longer wavelength could be effectively reflected. Moreover, due to well-known Bragg condition, reflection of X-rays with definite frequency ω in nanocrystals occurs at much lower incidence angles with respect to the crystallographic planes, affecting the tolerance to the deflection from the exact Bragg condition (‘rocking curve’ width). In the two-wave approximation of the dynamical theory of X-ray diffraction the solution of the equation system (4.3) satisfying the boundary conditions on the entrance surface to the crystal can be found in an analytical form. Let a wave be incident at an angle close to the Bragg angle with respect to the planes of the superlattice, and for the sake of simplicity we shall assume that the entrance surface is parallel to these planes. The coefficient of Bragg reflection from a large enough number of superlattice planes can be represented in the form [3]

$$\Re(\lambda, \delta\theta) = |\eta \pm (\eta^2 - 1)^{1/2}|^2 .\tag{4.9}$$

The sign in front of the parentheses is chosen from the condition $\Re \leq 1$. Here $\eta = \eta' + i\eta''$ is a complex parameter connected with $\chi(\omega, \mathbf{r})$ by the relations

$$\begin{aligned}\eta' &= \frac{-\delta\theta \sin 2\theta_B + \chi'_0}{|C| \chi'_{\mathbf{H}}} , \\ \eta'' &= -\frac{\chi''_{\mathbf{H}}}{\chi'_{\mathbf{H}}} \left(\eta' - \frac{1}{|C|} \frac{\chi''_0}{\chi''_{\mathbf{H}}} \right) ,\end{aligned}\tag{4.10}$$

Fig. 25. Contour plot of the Bragg reflection coefficients from a nanotube superlattice, versus the wavelength λ and the deviation $\delta\theta$ from the exact Bragg direction (room temperature, (10, 10) nanotubes, (1, 0) planes, σ -polarization).

where $C = 1$ for radiation polarized perpendicular to the plane of incidence (σ -polarization), $C = \cos 2\theta_B$ for the polarization in the plane of incidence (π -polarization), $\lambda = 2\pi/\omega$ is the radiation wavelength. The kinematic Bragg angle is determined by the equality $\sin \theta_B = H/(2\omega)$, and $\delta\theta = \theta - \theta_B$ is the angular deviation from the kinematic Bragg direction. Note that in the kinematic theory (Born approximation) $1/(2\eta')$ is the reflection amplitude r from an infinite number of planes; for a small number of N of planes, the reflection coefficient $\mathfrak{R}_N$ oscillates between zero and $4r^2$, therefore the unitarity condition $\mathfrak{R}_N < 1$ is violated at $|\eta'| < 1$. Formula (4.9), which results from the dynamical theory, satisfy unitarity and, neglecting η'' (absorption), gives $|\mathfrak{R}| = 1$ in the “unitarity plateau” $|\eta'| < 1$.

Expressions (4.9) and (4.10) with $C = 1$ are applicable to the case of thermal neutron as well. Another important characteristic is the integral coefficient of Bragg reflection

$$\mathfrak{R}_i(\lambda) = \int_{-\infty}^{\infty} \mathfrak{R}(\lambda, \delta\theta) d(\delta\theta) . \quad (4.11)$$

Since $\mathfrak{R}(\lambda, \delta\theta)$ is a very sharp function of $\delta\theta$ about $\delta\theta = 0$, integration in (4.11) is expanded to infinite limits without loss of accuracy. The dependence of the reflection coefficient $\mathfrak{R}(\lambda, \delta\theta)$ on the deflection angle $\delta\theta$ and on the wavelength λ for σ polarization and symmetric Bragg reflection by (1, 0) planes of a superlattice of (10, 10) nanotubes is displayed in Fig. 25 where the values of the reflection coefficient are indicated on the level curves. As the wavelength increases, the reflection maximum undergoes increasingly larger displacements relative to the exact Bragg direction, due to the increasing X-ray absorption in the medium, and is broadened. On the whole, as the wavelength increases, the fixed-angle reflection coefficient $\mathfrak{R}(\lambda, \delta\theta)$ decreases, but it still remains substantial ($\mathfrak{R} \approx 0.3$) even for very soft X-rays with wavelength 15 Å.

The corresponding integral-over- $\delta\theta$ reflection coefficient is displayed in Fig. 26. It is interesting to note that near 20 Å (incidence angles close to the Brewster angle $\approx 45^\circ$) the reflection of a π -polarized wave is substantially suppressed with respect to σ polarization, i.e. a nanotube superlattice acts as a polarizer in this frequency range. The integral reflection coefficient is proportional to the effective angular width

Fig. 26. Integrated-over- $\delta\theta$ Bragg reflection coefficient from (1, 0) planes of a superlattice of (10, 10) nanotubes as a function of wavelength for σ -polarization (curve 1) and π -polarization (curve 2).

$(\delta\theta)_{\text{eff}}$ of $\Re(\lambda, \delta\theta)$ which can be estimated as the width of the unitarity plateau, $(\delta\theta)_{\text{eff}} \simeq 2|C\chi'_{\mathbf{H}}|/\sin 2\theta_B$. Remembering the Bragg condition $\omega = H/(2 \sin \theta_B)$ and varying θ_B in this relation, we find the effective frequency width of the Bragg reflection at fixed theta $(\Delta\omega/\omega)_{\text{eff}} \simeq |C\chi'_{\mathbf{H}}|/\sin^2 \theta_B$. The latter defines the frequency resolution power of a lattice when a well collimated but achromatic X-ray beam (e.g. synchrotron radiation) reflects from a crystal. Since hard X-rays reflect at relatively low Bragg angles, nanotube ropes may serve as broadband monochromators with an integrated over ω reflection coefficient much higher than from ordinary crystals. As will be shown in Section 6.4, this result is very important for the total yield of PXR.

The dependence of the Bragg reflection coefficient (4.9) from a fullerite on the angular deviation $\delta\theta$ and the wavelength λ is illustrated by the contour plots in Fig. 27, the first of which corresponds to σ - and the second to π -polarization. At wavelengths above $\lambda_m = 2d/\sqrt{3} \simeq 1.6$ nm, which corresponds to the normal incidence ($\theta_B = \pi/2$), the diffraction in a fullerite is impossible. All the other peculiarities of the Bragg reflection are similar to the case of nanotube ropes.

4.2. Possibilities of channeling for neutral particles

The case which should be considered specially is the incidence of X-rays or thermal neutrons at small angles to the nanotube axis or a closely packed fullerene row in a fullerite crystal. The standard two-wave approximation used in the previous section is inapplicable to this case because a great number of reciprocal lattice vectors contributes to particle scattering. Let us consider X-ray propagation along nanotubes first. Similarly to the continuum potential, we can introduce a susceptibility $\chi(\omega, \mathbf{r})$ averaged along the axis of the nanotubes (4.7). Thus the problem becomes to be close to the electromagnetic wave propagation in optical fibers [62].

Due to the smallness of $\chi(\omega, \mathbf{r})$ the Fresnel reflection of X-rays mainly occurs at small angles to a channel, i.e. when the electromagnetic wave propagates predominantly in the forward direction. It is well

Fig. 27. Contour plot of the Bragg reflection coefficients from a fullerite, versus the wavelength λ and the deviation $\Delta\theta$ from the exact Bragg direction (room temperature, (1 1 1) crystallographic planes. left: σ -polarization, right: π -polarization).

known that small-angle reflections are independent of the polarization of electromagnetic waves, therefore the modulus as well as the direction of the polarization vector are practically unchanged. Furthermore, the longitudinal wave number (or photon momentum) k_z is conserved, like for particle channeling in the continuous potential approximation. As a result, the electric field of definite frequency and k_z can be approximately factorized as

$$\mathbf{E}(\mathbf{r}, z, t) = \mathbf{e}F(\mathbf{r}) \exp(ik_z z - i\omega t) ,$$

where $\mathbf{e}$ is a unit vector orthogonal to the nanotube axis and $F(\mathbf{r})$ obeys the scalar wave equation

$$\Delta_r F + k_T^2 F = 0 . \quad (4.12)$$

where $k_T^2 = \omega^2[1 + \chi(\omega, \mathbf{r})] - k_z^2$ and Δ_r is the two-dimensional Laplacian. One can see that Eq. (4.12) is similar to (3.1) which describes the quantum channeling of charged particles and thus it can be solved using the same approach. In order of magnitude, the number of modes localized inside a nanotube is determined by the squared ratio of the nanotube radius R to the characteristic transverse wavelength $\lambda_T = \lambda_p$ where $\lambda_p = 1/\omega_p$ and the quantity $\omega_p = (4\pi n_e e^2 / m)^{1/2}$ is the so called *plasma frequency* of substance electrons. According to (4.1), in contrast to relativistic electrons and positrons, the characteristic value of λ_T for X-ray photons does not depend on the particle energy ω and is about 85 Å for a superlattice of (10, 10) nanotubes. It is obvious that localized modes, similar to the discrete transverse energy states

of electrons and positrons discussed in Section 3.1, can exist only in multi-wall nanotubes with radius comparable or higher than the above value of λ_p .

To estimate more precisely the nanotube radius needed for the existence of localized modes let us consider [46] simplified step profile of $\chi(\omega, \mathbf{r})$: electron density $n_e = 0$ inside the tube and $n_e = n_0$ in the surrounding medium, which corresponds to a nanotube with very thick wall or a MWNT with a very large number of layers. In this case Eq. (4.12) can be solved analytically. Owing to the cylinder symmetry one can take F of definite angular momentum l , which is expressed as $F(\mathbf{r}) = f(r) \exp(il\varphi)$. The matching conditions of the transverse components of the fields and their derivatives on the nanotube internal wall imply the continuity of the logarithmic derivative of f at $r = R$:

$$k_T J'_l(k_T R) / J_l(k_T R) = \kappa_1 K'_l(\kappa_1 R) / K_l(\kappa_1 R) . \quad (4.13)$$

Here J_l is a Bessel function, K_l a modified Bessel function of second kind, $k_T = (\omega^2 - k_z^2)^{1/2}$ is the transverse momentum in the hole ($r < R$), $\kappa_1 = (\omega_p^2 - k_T^2)^{1/2}$ is the transverse attenuation coefficient in the wall ($r > R$). This equation gives discrete values of k_T . For each value (mode), the frequency ω and the longitudinal wave number k_z are linked by the dispersion relations $\omega^2 = k_z^2 + k_T^2$. There is at least one mode with $l = 0$, even at small R . When R increases, new modes appear. The second one appears in the wave $l = 1$ at $\kappa_1 = 0$, i.e. is determined by the smallest zero of $J_0(k_T R)$. This gives $R \simeq 2.4\lambda_p$ for the nanotube radius.

The above treatment, where polarization has been factorized out, neglects the coupling between polarization and orbital momentum. The latter was taken into account in [46] in terms of TE and TM modes. The dependence of k_T on the nanotube internal radius R for various exact modes (which are superpositions of TE and TM), calculated in [47], is presented in Fig. 28 where $\delta = k_T/\omega_p$. The fundamental mode designated as $(1, 1, -1)$ exists at any radius, but since the electromagnetic field of the mode inside the wall behaves like $\exp(-\kappa_1 r)$ this mode is not well localized at $r \leq R$ if nanotube radius is below $\simeq \lambda_p$. The second mode which appears at large enough nanotube radius $R \simeq 2.4\lambda_p$ is triply degenerate in terms of $E-H$ coupling model. This agrees with the corresponding result of the first approximation where the coupling is ignored. It can be seen that in the range $\lambda_p < R < 2.4\lambda_p$ the nanotube acts as a monomode X-ray waveguide with well localized field of the mode.

The leakage of the modes through the wall can be estimated using the WKB method. For axially symmetrical modes ($l = 0$) we may use the well-known results for the probability of tunneling through a one-dimensional potential barrier $w \simeq \exp(-2\kappa_1 \Delta a)$, where Δa denotes the effective width of a nanotube wall. The probability w must be small enough which implies the inequality $\Delta a \gtrsim \lambda_p$. Thus, the modes can be well localized inside a single nanotube, irrespective of the value of ω , only for sufficiently thick nanotube walls ($\sim 100 \text{ \AA}$). The above conclusions apply to thermal neutrons as well, since in this case $\lambda_T = (4\pi a \rho_0)^{-1/2}$ is about $138 \text{ \AA}$.

More accurate calculations of the modes, taking into account the tunneling of waves between the neighboring nanotubes, can be performed using a multiwave diffraction approach (4.3), similarly to the case of charged particles discussed above in Section 3.1. In this approach, solutions of Eq. (4.12) are looked for in the form

$$F(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} \sum_{\mathbf{G}} F_{\mathbf{G}} e^{i\mathbf{G}\mathbf{r}} .$$

Fig. 28. Discrete values of the internal transverse momentum k_T (in units of ω_p) of X-rays trapped in thick-wall carbon nanotubes, as a function of the internal radius R (in units of λ_p).

As a result, we obtain a system of equations for the coefficients $F_{\mathbf{G}}$ that describes the multiwave diffraction of X-rays in a nanotube superlattice:

$$[-(\mathbf{\kappa} + \mathbf{G})^2 + (\omega^2 - k_z^2)]F_{\mathbf{G}} + \omega^2 \sum_{\mathbf{H}} F_{\mathbf{G}-\mathbf{H}} \chi_{\mathbf{H}} = 0 . \quad (4.14)$$

The zeros of the determinant of system (4.14) determine the modes of the electromagnetic field propagating freely along the nanotubes or along the planes of the superlattice.

It should be noted that single-wall nanotubes, not only have insufficiently thick walls, but are mechanically unstable at large ($\gtrsim 5$ nm) radii, therefore they are completely unsuitable for the channeling of neutral particles, in contrast to the results of [50]. However X-ray waveguiding may be possible in multiwall nanotubes like those produced using catalytic pyrolysis of hydrocarbons on quartz substrates [63]. Such MWNTs had external diameters from 30 to 40 nm and internal ones from 10 to 15 nm, thus their walls are thick enough to prevent the leakage of the localized modes. Evidently, X-ray or neutron waveguiding in fullerenes (as well as in ordinary crystals) is impossible at all. It is also noteworthy that X-ray and neutron waveguiding (but with very large number of supported modes) was observed in straight and bent glass capillaries reviewed in [64] and micro-channel plates [65]. Other theoretical possibilities for this phenomenon, like in a void superlattice of neutron irradiated metals or artificial multilayered structures, were discussed in [9] and references therein.

5. Incoherent scattering of channeled particles and dechanneling mechanisms

5.1. Mathematical methods for dechanneling

The continuum potential introduced in Section 3 describes totally coherent scattering of particles by carbon atomic or fullerene rows conserving the transverse energy. We discuss now how the equations of motion should be modified to take into account incoherent scattering which violates the conservation of the transverse energy and eventually leads to *dechanneling*.

For this purpose, following [66], let us consider with more details the scattering of a fast particle by a row of vibrating atoms. Let ρ_0 and z be the transverse radius-vector and the longitudinal coordinate of the particle, ρ_i the vector displacement of the i th atom from the axis of the row due to the thermal vibrations, $w(\rho_i)$ the probability of the displacement, $N = \Delta z/d_R$ the number of atoms with which the particle interacts on its path Δz along the row, and d_R the mean inter-atomic distance along the row. The potential acting on the fast particle from i th atom is $U_1(r_i)$, where $r_i = \sqrt{|\rho_i - \rho_0|^2 + (z - id_R)^2}$ is the distance between the particle and the carbon atom (we can assume that the row is made of equidistant atoms). The transverse momentum $\mathbf{q}$ transferred to the particle due to the scatterings on N atoms of the row, on the assumption that the scatterings are independent, may be presented as a sum

$$\mathbf{q} = \sum_{i=1}^N \mathbf{q}_i ,$$

where $\mathbf{q}_i$ refers to the momentum transfer by the i th individual atom. If we assume that the variations of the transverse coordinate of the particle $|\Delta \rho_0|$ over the path Δz along the row is small compared to the distance at which the atomic potential changes significantly, we find the following expression:

$$\mathbf{q}_i = -\nabla \int_{-\infty}^{\infty} U_1 \left(\sqrt{|\rho_i - \rho_0|^2 + z^2} \right) dz ,$$

where ∇U_1 denotes the gradient of atomic potential in the transverse plane.

We may represent the mean (over thermal vibrations) momentum transfer $\langle \mathbf{q}(\rho_0) \rangle$ as the sum of the corresponding values for the individual atoms:

$$\langle \mathbf{q} \rangle = \sum_{i=1}^N \langle \mathbf{q}_i \rangle ,$$

where

$$\langle \mathbf{q}_i(\rho_0) \rangle = -\nabla \int_0^\infty \int_0^\infty U_1 \left(\sqrt{|\rho_i - \rho_0|^2 + z^2} \right) w(\rho_i) dz d\rho_i . \quad (5.1)$$

Hence, the mean value of momentum transfer is defined by the atomic potential U_1 averaged along the atomic row and over the transverse thermal vibrations of the carbon atoms. It is the basis of the existing channeling theory used in the previous sections.

In the next approximation we should take into account the deviations $\Delta \mathbf{q}$ of $\mathbf{q}$ from the mean value $\langle \mathbf{q} \rangle$ caused by atomic vibrations and the presence of the electron gas. Neglecting correlations between the

thermal vibrations of neighboring atoms, we can add the mean-squared fluctuations of the corresponding vector $\mathbf{q}_i$:

$$\langle(\Delta\mathbf{q})^2\rangle = \sum_{i=1}^N (\langle\mathbf{q}_i^2\rangle - \langle\mathbf{q}_i\rangle^2), \quad (5.2)$$

where $\langle\mathbf{q}_i^2\rangle$ is the mean-squared momentum transfer from a single atom. The mean deviation by the angle $\langle\mathbf{q}\rangle/E$ corresponds to coherent scattering by the N atoms, whereas the fluctuating part corresponds to incoherent scattering. In the following, we will neglect the $\langle\mathbf{q}_i\rangle^2$ terms in the right-hand side of (5.2). This leads to an over-estimation, but not too drastic, of $\langle(\Delta\mathbf{q})^2\rangle$. Note that relatively close collisions of the particles with nuclei, where screening of the latter by the medium electrons is weak, give the main contribution to $\langle(\Delta\mathbf{q})^2\rangle$. So, we can assume that the intensity of incoherent scattering on nuclei depends on the local density $n_a(\mathbf{r})$ of the nuclei. A similar assumption will be done for incoherent scattering on the electrons of the material with local density $n_e(\mathbf{r})$. On these assumptions the mean-squared momentum transfer during a longitudinal step Δz (containing many atomic distances, but such that $n_a(\mathbf{r})$ and $n_e(\mathbf{r})$ do not vary too much) may be found similarly to the case of multiple scattering in amorphous media. In terms of the multiple scattering angle $\theta_s = \Delta\mathbf{q}/E$, we have then

$$\langle\theta_s^2(\mathbf{r})\rangle = 16\pi e^4 (\Delta z/E^2) [n_a(\mathbf{r})Z^2 L_n + n_e(\mathbf{r})L_e] \quad (5.3)$$

with Coulomb logarithms [67] $L_n = \ln(191Z^{-1/3})$, $L_e = \ln(1194Z^{-2/3})$ for electron–nucleus and electron–electron scattering, respectively. Unlike in amorphous media [67], here $n_a(\mathbf{r})$ and $n_e(\mathbf{r})$ are the local number density of carbon nuclei and medium electrons as a function of the transverse coordinates $\mathbf{r}$. These quantities, therefore $\langle(\Delta\mathbf{q})^2\rangle$ also, vary strongly with $\mathbf{r}$ and are concentrated near the row axis. From the equality $\mathbf{q} = \langle\mathbf{q}\rangle + \Delta\mathbf{q}$ we may consider the transverse motion of a fast particle in a nanotube rope as a relatively smooth motion in the continuum potential on which stochastic perturbations are superimposed due to the incoherent scattering on atomic vibrations and electrons of the medium. Similar considerations can be performed in the case of axial channeling in fullerites [37] where additional averaging over the fullerene angular coordinates should be included.

The stochastic character of the perturbations of the particle trajectories prevents us from formulating exact equations of motion. However, we may apply the following calculation algorithm. Since the entrance points $\mathbf{r}_0$ of the particles into the channels are randomly distributed over the transverse plane, we can use the Monte-Carlo method to determine the initial transverse coordinate of the particle. Then we integrate numerically the equations of motion (3.12) in the averaged potential of the nanotube rope $U(\mathbf{r})$ over time interval Δt and obtain the values of the transverse coordinate $\mathbf{r}_1$ and momentum $\mathbf{p}_{\perp 1}$ at time $t_1 = \Delta t$. The integration interval Δt_1 should be chosen so short that the nuclear number density $n_a(\mathbf{r})$ as well as the electron number density $n_e(\mathbf{r})$ are practically constant in this interval. At the same time the number of collisions should be large enough for the validity of the Gaussian distribution of $\Delta\theta$. Then, using the Monte-Carlo method we generate a random value of the incoherent multiple scattering angle $\Delta\theta = \{\Delta\theta_x, \Delta\theta_y\}$ due to incoherent scattering on path $\Delta z \approx \Delta t$ according to the probability distribution

$$P(\Delta\theta) = 2 \frac{|\Delta\theta| \exp(-(\Delta\theta)^2/\langle\theta_s^2\rangle)}{\langle\theta_s^2\rangle} \quad (5.4)$$

(the use of this formula will be discussed below), $\langle\theta_s^2\rangle$ being given above. The random value of $\Delta\mathbf{q} = E\Delta\theta$ is then added to $\mathbf{p}_{\perp 1}$, and the sum is considered as the actual value of the transverse momentum at time

Fig. 29. Number density distribution for nuclei (curve 1) and electrons (curve 2) as a function of the distance from the $[1\ 0\ 0]$ axis along the straight line connecting two adjacent $[1\ 0\ 0]$ axes spaced by the maximum distance. The distribution density is normalized to the values averaged over the volume; the distance is measured in units of the fullerene radius.

t_1 . The above procedure concerning the transverse momentum is repeated for the next time interval from t_1 to $t_2 = t_1 + \Delta t_2$ and so on.

This method of taking into account incoherent scattering (sometimes referred to as the method of aggregated collisions [68]) is much faster than other ones, e.g. the method of kinetic equations [9] or the binary collisions method [18], at least in the case of axial channeling, where the phase space for the transverse motion is four-dimensional and kinetic equations are too complicated, and in the case of high-energy particles where an extremely large number of binary collisions must be taken into consideration.

The results of specific numerical calculations obtained with this method will be discussed in Section 5.2. Let us do some qualitative analytical estimations of the effect of the incoherent scattering on the channeling of a particle beam. The dechanneling length l_{dc} is often defined as the length of a channel at which a half of the particle beam primarily captured into this channel leaves it due to the incoherent scatterings. It can be roughly estimated by equating the mean square angle of multiple scattering over this length to the square of the Lindhard angle. This leads to the relation

$$l_{dc} \approx \frac{U_0 E}{8\pi e^4} (Z^2 \langle n_a \rangle L_n + \langle n_e \rangle L_e)^{-1}. \quad (5.5)$$

Here $\langle n_a \rangle$ and $\langle n_e \rangle$ are the averages of $n_a(\mathbf{r})$ and $n_e(\mathbf{r})$ along the particle trajectory, which may be very different from the averages over the crystal volume. For example, Fig. 29 shows the profiles of the nuclear, $n_a(\mathbf{r})$ (curve 1) and electron, $n_e(\mathbf{r})$ (curve 2), number densities along the $[1\ 1\ 0]$ direction (straight line connecting next-to-nearest $[1\ 0\ 0]$ channels in fullerite). They are expressed in terms of the corresponding

Fig. 30. Distribution of the number density of carbon nuclei (curve 1) and medium electrons (curve 2) along the line between the nearest neighbor nanotubes in the rope (11, 9).

values in an amorphous medium n_a of same volume density, ρ is the distance from axis of the row and R is the fullerene radius. The amplitude of thermal vibrations of fullerenes was calculated in the framework of the Debye model with a Debye temperature $T_D = 55.4$ K measured in experiments [38], the fullerite target was assumed to be at room temperature. Both nuclear and electron densities are significantly reduced between the rows, but inside the rows they are comparable with the corresponding values in randomized (amorphous) medium. For a nanotube rope, Fig. 30 shows the number density of carbon atoms (curve 1) and medium electrons (curve 2) along the line between two nearest neighbor (11, 9) tubes. Here ρ/R is the distance from the nanotube axis measured in units of the nanotube radius $R = 6.79$ Å. One can see that in nanotubes the density of vibrating atoms and medium electrons is concentrated in the vicinity of the nanotube wall while in the remaining part of the channels the density of scatterers is negligibly small. We may conclude, using (5.5) that positive particles channeled in nanotubes or between the fullerene rows in fullerites have much longer dechanneling lengths than in ordinary crystals like diamond for the same total energy E of the ultrarelativistic particle. For a given target, the dechanneling length is proportional to E , according to (5.5).

It should be noted that due to the Coulomb character of the atomic field at small distance $|\rho_i - \rho_0|$ to a nucleus, $\langle \mathbf{q}_i^2 \rangle$, and consequently $\langle (\Delta \mathbf{q})^2 \rangle$ in (5.2), is logarithmically divergent. Formally, this singularity was cut-off at $\mathbf{q}_i \simeq 1/R_{\text{nuc}}$ where R_{nuc} is the nuclear radius (at $\mathbf{q}_i \simeq 1$ for the collisions on an electron). On the other hand, a single collision at an angle $\theta_s \geq \theta_L$, corresponding to $|\mathbf{q}_i| \geq q_{\text{dc}} = \sqrt{2U_0 E}$, produces dechanneling at once. Therefore the dechanneling by multiple collisions should involve the $\mathbf{q}_i$ distribution weighted by $\mathbf{q}_i^2$ only up to $q_i \simeq q_{\text{dc}}$. For this reason and for having neglected the $\langle \mathbf{q}_i \rangle^2$ terms in the right-hand side of (5.2), Eqs. (5.4) and (5.5), which involve $\langle \mathbf{q}_i^2 \rangle$, overestimate the dechanneling. Similar problem of the Coulomb tails exists in the case of amorphous media [69] as well. A more involved simulation method of channeling taking into account the Coulomb tails can be found in [70].

Besides incoherent scattering there may be other factors changing the transverse energy. For example, according to the recent experiments at CERN [71], radiation energy loss of electrons and positrons with energy of the order of 10^2 GeV channeled in diamond crystals may be two orders higher than in the amorphous medium (randomly oriented diamond). This is due to a significant enhancement of the electromagnetic radiation from channeled particles in a wide spectral region, including photon energies ω comparable to the particle energy E . If the radiation length, which determines the radiative energy loss, is so short that it is comparable to the penetration depth of particles into a nanotube rope or a fullerite, we should take into account the influence of the energy loss on the transverse motion of channeled particles. The expression for the energy loss rate depends on the ratio $\chi = E/E_{\text{cr}}^{(2)}$ where $E_{\text{cr}}^{(2)} = 1/|\nabla U|$. It can be written as

$$\frac{dE}{dt} = -e^2 f(\chi) , \quad (5.6)$$

where $f(\chi)$ has a simple form in two limits:

$$\begin{aligned} f(\chi) &= \frac{2\chi^2}{3}, & \chi \ll 1 \text{ (classical limit)} , \\ f(\chi) &\simeq 0.82\chi^{2/3}, & \chi \gg 1 \text{ (ultra-quantum limit)} , \end{aligned}$$

χ being calculated at the particle locus $\mathbf{r} = \mathbf{r}(t)$.

Radiation can also decrease the transverse energy ε . Calculating the work of radiative friction force against the particle we can find the following relation between the total energy loss (5.6) and the transverse energy loss [9]:

$$\frac{d\varepsilon}{dt} = (E^{-2} + \mathbf{v}_{\perp}^2/2) \frac{dE}{dt} , \quad (5.7)$$

where $\mathbf{v}_{\perp}$ is the transverse velocity. One may attribute one part of this energy loss to a friction force collinear to the velocity, the other part to a “side-slipping” [74,75] of the electron deeper into the potential well. At relatively high energy $E \gg E_{\text{cr}}^{(1)} = 1/U_0$ the second term in the brackets of (5.7) dominates and $d\varepsilon/dt$ occurs to be proportional to E . In this limit the quantum theory gives [9] the same result (5.7). The decreasing of ε called “transverse energy cooling” [72,73] can overcome the transverse energy “heating” of incoherent multiple scattering which according to (5.6) is inversely proportional to E . This effect makes the electron travel deeper into the potential well where the electric field (gradient of the potential) is stronger, therefore the electron radiates more and more intensely [70,73]. It can loose most of its energy on a length 100 times shorter than the ordinary radiation length. Such a dramatic enhancement of the electromagnetic radiation intensity was first observed for axial channeling in ordinary crystals [76] and has been studied more systematically in CERN [71].

Fortunately, as calculations showed [37,66], energy loss of channeled positrons and electrons in nanocrystals are significantly lower than in diamond crystal and its influence on the channeling may be neglected up to electron or positron energies of 10^3 GeV. Consequently, the transverse energy cooling effect is weaker, however one should keep in mind that multiple scattering heating is weaker too. As far as heavier particles (e.g. protons or π -mesons) are concerned, there is no need to take into account the radiative energy losses at all. Indeed, returning in (5.6) to usual units, we find out that the energy loss rate is inversely proportional to the fourth power of the particle mass. Below we consider the cases where the backward reaction of radiation on particle motion may be neglected.

5.2. Discussions of the computer simulation results

5.2.1. Case of nanotubes

The method of aggregated collisions outlined above was applied in [66] to the computer simulations of the propagation of ultra-relativistic positively charged 150 GeV particles (e.g. positrons, π^+ -mesons or protons) through a (11, 9) nanotube rope made of a hexagonal 2D lattice of nanotubes. The simulated beam of particles consists in of $N = 10^3$ particles, has zero initial angular spread and enters into the nanotube rope at an angle $\theta_0 = \theta_L/2$ equal to the half of the Lindhard angle $\theta_L = 2.83 \times 10^{-5}$. The penetration depths of the particles into the rope are measured in units of $L_0 = R/\theta_L = 24 \mu\text{m}$ which represents the typical path of the particle in the rope between two subsequent encounters with the nanotube wall. The angular distribution of the beam at various depths is illustrated in Figs. 31–33 by series of scattering plots. The values of the penetration depth are shown in the upper-right corner of the corresponding plot, θ_x and θ_y are the angular coordinates of particles in the transverse (with respect to the nanotube axis) plane.

Three stages of the transformation of the angular distribution may be distinguished. At the first stage from $z = 0$ to $z \approx L_0$ the initial distribution quickly broadens due to the strong coherent scattering of the beam by the atomic rows. The influence of the incoherent scattering at this stage is relatively small. At the second stage from $z \approx L_0$ to $z \approx 20L_0$ the angular distribution tends to the ring-like pattern, the radius of which corresponds to the angle of incidence (equal to the half of θ_L). The thickness of the ring is determined by the thickness of the nanotube wall. The ring appears as a result of the multiple reflections of the beam on nanotube walls which lead to rotations of the transverse momentum of the particles at different azimuthal angles. At the third stage due to the increasing influence of the incoherent scattering the ring-like pattern broadens and at very large depth $z \approx 10^3 L_0$ it is hardly noticeable.

The variation of the relative number N_{ch}/N of particles bound inside the nanotubes as a function of z is shown in Fig. 34 for 150 GeV positive particles. At entrance about 60% of the beam is captured into the nanotubes, but after a few decimeters only a small part of them remains bound inside the channels. The dechanneling length in nanotube ropes estimated from this figure is close to 250 mm for 150 GeV positive particles, which is one order of magnitude higher than in ordinary crystals at similar conditions.

The spatial distribution of the beam over the transverse coordinates strongly varies with the penetration depth as well. The transformation of the spatial distribution of the beam in the hexagonal two-dimensional lattice cell of the rope is illustrated in Fig. 35. Initially at $z \approx 0$, the beam is uniformly distributed over the unit cell. A significant redistribution of the spatial distribution may be noticed already at $z \approx L_0$. It is noteworthy that, like in ordinary crystals, this effect may serve for the location of impurity atoms inside relatively short ($z \sim L_0$) nanotubes, using secondary processes sensitive to the close collisions of the particles with the impurity atoms, i.e. backward Coulomb scattering, characteristic X-ray production or nuclear reactions.

Fig. 31. Angular distribution of the beam at various depths (the first stage).

The simulated angular distribution of the beam passing through (11, 9) nanotubes bent with a curvature radius R_b equal to Tsyganov critical radius $R_c = 1.70$ m, at various penetration depths, is shown in Fig. 36. The point $\theta_{0x} = \theta_{0y} = 0$ is the direction of the initial beam, supposed to be extremely collimated. It can be seen that a noticeable part of the beam follows the curved channel and thus is deflected at an angle $\alpha = z/R_b$ which can be equal to several times the Lindhard angle. This part has an angular divergence close to the Lindhard angle. The remaining particles contains non-deflected and partially deflected particles, the latter travelling preferably along the major superlattice planes.

The relative number of particles following the curved nanotubes is shown in Fig. 37 as a function of the deflection angle $\alpha = z/R_b$. This figure clearly shows that about 20% of the beam may be deflected at angles $\alpha \simeq 10$ milliradians which are two orders higher than the Lindhard angle at $E = 150$ GeV. As pointed out above, the channeling of high-energy particles in curved nanotube ropes is of special interest due to the possibilities of beam deflection at comparatively large angles.

Fig. 32. Angular distribution of the beam at various depths (the second stage).

The comparison between the channeling of 1 GeV electrons and positrons along (10, 10) nanotube rope and along [1 1 0] axial direction in diamond is carried out in [77] using the simulation method similar to the described above. The continuum potential of diamond at room temperature is shown in Fig. 38 which should be compared to that of (10, 10) nanotube rope in Fig. 4a. The dependence of the channeling fraction of the beams, having the initial angular spread $\Delta\theta_0 = \theta_L/4$, on the penetration depth z is illustrated in Fig. 39 for positrons and in Fig. 40 for electrons. It can be seen that dechanneling of positrons in a nanotube rope (curve 1) is substantially slower than in diamond (curve 2) due to the much deeper potential well and lower substance electron density inside the channels in a nanotube rope compared to diamond. Electrons (Fig. 40) have always much shorter dechanneling length than positrons (Fig. 39). Dechanneling length of electrons in a nanotube rope (curve 1) has the same order of magnitude as in diamond (curve 2). This is due to the fact that channeled electrons, both in nanotubes and diamond, move back and forth through the region of atomic thermal vibrations which in this case become the main reason for relatively high incoherent scattering.

The comparative results for positrons passing through a bent (10, 10) nanotube rope and through a bent [1 1 0] channels of diamond crystal is shown in Fig. 41 as the scattering plots for a set of the penetration depths proportional to the deflection angle equal to 5, 10 and 20 mrad. At relatively small depths a noticeable part of the beam follows the bend axial channels both in nanotube rope and diamond. However, in nanotubes the beam deflects due to true channeling, while in diamond the deflection is caused rather by multiple scattering of positrons on bent atomic strings [57,77]. When the penetration depth into diamond (deflection angle) increases a considerable part of positrons leaves the axial channels. However, some of dechanneled positrons them can be recaptured into bent planar channels and follow them further

Fig. 33. Angular distribution of the beam at various depths (the third stage).

giving “whiskers” in the angular distributions of the beam. The planar effect (“whiskers”) can be also seen in the case of nanotube ropes, but they are much less distinctive than in ordinary crystals.

The dependence of the fraction of a deflected beam on the deflection angle α is presented in Fig. 42. Particles are considered as “deflected” if the angle between their velocity and the direction of the axis of bent nanotubes (or bent $[1\ 1\ 0]$ diamond axes) are below the Lindhard angle. The simulation is performed for 1 GeV positrons (Fig. 42a) and electrons (Fig. 42b) passing through a nanotube rope and a diamond crystal, both bent with the curvature radius $R_b = 2$ cm.

It can be seen that beam deflection is possible both for positively and negatively charged particles. However, in the case of a nanotube rope and positrons the part of the beam deflected at α larger than $\simeq 10^{-2}$ is relatively large and it varies slowly with increasing α . Electrons are deflected less efficiently both by a nanotube rope and diamond. Only a small fraction of them can be deflected at angles α larger than $\simeq 10^{-3}$. This is obviously due to the fact that incoherent scattering of channeled negative particles is always more intense than of positive.

Fig. 34. Relative number of 150 GeV positive particles remaining inside the nanotubes at different penetration depths into the nanotube rope.

5.2.2. Case of fullerites

The method of aggregated collisions was also applied in [37,78] to the case of the propagation of high-energy particles along $[1\ 0\ 0]$ axial channels in fullerites. The results for particles with different energies E are given below. For each value of total energy E , the trajectories of $N = 10^3$ particles with random entrance positions were calculated. The incident beam was supposed without divergence and parallel to the fullerite crystallographic axis. The continuum potential governing the particle motion is shown in Fig. 6. Fig. 43 illustrates the decrease of the relative number N_{ch}/N of ultrarelativistic positively charged particles remaining in $[1\ 0\ 0]$ axial channels as a function of the depth z . About 80% of the beam is initially captured into the channels both between and inside fullerene rows. Curves 1–3 correspond to particle energies $E = 150, 50$ and 10 GeV, respectively. The comparison of their slopes confirms that the dechanneling length is proportional to E , in accordance with the simple estimate (5.5). There is a slowing down of dechanneling at relatively large depths, apparently associated with the fact that at such depths channeling predominantly occurs between the fullerene rows (“square” channels of Fig. 6), where the effect of incoherent scattering is weaker than inside the rows (circular channels of Fig. 6). However, in average, the dechanneling length in fullerites occurs to be about one decimal order shorter than in nanotubes (at the same particle energies).

Fig. 35. Transformations of the spatial distribution of the beam over the transverse coordinates at various depths.

The comparison of channeling of positive and negative particles in fullerenes is illustrated in Fig. 44. Curve 1 shows the relative number of 10 GeV ultrarelativistic negatively charged particles remaining in $[110]$ axial channels (Fig. 7) as a function of the depth z while curve 2 shows the similar results for 10 GeV positively charged particles in $[100]$ axial channels. About 80% of negative particle can be

Fig. 36. Angular distribution of the beam passing through (11, 9) nanotubes bent with the Tsyganov curvature radius at various penetration depths.

captured in [1 1 0] channels. The dechanneling length for negative particles is about 0.2 mm which (as contrasted to the nanotube case) is only about two times less than for positive particles in [1 0 0] channels.

The angular and spatial distributions of 10 GeV positron beam at various depths in a fullerite is illustrated in Fig. 45 by series of scattering plots. Initially the beam has zero angular spread and zero entrance angle to [1 0 0] axial channels. The penetration depths z of the particles into the fullerite (indicated by numbers in the upper side of the figures) are measured in units of $L_0 = R/\theta_L = 6.786 \mu\text{m}$, where R is the fullerene radius and θ_L is the Lindhard angle corresponding to the channeling in the deepest “square” well. The circle in all the left figures corresponds to the Lindhard angle. Similarly to the case of a

Fig. 37. Relative number of particles following the curved nanotubes as a function of the deflection angle.

Fig. 38. Continuum potential of [110] channels in diamond.

Fig. 39. Dependence of the channeling fraction of 1 GeV positrons on the penetration depth into (10, 10) nanotubes.

Fig. 40. Dependence of the channeling fraction of 1 GeV electrons on the penetration depth into (10, 10) nanotubes.

nanotube rope discussed above, at the first stage from $z = 0$ to $z \approx L_0$ the initial distribution, which is represented by the point $(0, 0)$ in the transverse momentum space, quickly broadens due to the strong coherent scattering of the beam by the molecular rows. The central almost axially symmetrical core of the angular distribution is probably formed by the coherent scattering of particles moving inside the more shallow ($U_0 \simeq 7$ eV) circular channels while the broader star-like distribution is due to the scattering of particles moving between the fullerene rows in almost twice deeper ($U_0 \simeq 13.5$ eV) “square” channels. At larger z the dechanneling brings some part of the beam outside the ring. It is interesting to note that at $z \simeq 4L_0$ and $8L_0$ the re-focusing of the beam is observed. This is due to the closeness of the potential of the circular channels to the parabolic one. Indeed, it is known that in a two-dimensional parabolic

Fig. 41. Angular distribution of 1 GeV positrons passing through a bent (10, 10) nanotube rope and through a bent [1 1 0] channels of diamond crystal at various depths.

potential oscillation periods of the particles with zero angular momentum do not depend on their oscillation amplitudes, thus after one oscillation period the beam can become parallel again. However, with the increasing penetration depth the focusing effect becomes weaker both due to the anharmonic

Fig. 42. Relative number of 1 GeV positrons (a) and electrons (b) deflected by bent (10, 10) nanotubes (curves 1) and bent [1 1 0] diamond axes (curves 2) as a function of the deflection angle.

Fig. 43. Dependence of the relative number N_{ch}/N of ultrarelativistic positively charged particles remaining in [1 0 0] axial channels of a fullerite at the depth z . Curve 1 for $E = 150$ GeV, curve 2 for 50 GeV, and curve 3 for 10 GeV.

part of the potential and the influence of the incoherent scattering giving non-zero angular momenta to the particles.

The spatial distribution of the beam, shown in the limits of the square unit cell of the transverse lattice, at the entrance to a fullerite is homogeneous, but it rapidly transforms to extremely inhomogeneous already at $z \simeq 0.6L_0$. Due to the approximate conservation of the phase-space volume of the beam one can see strong correlations between the angular and the spatial distributions.

Fig. 44. Dependence of the relative number N_{ch}/N of ultrarelativistic 10 GeV charged particles remaining in axial channels of a fullerite at the depth z . Curve 1 for electrons and $[1\ 1\ 0]$ channels, curve 2 for positrons and $[1\ 0\ 0]$ channels.

Bent fullerites can effectively deflect both positive and negative particles. The angular distribution of 10 GeV positron beam (with negligibly small initial angular divergence) passed along $[1\ 0\ 0]$ axial channels of a fullerite with thickness $z = 10L_0$ curved with radius R_b equal to Tsyanov critical radius R_c is shown in Fig. 46 as a scattering plot. The similar distribution for the case of 10 GeV electrons and $[1\ 1\ 0]$ channels is shown in Fig. 47. It can be seen that a noticeable part of the both beams can be deflected at angles about five Lindhard angles.

6. Emission of radiation by charged particles passing through nanocrystals

Propagation of electrons and positrons through ordinary crystals as well as nanocrystals is accompanied by various types of electromagnetic radiation. They arise both from the non uniform motion of the charged particles in the electrostatic potential of aligned atoms and from the transient polarization of the medium by the particles. In this chapter we present the general properties of these radiations and their particular features in the nanotube and fullerite cases.

6.1. Radiative transitions (channeling radiation) between the transverse energy levels of MeV electrons and positrons

In this subsection we consider e^+ and e^- of energies sufficiently low so that channeling has an essentially quantum character. Spontaneous radiative transitions between the transverse states of channeled particles give rise to the so-called *channeling radiation* (CR). As shown above in Section 3.1, at relatively low energies of positrons and electrons, there are transverse energy bands $\varepsilon_n(\kappa)$, which, in the limit of infinitely

Fig. 45. Angular (left) and spatial (right) distributions of the positron beam at different depths of channeling in a fullerite.

small transmittance by tunneling of the potential barrier separating neighboring nanotubes, degenerate into discrete levels. The electromagnetic radiation can be treated as being due to dipole radiative transitions between the bands (levels). Due to the Doppler effect caused by the relativistic longitudinal motion of the particles the energy of an emitted photon is high compared to the transverse energy difference, but in usual circumstances it is small compared to the energy of the particle ($\omega \ll E$) in the region of E under consideration. Electromagnetic radiation under quantum channeling of electrons and positrons is a well-known phenomenon and several review articles, e.g. [9], describe the various theoretical approaches and the corresponding experimental results. In this subsection we discuss some features the channeling radiation may have in nanocrystals.

The spectral-angular probability density of photon emission per unit time due to a spontaneous transition of a particle from a band i into a band f with lower transverse energy can be represented in the form [41]

$$\frac{d^2 w}{d\omega d\Omega} = \frac{e^2 \omega^3}{8\pi} \sum_f \left[(\theta^2 + E^{-2})^2 |\mathbf{n}_\perp \times \mathbf{r}_{if}|^2 + (\theta^2 - E^{-2})^2 |\mathbf{n}_\perp \cdot \mathbf{r}_{if}|^2 \right] \times \delta \left[\frac{\omega}{2} (\theta^2 + E^{-2} - \chi'_0(\omega)) - \omega_{if} \right]. \quad (6.1)$$

Fig. 46. Angular distribution of the positron beam passing through the $[1\ 0\ 0]$ channels of the fullerite bent with the Tsyganov curvature radius at penetration depth $z = 10L_0$.

Fig. 47. Similar to Fig. 46, but for electrons and $[1\ 1\ 0]$ channels.

Here $(\omega, \theta, \varphi)$, with $\theta \ll 1$, represent the photon momentum in polar coordinates about the crystallographic axis. $d\Omega \simeq \theta d\theta d\varphi$ is the differential of the solid angle of emission, $\mathbf{n}_\perp = \{\cos \varphi, \sin \varphi\}$ is the unit vector collinear to the transverse momentum of the photon, $\varepsilon_n(\mathbf{k})$ is the transverse energy of the particle with quasi-momentum $\mathbf{k}$ in the n th band, $\omega_{if} = \varepsilon_i(\mathbf{k}) - \varepsilon_f(\mathbf{k})$ is the transition frequency, and δ is the Dirac function. The matrix element of a dipole transition between the bands has the form

$$\mathbf{r}_{if} = \int_S \phi_{f\mathbf{k}}^*(\mathbf{r}) \mathbf{r} \phi_{i\mathbf{k}}(\mathbf{r}) d^2r ,$$

where $\phi_{i\mathbf{k}}$ denotes the periodical part of the transverse wave-function (3.2), S is the area of the transverse lattice cell. The quasi-momentum of the particle is conserved (up to a reciprocal lattice vector) during the dipole transitions. Wavefunctions $\phi_{i\mathbf{k}}$ are normalized according to the relation

$$\int_S \phi_{f\mathbf{k}}^*(\mathbf{r}) \phi_{i\mathbf{k}}(\mathbf{r}) d^2r = \delta_{if} .$$

Following [79], we have taken into account the complex Doppler effect through the volume-averaged real part of the dielectric susceptibility of the medium $\chi'_0(\omega) \ll 1$. Formula (6.1) corresponds (for each f) to a quantum dipole moving with a relativistic speed in the dielectric medium. In contrast to ordinary crystals, the polarization can indeed have a large effect on the spectrum of emitted frequencies via the complex Doppler effect determined by zeros of the Dirac function in (6.1). The characteristic channeling radiation frequencies can be estimated as $\omega \sim \omega_{if} E^2$. If ω is substantially higher than the K-shell ionization threshold of carbon ($\hbar\omega_K \approx 284$ eV), we can use the “plasma” formula $\chi'_0(\omega) = -\omega_p^2/\omega^2$ where ω_p (see 4.2) is the plasma frequency of the medium. In this case the relation between the radiation frequency and the polar angle of the radiation takes on the form

$$\theta^2 = \frac{2\omega_{if}}{\omega} - E^{-2} - \frac{\omega_p^2}{\omega^2} . \quad (6.2)$$

In ordinary crystals the influence of the last term in (6.2) is negligibly small due to relatively high values of the energy level difference ω_{if} at any particle energy E . However, the situation can change in nanocrystals where ω_{if} is smaller than in ordinary crystals by one order of magnitude. In the general case the allowed frequencies are determined by the condition that the right-hand side of (6.2) is positive, which gives the following limitations:

$$\begin{aligned} \omega_{\min} &\leq \omega \leq \omega_{\max} , \\ \omega_{\min} &= E^2[\omega_{if} - (\omega_{if}^2 - \omega_p^2 E^{-2})^{1/2}] , \quad \omega_{\max} = E^2[\omega_{if} + (\omega_{if}^2 - \omega_p^2 E^{-2})^{1/2}] . \end{aligned} \quad (6.3)$$

Radiation with frequency $\omega_{\min}$ or $\omega_{\max}$ is emitted at zero angle θ . It is important that the expression in the brackets of (6.3) must be positive, otherwise radiation becomes impossible at all, in other words, the particle energy E must be high enough to satisfy the condition

$$E\omega_{if} \gg \omega_p , \quad (6.4)$$

where ω_{if} is E -dependent due to the relativistic mass in (3.1). Note that according to (3.1) ω_{if} depends on E via the parametric dependence of the transverse energy levels on E . It should be taken into account that, if $\omega_{\min}$ and $\omega_{\max}$ happen to be outside the validity of plasma formula for the real part of the dielectric

susceptibility, the dependence of the latter on ω can be more complicated giving rise to a more complex Doppler effect. Moreover, below or not far above the K-edge the absorption of radiation inside nanocrystals may be of importance. For example, the analysis based on energy level scheme in Figs. 8 and 9 shows that 1 MeV electrons and positrons channeled in a nanotube rope can emit only in the ultraviolet range, where radiation is almost completely absorbed in the matter itself and it is hardly possible to observe the radiation. Electrons with higher energy (3 MeV) can emit several lines in the range 290–311 eV at zero angle of observation and increasing again the electron energy (9 MeV), radiation at even higher frequencies (1.3–2.2 keV) becomes possible. As for the intensities of the lines, they depend, besides the dipole matrix elements, on the lifetime and the populations of the levels. The initial populations depend on the entrance angle of the beam with respect to the channels while a redistribution between the levels occurs due to the incoherent scatterings of the beam on substance electrons, fluctuations of the potential caused by thermal vibrations and other reasons which are superimposed on the radiative transitions. More detailed information on this problem can be found in [9] and references therein.

Expression (6.1) describes radiative transitions between the above-barrier transverse energy bands of low energy particles as well. If the transverse energy is high above the barrier, i.e. the entrance angle of the particles substantially exceeds the Lindhard critical angle, we can consider the continuum potential as the source of a small perturbation of the incident wave function (plane wave) of the particle and use the first Born approximation to calculate such a perturbation. This regime of the radiation mechanism is called coherent bremsstrahlung (CB). In the first Born approximation the radiation probability is proportional to the *squared* charge of the particle, therefore in contrast to CR discussed above, there is no difference in the radiation spectra from electrons and positrons. Historically CB was predicted and investigated experimentally in ordinary crystals [80] early before channeling, however only with the discovering of the latter a unified approach to the problem of radiation of fast particles in crystals was developed enabling to define the limits for the old theory of CB based on the Born approximation. We discuss this theory below in conjunction with CB and CR from ultra-relativistic electrons and positrons in nanocrystals.

6.2. Coherent bremsstrahlung and channeling radiation from ultra-relativistic electrons and positrons

In this subsection we consider electrons and positrons of sufficiently high energies. In particular, the channeling motion can be treated classically. As we shall see however, it does not mean that the radiation mechanism is always classical.

6.2.1. Different regimes of radiation

As mentioned above, the standard theory of coherent bremsstrahlung (CB) is based on the Born approximation, which implies, as a first condition $\varepsilon \gg U_0$, equivalently, $\theta_0 \gg \theta_L$. Besides, one must assume that the variations ϑ_{dev} of the direction of the particle momentum due to the fields of the atomic rows or planes is small in comparison with the effective angle $\theta_{\text{eff}} \sim E^{-1}$ for the emission of radiation by ultra-relativistic particles. In fact, it is well known [81] that the character of the electromagnetic radiation from a charged particle in an external electromagnetic field substantially depends upon the relation between the angular deviation ϑ_{dev} of the particle from the initial direction of motion and the effective angle of radiation θ_{eff} . Thus two regimes have to be considered:

If the deviation is relatively small ($\vartheta_{\text{dev}} \ll E^{-1}$), the radiation spectrum has a dipole character, i.e. it is determined by the Fourier expansion of particle velocity with respect to time. In this case the

radiation is formed over a relatively long path $l_{\text{coh}} = 2\pi/(\omega - \mathbf{k}\mathbf{v})$ called *the coherence length* [80] (or the formation zone) of radiation. For radiation in vacuum ($k = \omega$) and in the direction close to the particle velocity we may estimate the coherence length as $l_{\text{coh}} \sim \lambda E^2$ which substantially exceeds the radiation wavelength λ . The CB arises if the coherence length coincides with the path between the successive collisions of the particle with atomic rows or planes. For ultrarelativistic particles the CB condition can be satisfied when they move at small angle to the crystallographic plane or axis, but not too small otherwise the angular deviation ϑ_{dev} of the particle can increase due to the channeling effect.

In the opposite case of large deviation angles ($\vartheta_{\text{dev}} \gg E^{-1}$) the analysis of the problem can be simplified significantly. Indeed, a piece of trajectory of length $l_{1/E} = 1/|\nabla U|$, where the direction changes by $1/E$, occupies a small region of the transverse coordinate r , where the field is approximately uniform and the trajectory almost circular. So, one can estimate that the radiation emitted from this piece has the spectrum of synchrotron radiation corresponding to the local acceleration, except for low frequencies where the formation length $l_f \sim l_{1/E}(\omega_m/\omega)^{1/3}$ may be too large ($\omega_m \sim E^2|\nabla U|$ is the synchrotron peak frequency). The detailed shape of the trajectory is not important for the radiation spectrum, however, since the acceleration is not constant, the whole spectrum is obtained by averaging the local synchrotron-like spectra over time along the trajectory.

The characteristic deviation angle ϑ_{dev} is equal to the Lindhard critical angle $\theta_L = (2U_0/E)^{1/2}$ for channeled particles ($\theta_0 \lesssim \theta_L$) and to $\vartheta_{\text{dev}} \simeq U_0/(E\theta_0)$ for above-barrier particles ($\theta_0 \gtrsim \theta_L$), where θ_0 is the entrance angle with respect to the channel. Therefore, the condition of synchrotron regime ($\vartheta_{\text{dev}} \gg E^{-1}$) may be generally rewritten (in order of magnitude) as $E \gg E_{\text{cr}}^{(1)} = 1/U_0$ and $\theta_0 \lesssim U_0$. This defines a horizontal strip in the (E, θ_0) plane. On the opposite condition, $E \lesssim E_{\text{cr}}^{(1)} = 1/U_0$ or $\theta_0 \gtrsim U_0$, we have the dipole regime. For example, according to Fig. 4, in chiral nanotubes $U_0 \simeq 60$ eV and $E_{\text{cr}}^{(1)} \simeq 4.3$ GeV. For zigzag and armchair nanotubes the height of the peaks in Figs. 4a and 4b, rather than the well depth U_0 , should be taken in the above estimations. Between these limiting cases there is an intermediate region $\vartheta_{\text{dev}} \sim E^{-1}$ where the details of the particle trajectory are of importance and it is the most difficult case for the theoretical analysis of the radiation spectrum. Note that both dipole and synchrotron regions of the (E, θ_0) plane are further separated in channeling and above-barrier regions, the line $\theta_0 = \theta_L(E)$ passing approximately at upper left corner of the “synchrotron strip”. Thus it is clear that the standard theory of CB may fail not only at entrance angles compatible with the Lindhard angle, where channeling effects are dominant, but even at much larger angles.

According to the classical theory of synchrotron radiation, the maximum of the spectrum is around $\omega_m \sim (3/2)E\chi$, where χ is defined in Section 5.1. At $\chi \simeq 1$ or $E \simeq E_{\text{cr}}^{(2)} = 1/|\nabla U|$ the radiation spectra can reach a photon energy ω comparable to the particle energy E and quantum recoil and spin-flip effects must be taken into account. In the coordinate system moving uniformly along the channel with the particle the electromagnetic field acting on the particle is E times stronger than in the lab system. At $E = E_{\text{cr}}^{(2)}$ this field has the strength of the Schwinger field $H_0 = m^2c^3/(e\hbar) = 4.41 \times 10^{10}$ T. The value of $E_{\text{cr}}^{(2)}$ for nanotubes is of the order of 10^3 GeV which is three decimal orders higher than $E_{\text{cr}}^{(1)}$. In other words, in the dipole approximation region the quantum recoil effects can be neglected and we can use classical electrodynamics (with the exception of hard coherent bremsstrahlung). The general theory of radiation (and e^+e^- -pair production) in aligned crystals, applicable at arbitrary ratio between ϑ_{dev} and E^{-1} was developed in [82,83]. So calculating radiation spectra we must distinguish ultra-relativistic particles according to the ratio of their energies to $E_{\text{cr}}^{(1)}$ or $E_{\text{cr}}^{(2)}$.

Fig. 48. Radiation spectra from positrons (lower curve) and electrons (upper curve) channeled in (11, 9) chiral nanotubes.

6.2.2. Classical dipole radiation of channeled particles

Let us first consider the most simple case of channeled particles with relatively low ($E \lesssim E_{\text{cr}}^{(1)}$) energies (but high enough to use classical mechanics). In the frame of the dipole approximation the CR spectrum from particles moving inside the chiral nanotubes was calculated in [46]. In this case the particle trajectories are determined by Eqs. (3.15)–(3.17). The energy $I(\omega)$ radiated by a single channeled particle per unit path in a nanotube and per unit frequency interval can be written as

$$I(\omega) = (e^2 \omega / 2) \sum_{n=0}^{\infty} \{ \omega_n^{(+2)} |\rho_n^{(+)}|^2 f[\omega / (2\gamma^2 \omega_n^{(+)})] + \omega_n^{(-2)} |\rho_n^{(-)}|^2 f[\omega / (2\gamma^2 \omega_n^{(-)})] \}, \quad (6.5)$$

where $\omega_n^{(\pm)} = n\omega_\rho \pm \Omega$, $f(\xi) = (1 - 2\xi + 2\xi^2)\eta(1 - \xi)\eta(\xi)$, η is the Heaviside step-function and

$$\rho_n^{(\pm)} = [2 / (2\pi n \pm \Delta\phi)] \text{Im} \int_0^{T_\rho/2} \exp[-i(n\omega_\rho \pm \Omega)t] (d/dt) \{ \rho(t) \exp[\pm i\phi(t)] \} dt \quad (6.6)$$

originate from the Fourier expansion of the linear combinations $v_x \pm iv_y$ of the Cartesian components of the transverse velocity of the particle [84].

The radiation spectra from channeled positrons and electrons are shown in Fig. 48 in the case of a beam with zero angular divergence entering (11, 9) nanotubes at half of the Lindhard angle. The target thickness is considered to be small compared to the dechanneling length and spectrum (6.5) was averaged over the random values of the initial coordinates. To emphasize the scaling of the dipole spectrum we introduced the characteristic frequency $\omega_c = 4E^2 \theta_L / d \sim E^{3/2}$ and spectral density $I_c = P e^2 \omega_c \theta_L^2 / 2 \sim E^{1/2}$, where P is the probability of particle capturing into the potential well. Compared to positrons, channeled electrons

produce, along with the peak near $\omega \approx \omega_c$ associated with the azimuthal motion of the orbits, more intense and hard radiation at $\omega \approx 8\omega_c$ due to the relatively fast radial oscillations.

The calculated spectra does not take into account the input from positrons moving between the nanotubes as well as from above-barrier particles, however it shows a substantial difference in the shape and intensity of CR spectra from electrons and positrons, in other words, the spectra are strongly charge-dependent.

6.2.3. Coherent bremsstrahlung

CB in nanotubes has a number of peculiarities which we shall discuss below. Here electrons or positrons are scattered by a nanotube as a whole and since nanotubes in a rope make a two-dimensional superlattice, they can act coherently in the formation of CB, similarly to the atomic rows in ordinary crystals. It should be noted that if the entrance angle is above but still comparable to the Lindhard angle ($\theta_L < \theta_0 \lesssim 2\theta_L$), then particles may deflect significantly *in the transverse plane* destroying the coherence, similarly to the case of the ordinary crystals [83]. The significant coherence between nanotubes (or atomic rows in ordinary crystals) may exist only at higher entrance angles $\theta_0 \gtrsim 2\theta_L$ where standard theory of CB is applicable.

A special situation occurs when the particles move at low angles to the planes of the two-dimensional lattice of a nanotube rope, but far from the nanotube axis. In this case, as in ordinary crystals, the coherence may exist between the different planes. As regards CB in fullerenes, it is quite similar to the case of ordinary crystals with the exception that instead of collisions of charged particles with atoms there are collisions with C_{60} fullerenes.

According to the standard theory of CB in the ordinary crystals [6], the emission probability per unit path of electron (positron) moving in a crystal at small angle to atomic rows or planes, differential with respect to the photon energy ω , can be related to the Fourier component of the continuum potential of the atomic row $V_{\mathbf{H}}$

$$\frac{dw}{d\omega} = \frac{e^2}{E^2} \sum_{\mathbf{H}} \frac{H^2}{(\mathbf{H} \cdot \mathbf{v})^2} |V_{\mathbf{H}}|^2 \left[1 + \frac{u}{2(1+u)} - 2\Omega_{\mathbf{H}} + 2\Omega_{\mathbf{H}}^2 \right] \eta(1 - \Omega_{\mathbf{H}}) . \quad (6.7)$$

Here we use the following notations: $\mathbf{v}$ is the unit vector along the direction of the initial momentum of the charged particle, $u = \omega/(E - \omega)$, $\Omega_{\mathbf{H}} = u/(2E\mathbf{H} \cdot \mathbf{v})$, η is the Heaviside step function. The summation in (6.7) is performed over all reciprocal lattice vectors $\mathbf{H} = \{H_x, H_y\}$ orthogonal to the chosen family of the rows (directed along z). In its turn, in monatomic crystal $V_{\mathbf{H}}$ is connected with the Fourier expansion of the atomic potential $f(\mathbf{k})$ (2.12) by the simple relation

$$V_{\mathbf{H}} = \mathfrak{V}^{-1} \exp(-H^2 u_1^2) f(H_x, H_y, 0) ,$$

where $\mathfrak{V}$ is the unit cell volume of the crystal and u_1^2 is the squared amplitude of the thermal vibrations. If atomic rows are chaotically spaced, or the direction of $\mathbf{v}$ is far from the direction of closely packed atomic planes, we may substitute the summation in (6.7) by an integration according to the rule

$$\sum_{\mathbf{H}} \Rightarrow \frac{S \cdot d^2 H}{(2\pi)^2} .$$

S is the transverse cell area. Eq. (6.7) includes the case where the charged particle moves far from the closely packed atomic rows but at small angle to a closely packed atomic plane. On this condition

Fig. 49. The frequency distribution of the coherent bremsstrahlung energy from 1 GeV electron (positron) entering at angle $\theta_0 = 2\theta_L$ with respect to the planes (1, 0) of a superlattice of (10, 10) nanotubes.

we may restrict the summation in (6.7) to the one-dimensional family of reciprocal lattice vectors orthogonal to the corresponding atomic plane.

In order to calculate CB from nanotube superlattices we must generalize Eq. (6.7) [17]. Since different nanotubes in a rope have different azimuthal orientations we may first average the nanotube potential (2.9) over azimuth φ . Considering the continuum potential of a nanotube as azimuthally symmetric, the generalization reduces to the substitution of the Fourier expansion of the string potential $V_{\mathbf{H}}$ by the expansion of the continuum potential of the nanotubes $U_{\mathbf{H}}$ (3.8) over the reciprocal superlattice vectors $\mathbf{H}$ defined above (3.6). The difference between the exact potential (2.9) and the averaged over azimuthal angles gives rise, for not too large θ_0 , to a semi-coherent radiation (incoherent between nanotubes, but coherent between atoms of the same row), due to scatterings on separate atomic rows. As follows from Fig. 4, this semi-coherent radiation may be significant for zigzag or armchair nanotubes, but it should be relatively small for chiral nanotubes due to the relatively weak dependence of the continuum potential on the azimuthal angle. Similarly, in a fullerite CB is described by (6.7) where $V_{\mathbf{H}}$ must be replaced by the Fourier expansion (3.10).

One should distinguish the case where the charged particle moves at small angle to a nanotube row and the case where it moves at small angle to the plane of the two-dimensional lattice of the rope. The per-unit-path frequency distribution of the coherent bremsstrahlung energy $dW/d\omega = \omega dw/d\omega$ from 1 GeV electron (positron) entering at angle $\theta_0 = 2\theta_L^{(p)} = 3.04 \times 10^{-4}$ with respect to the planes (1, 0) of a superlattice of (10, 10) nanotubes is illustrated in Fig. 49 ($\theta_L^{(p)}$ is the Lindhard angle for planar channeling). This case corresponds to the particles moving above the potential barrier shown in Fig. 8 or Fig. 9. The maximum near 2 MeV originates from the fundamental harmonic of CB, but in this case the maxima of the higher order harmonics (right up to the tenth) occur to be comparable to that of the first harmonic. Such a behavior of the CB spectrum is due to the relatively slow decrease of $U_{\mathbf{H}}$ in the region

Fig. 50. The frequency distribution of the coherent bremsstrahlung from 1 GeV electron (positron) entering at $\theta_0 = 2\theta_L^{(s)}$ to the rows of nanotubes laying in $(1, 0)$ planes of the rope.

$2\pi/R < H < 2\pi/a_{TF}$. In that region U_H is essentially governed by $J_0(RH)$, which is the form factor of a rigid hollow tube (3.7). A different case is illustrated in Fig. 50. Here the frequency distribution of the coherent bremsstrahlung is shown for 1 GeV electron (positron) entering parallel to the $(1, 0)$ planes of the rope and at $\theta_0 = 2\theta_L^{(s)}$ to the nanotube axes, where $\theta_L^{(s)}$ is the Lindhard angle for channeling inside nanotubes. The dashed line represents the bremsstrahlung in case of randomized positions of carbon atoms (amorphous medium). It can be seen that in the case of nanotube row the radiation is much higher than in the planar case due to the higher strength of the potential (Figs. 3 and 4) acting on the particle.

6.3. Reflection or Bragg diffraction of the proper electromagnetic field of fast charged particles

A charged particle moving rectilinearly in a homogeneous medium of refractive index $n(\omega) = \sqrt{1 + \chi(\omega)}$ at velocity less than the phase velocity of light $1/n(\omega)$ cannot emit any radiation. It only carries its own electromagnetic field from one point of space to another. In terms of quantum electrodynamics this field can be decomposed in a spectrum of virtual photons. In inhomogeneous dielectric media the virtual photons can be converted into real photons due to momentum transfer from the photons to the medium. In other words, radiation is emitted. The conversion of the virtual photons takes a time equal to $\tau_{coh} = 2\pi/(\omega - \mathbf{k} \cdot \mathbf{v})$ during which an ultra-relativistic particle passes the coherence length $l_{coh} \simeq \tau_{coh}$ introduced in the previous subsection. Besides, in absorbing media it may happen that photons are absorbed (due to the photo-electric effect or e^-e^+ pair production) at lengths shorter than l_{coh} . In this case no radiation is really emitted, when the possibility of radiation exists.

The simplest example of inhomogeneous media is the boundary between two layers with different dielectric susceptibility and the arising radiation is known as *transition radiation*. A more complicated case of inhomogeneous media is represented by crystals and periodic multilayered structures (MLS). The X-ray radiation from relativistic charged particle arising from the Bragg diffraction of the own electromagnetic field of a particle in crystals or MLS is called *parametric X-ray radiation* (PXR). It was predicted by Ter-Mikhaelyan [80] who developed the theory based on the kinematic diffraction of

virtual photons in infinite nonabsorptive media. The influence of absorption and extinction of X-rays inside crystals was taken into account later [85] using the two-wave dynamic diffraction method. PXR in ordinary crystals was discovered and investigated experimentally [86–88]. The modern state of the theory and experiments in this field was presented recently in a review article [89] where a comprehensive list of works devoted to PXR can be found. It should be noted that PXR is often referred to as *quasi-Cherenkov, resonance transition* or even *diffraction X-ray radiation*. The peculiarities of PXR from nanocrystal were investigated quite recently [90,91]. It should be noted that PXR may be also treated as a kind of *coherent* transition radiation, similar to the coherent bremsstrahlung discussed in the previous subsection.

The properties of transition radiation and PXR can be understood from simple considerations using the method of “equivalent quanta” developed by Fermi [92] to calculate the interactions of charged particles with matter. This method is widely used today under the name of the Weizsäcker–Williams method [93,94]. It is based on the observation that the electric and magnetic fields of a fast-moving charged particle are nearly transverse to the direction of motion. Consequently, the electromagnetic effects caused by these fields are nearly identical to those caused by a passing electromagnetic plane wave. The equivalent photons may be defined as those which turn to real photons of radiation at a sudden stop of the particle. Using classical electrodynamics we can easily calculate the frequency and angular distribution of radiation energy at a sudden stop of the particle and, dividing it by the photon energy ω , obtain the corresponding distribution of equivalent photons:

$$\frac{d^2 N_{\text{eq}}}{d\omega d\Omega} = \frac{e^2 \omega}{4\pi^2} \left(\frac{\boldsymbol{\varepsilon} \cdot \mathbf{v}}{\omega - \mathbf{k} \cdot \mathbf{v}} \right)^2. \quad (6.8)$$

Here $\mathbf{k}$ and $\boldsymbol{\varepsilon}$ are the photon momentum and the unit vector of the photon polarization, respectively, $k = \omega n(\omega)$, e and $\mathbf{v}$ are the particle charge and velocity. The cornerstone of the Weizsäcker–Williams method is thus the approximation that the virtual photons of the field can be replaced by the real photons with spectral-angular distribution (6.8) and the physics of the interactions between the charged particles and matter is simplified to that of the interactions between photons and matter.

At first, let us consider the case of a single smooth and flat interface between two media with different dielectric susceptibility $\chi_1(\omega)$ and $\chi_2(\omega)$. When a charged particle traverses the interface at a grazing angle ψ , some of the virtual photons reflect back into the first medium and become real, giving rise to the so-called backward transition radiation. We introduce the Fresnel coefficient R_s of the photon reflection at the boundary and count the polar angle θ of transition radiation from the specular direction of the particle velocity and the azimuth angle ϕ from the incidence plane. The charged particle is considered as ultra-relativistic and the dielectric susceptibility in the X-ray region as relatively small $\chi \ll 1$ and negative. Multiplying the right-hand side of (6.8) by the reflection coefficient R_s , we find the frequency and angular distribution of transition radiation photons from an ultra-relativistic particle

$$\frac{d^2 N_s}{d\omega d\Omega} = \frac{e^2}{\pi^2 \omega} \left(\frac{P_s \theta}{\theta^2 + E^{-2} - \chi_1} \right)^2 R_s \quad (6.9)$$

which is in agreement with more general results of transition radiation theory [95]. Here $s = \pi$ or σ denotes the photon polarization. The π and σ polarizations are, respectively, parallel and perpendicular to the incidence plane of the particle, $P_s = \cos \phi$ for $s = \pi$ and $P_s = \sin \phi$ for $s = \sigma$. If the particle grazing angle ψ is large compared to the Fresnel angle $\psi_F = |\Delta\chi|^{1/2} \ll 1$, where $\Delta\chi(\omega) = \chi_2(\omega) - \chi_1(\omega)$ is the

jump of the dielectric susceptibility, the Fresnel coefficient may be presented as

$$R_s = \frac{|\Delta\chi|^2 C_s^2}{16 \sin^4 \psi} . \quad (6.10)$$

Here $C_s = \cos 2\psi$ for π - and $C_s = 1$ for σ -polarization.

6.3.1. The case of parametric X-rays. Basic formula

It follows from (6.10) that at relatively large incidence angles $\psi \gg \psi_F$ the reflection coefficient is extremely low, consequently the number of transition radiation photons from a single interface (6.9) is low too. However this number can be considerably increased using many periodically spaced interfaces. As a simple model, one may take alternate layers of susceptibilities χ_1 and χ_2 of equal thicknesses. If the flight path $d/\sin \psi$ of the particle between two successive $1 \rightarrow 2$ interfaces coincides with the coherence length of radiation $l_{\text{coh}} = 2\pi/(\omega - \mathbf{k} \cdot \mathbf{v})$ for a given wave vector $\mathbf{k}$, the different interfaces reflect coherently and the number of radiated photons having this wave vector increases by the squared number of interfaces $(2N)^2$ (d is the spatial period, N the number of periods). At relatively large angles ψ but small θ the coherence length may be rewritten as $l_{\text{coh}} \approx \lambda/(2 \sin^2 \psi)$, where $\lambda = 2\pi/\omega$ is the radiation wavelength, and we find out that the full coherence takes place at *resonance* frequency ω close to the Bragg frequency $\omega_B = \pi/d \sin \psi$. To first order in θ , and neglecting terms of order χ and $1 - v$ the frequency shift $\Delta\omega = \omega - \omega_B$ is given by

$$\Delta\omega = -\omega_B \cot \psi \delta\psi \approx \omega_B \theta \cot \psi \cos \phi . \quad (6.11)$$

The most intense radiation may be observed at angles θ close to $\theta_{\text{opt}} = (E^{-2} - \chi_1)^{1/2}$, where the single-surface transition radiation intensity (6.9) is maximum. At fixed angle, the interference is constructive over a frequency interval $\Gamma \simeq \omega_B/N$ about the peak $\omega_B = \pi/(d \sin \psi)$. Considering $\Delta\chi$ as the modulation depth of the dielectric susceptibility and replacing χ_1 by the real part χ'_0 of the dielectric susceptibility averaged over the period we may apply the above estimates to arbitrary periodic media including ordinary crystals, MLS, nanotube ropes or fullerenes.

For a crystal with entrance and exit faces parallel to the reflecting atomic layers, the number of periods is simply the ratio T/d of the crystal thickness T to the interplane distance d . However, it is clear that the effective thickness T_{eff} divided by $\sin \psi$ is limited by the absorption length of X-rays in the medium $l_a = 1/[\omega\chi''_0(\omega)]$, where $\chi''_0(\omega)$ is the imaginary part of the averaged dielectric susceptibility. In the following, we will assume that the crystal is thick enough so that $T_{\text{eff}}/\sin \psi = l_a$, giving an effective number of periods $N_{\text{eff}} = \sin^2 \psi/[\pi\chi''_0(\omega_B)]$. At resonance frequencies the coherence between the interfaces increases the spectral angular distribution of radiation by the factor $(2N_{\text{eff}})^2$. However, integrating over the resonance peak of width $\Gamma = \omega_B/N_{\text{eff}}$, one loses a factor N_{eff} and we obtain for the angular distribution of PXR photons the following estimation:

$$\frac{dN_s}{d\Omega} = \frac{e^2}{4\pi^3 \sin^2 \psi} \frac{|\Delta\chi(\omega_B)|^2 C_s^2}{\chi''_0(\omega_B)} \left(\frac{P_s \theta}{\theta^2 + E^{-2} - \chi'_0(\omega_B)} \right)^2 . \quad (6.12)$$

A more accurate and general approach to the problem is based on the multi-wave diffraction theory. We expand the radiation electric field in a superlattice in series of Bloch waves (4.2) and from the wave equations (C.2,C.3) find the following infinite system of algebraic equations for the expansion

coefficients $\mathbf{E}_{\mathbf{K}}(\mathbf{k}, \omega)$:

$$\begin{aligned}
& (\mathbf{k} + \mathbf{K}) \times (\mathbf{k} + \mathbf{K}) \times \mathbf{E}_{\mathbf{K}}(\mathbf{r}, \omega) + \omega^2 \mathbf{E}_{\mathbf{K}}(\mathbf{r}, \omega) + \omega^2 \sum_{\mathbf{H}} \chi_{\mathbf{H}}(\omega) \mathbf{E}_{\mathbf{K}-\mathbf{H}}(\mathbf{k}, \omega) \\
& = 8\pi^2 i e \omega \mathbf{v} \delta(\omega - \mathbf{k} \cdot \mathbf{v}) \delta_{\mathbf{K}0} .
\end{aligned} \tag{6.13}$$

It differs from (4.3) only by the term in the right-hand side which represents the electric current of the uniformly moving electron. In most practical cases only two Bloch waves are of importance and the infinite system of equations (6.13) turns to the following two pairs of equations for each polarization (σ or π) of the electromagnetic field

$$\begin{aligned}
& [\omega^2(1 + \chi_0) - k^2] E_0 + C_s \omega^2 \chi_{\mathbf{H}} E_{\mathbf{H}} = 8\pi^2 i e \omega \theta P_s \delta(\omega - \mathbf{k} \cdot \mathbf{v}) , \\
& C_s \omega^2 \chi_{\mathbf{H}}^* E_0 + [\omega^2(1 + \chi_0) - (\mathbf{k} + \mathbf{H})^2] E_{\mathbf{H}} = 0 .
\end{aligned} \tag{6.14}$$

The exact solution of (6.14) corresponds to PXR of the two-wave dynamical diffraction theory. The more simple kinematic theory assumes $|E_{\mathbf{H}}|$ to be small compared to $|E_0|$. This assumption is reasonable if the ratio $r = |C_s \chi'_{\mathbf{H}}(\omega)|/\xi$, where $\xi(\theta) = \theta^2 + E^{-2} - \chi'_0(\omega)$, is small compared to unity. As shown in [91] (see also Fig. 51 below) for nanocrystals the ratio r is always small and the kinematic theory is sufficient. It is also reasonable to consider the case of relatively thick ($T/\sin \psi \gg l_a$) medium where the output of PXR is maximum. In this case the solution of (6.14), using the relative smallness of the diffracted field, leads to the following spectral-angular distribution of PXR photons both for the symmetric Bragg case ($\mathbf{H}$ orthogonal to the entrance surface) and symmetric Laue case (radiation through the backward crystal interface, this one being parallel to $\mathbf{H}$ and $\mathbf{H} \times \mathbf{v}$):

$$\frac{d^2 N_s}{d\omega d\Omega} = \frac{\omega}{(2\pi)^6} |E_{\mathbf{H}}^{(-)}|^2 = \frac{e^2 \theta^2}{4\pi \chi''_0(\omega) \sin^2 \psi} \frac{|P_s C_s \chi'_{\mathbf{H}}(\omega)|^2}{\xi^2(\theta)} A(\omega, \theta) , \tag{6.15}$$

where $E_{\mathbf{H}}^{(-)}$ is $E_{\mathbf{H}}$ without multiplier $\delta(\omega - \mathbf{k} \cdot \mathbf{v})$, $\pi/2 + \psi$ is the angle between the particle velocity $\mathbf{v}$ and the reciprocal vector $\mathbf{H}$, $\chi'_{\mathbf{H}}(\omega)$ is determined by (4.4) and it is supposed that ψ is much higher than the “Fresnel angle” $\sim |\chi'_0(\omega)|^{1/2}$ (the grazing incidence case will be considered in Section 6.3.3). The line shape of spectrum (6.15) is determined by the normalized Lorentz curve

$$A(\omega, \theta) = \frac{\Gamma}{2\pi} \frac{1}{[\omega - \omega_B(1 - \theta \cos \phi \cot \psi)]^2 + (\Gamma/2)^2} , \tag{6.16}$$

where $\omega_B = H/(2 \sin \psi)$. The line width Γ of PXR radiated in a sufficiently small solid angle around the direction (θ, ϕ) is determined by the imaginary part of the volume-averaged dielectric susceptibility:

$$\frac{\Gamma}{2} = \frac{\omega_B}{4 \sin^2 \psi} \chi''_0(\omega) . \tag{6.17}$$

Integrating (6.15) over ω we can replace $A(\omega, \theta)$ by the Dirac function $\delta[\omega - \omega_B(1 - \theta \cos \phi \cot \psi)]$, therefore the angular distribution of PXR takes on the form

$$\frac{dN_s}{d\Omega} = \frac{e^2 \theta^2}{4\pi \chi''_0(\omega_B) \sin^2 \psi} \frac{|P_s C_s \chi'_{\mathbf{H}}(\omega_B)|^2}{\xi^2(\theta)} . \tag{6.18}$$

Fig. 51. Total number of polarized PXR photons radiated by an electron with Lorentz factor $\gamma = 10^3$ in the effective solid angle (see text) from various periodic media as a function of the radiation frequency: (a) σ -polarization, (b) π -polarization. The target types are indicated by letters: **N**—reflection from (1, 0) planes of (10, 10) nanotube ropes; **F**—(1 1 1) planes of fullerite; **C-W**—carbon–tungsten MLS; **D** and **Ge**—(2 2 0) planes of diamond and germanium, respectively.

According to [91], in the case of MLS consisting of layers with complex dielectric susceptibility $\chi^{(1)}(\omega)$ and thickness αd alternating with layers of complex dielectric susceptibility $\chi^{(2)}(\omega)$ and thickness $(1 - \alpha)d$, the Fourier coefficients of the periodic complex dielectric susceptibility $\chi(\omega, \mathbf{r})$ can be presented as

$$\chi_0(\omega) = \alpha\chi^{(1)}(\omega) + (1 - \alpha)\chi^{(2)}(\omega), \quad |\chi_{\mathbf{H}}(\omega)| = |\Delta\chi(\omega) \sin(\pi n \alpha) / \pi n|, \quad (6.19)$$

where $\mathbf{H} = (2\pi n/d)\boldsymbol{\tau}$, $\boldsymbol{\tau}$ is the unit vector normal to the interfaces and n is integer. For equal thicknesses ($\alpha = 1/2$) and $n = 1$, one recovers result (6.12). For nanocrystals the corresponding expressions of $\chi_{\mathbf{H}}(\omega)$ are determined above (Eqs. (4.5–4.7)). Another theoretical treatment of PXR, based on the reciprocity theorem, can be found in [136].

Integrating (6.18) over azimuth angles ϕ , and polar angles from zero to some $\theta_m \sim [E^{-2} - \chi'_0(\omega)]^{1/2}$, corresponding to a detector aperture of the order of the virtual photon angular spread, we find the total

number of PXR photons N_s per electron

$$N_s = \frac{e^2 \omega_B^2}{2H^2} \frac{|C_s \chi'_H(\omega_B)|^2}{\chi''_0(\omega_B)} \left[\ln \frac{\xi_m}{\xi_0} - \frac{\theta_m^2}{\xi_m} \right]. \quad (6.20)$$

Here we introduced the following notations $\xi_m = \xi(\theta_m)$, $\xi_0 = \xi(0)$. More general results for non-symmetrical Bragg and Laue cases and the dynamical diffraction were obtained by Afanas'ev and Aginyan [85]. It was also shown by these authors in other paper [96] that in mosaic crystals the total number of PXR photons does not differ substantially (only by the argument of the logarithm in (6.20)) from that in perfect crystals even in the case where the angular spread of monocrystalline blocks in a thick mosaic crystal is high compared to the natural angular width of expression (6.16).

Assuming that the modulation depth of the crystal electron density does not depend substantially on the modulation period (which strictly holds for MLS) the number of photons with energies $\approx \omega_B$ is proportional to the squared interplanar space $d_p^2 \sim H^{-2}$. According to (6.11), the maximum shift $\Delta\omega_{\max}$ of the photon energy ω from ω_B corresponding to $\phi = \pm\pi$ depends on the detector acceptance angle θ_m and the incidence angle of electrons ψ through the relation

$$\frac{\Delta\omega_{\max}}{\omega_B} = \theta_m \cot \psi. \quad (6.21)$$

This relation determines the width $\Delta\omega$ of PXR spectrum captured by a detector with relatively large (compared to the natural width) acceptance angle. Relation (6.21) shows that photons the number of which is determined by (6.20) are rather monochromatic until the incidence angle ψ becomes close to the ‘‘Fresnel angle’’ $\sim |\chi'_0(\omega)|^{1/2}$.

6.3.2. Numerical results for PXR

Fig. 51 shows the total number of PXR photons (6.20) with frequencies around ω_B radiated by one electron with $\gamma = 10^3$ into the *effective solid angle* $0 \leq \theta \leq \theta_{\text{eff}} = 2[E^{-2} - \chi'_0(\omega)]^{1/2}$, $0 \leq \phi \leq 2\pi$ from nanocrystals as a function of the peak radiation frequency ω_B (determined by the incidence angle ψ to the crystal planes) for the two polarization cases.

For comparison, corresponding results are also given for ordinary crystals: (2 2 0) planes of diamond and germanium crystals at room temperature, and for the carbon–tungsten multilayered structure with period $d = 16 \text{ \AA}$ and equal thickness of the adjacent layers (in diamond-like crystals (1 1 0) reflection is suppressed due to the structure factor). Solid curves represent the results based on the dynamic diffraction theory and broken ones on the kinematic theory (6.20). For the nanocrystals and diamond the results of the dynamic and kinematic theory coincide with the accuracy corresponding to the curve thickness. Some difference may be noticed in case of C – W MLS and for germanium (and probably other high Z crystals) the difference is substantial. The narrow dips are due to absorption lines. In addition, for the parallel (π) polarization, each curve has a wider dip: at this photon energy the Bragg angle is close to the Brewster angle $\simeq 45^\circ$ of X-rays and PXR is linearly polarized perpendicular to the incidence plane.

In the photon energy interval from 1 to 30 keV both nanocrystals and MLS are more efficient, by two orders of magnitude in photon yield, than ordinary crystals. This can be foreseen if we remember that virtual photons have extremely narrow angular and very broad frequency distribution (6.8), periodic structures act as a spectrum analyzer of the virtual photons and according to the results of Section 4.1 nanocrystals are X-ray mirrors with a substantially broader frequency band than ordinary crystals.

Fig. 52. The relative width of PXR photon spectra from various media as a function of the radiation frequency.

At photon energies higher than 10 keV the nanotube ropes dominate over fullerite and carbon–tungsten MLS. For $\omega_B \simeq 3$ keV, the total number of photons (in the above-defined effective solid angle) per electron from a nanotube superlattice is about 10^{-5} which is comparable to that from the carbon–tungsten MLS, while ordinary crystals like diamond or germanium are unable to emit PXR at such low frequencies at all.

The relative widths of the photon spectra from various media calculated using (6.21) are illustrated in Fig. 52. One can see that PXR from ordinary crystals have much narrower photon energy distributions than from superlattices. However, it should be noted that for some applications, such as X-ray lithography, the whole number of photons is more important than high monochromaticity.

6.3.3. “Channeled” transition radiation

A transition radiation of quite different character may arise [91] at a grazing incidence angle smaller than the Fresnel angle. Let us consider a bundle of micro-capillaries which qualitatively describes a rope of thick and wide enough multi-wall nanotubes. Let a fast charged particle traverse a capillary at small angle ψ_0 to the axis and at impact parameter b and consider more particularly the radiation arising when the charged particle impinges the capillary wall from inside of the capillary (vacuum). If the particle energy is high enough ($E \gg \psi^{-1}$), we may neglect the angular divergence of the equivalent photon beam compared to the incidence angle and present the frequency and angular distribution of radiated photons, due to the reflection from the wall, in the following form:

$$\frac{d^2 N_s}{d\omega d\Omega} = \frac{e^2}{\pi^2 \omega} \left(\frac{P_s \theta}{\theta^2 + E^{-2}} \right)^2 R_s(\psi) . \quad (6.22)$$

The reflection coefficient $R_s(\psi)$ depends on the actual angle of incidence $\psi = \psi_0(1 - b^2/r^2)^{1/2}$ to the wall, r being the internal radius of the capillary. The small-angle reflection coefficient from an absolutely

smooth surface does not depend on the polarization and may be written in the simple form

$$R_s(\psi) = \left| \frac{\psi - (\chi + \psi^2)^{1/2}}{\psi + (\chi + \psi^2)^{1/2}} \right|^2, \quad (6.23)$$

where χ is the complex dielectric susceptibility of the wall substance. Since the capillary diameter is considered as small compared to the diameter of the beam, expression (6.22) should be averaged over all impact parameters b . The frequency distribution of radiation is determined exclusively by the frequency dependence of the averaged coefficient $\langle R_s \rangle$ and may be written in the form

$$\frac{dN}{d\omega} = \frac{e^2}{\pi\omega} \langle R_s \rangle \left[\ln(1 + (E\theta_m)^2) - \frac{(E\theta_m)^2}{1 + (E\theta_m)^2} \right]. \quad (6.24)$$

The upper limit θ_m of the integration over θ is chosen to be comparable to the Fresnel angle ψ_F (due to the logarithmic divergence of (6.24) at large θ_m there is no need to define θ_m more accurately).

In addition to backward transition radiation (BTR) when the electron leaves the hole, there is also the forward transition radiation (FTR) when it enters the hole. At $E \gg \psi^{-1}$ the two radiations are nearly equal. Inside the hole, FTR travels nearly parallel to the electron, is reflected on the opposite wall near the specular direction and thereafter interfere with BTR. The interference is destructive when the electron path in the hole is smaller than the FTR coherence length in vacuum, $l_{\text{coh}} = 2\pi/(\omega - \mathbf{k}\mathbf{v}) \approx 2\lambda/(\theta^2 + E^{-2})$, divided by 4. To avoid such an effect the inner diameter d of the nanotube should be larger than $d_{\text{min}} = \psi E^2 \lambda/4$.

The most interesting point is that radiation is emitted back into the capillary and propagates almost totally inside it, suffering multiple reflections from the wall (X-ray channeling). During that time the charged particle passes through the capillary wall and traverses many other capillaries. Since radiation does not pass through the capillary (MWNT) walls, it is not absorbed as much as PXR. The attenuation of radiation is determined only by a small difference of R_s from unity. If $\psi \ll \psi_F$, then (6.23) gives $R_s \simeq 1 - \delta$, where $\delta = 2\psi\chi''/(\psi_F|\chi'|)$ and the effective number of reflections inside the capillary may be estimated as $N_e \simeq 1/\delta$. The number of capillaries passed by the charged particle during that time is comparable to N_e in order of magnitude. Thus the resulting *channeled transition radiation* (CTR) from a bundle of capillaries can be N_e times higher than transition radiation from a single capillary or MWNT. However, it is important that the grazing angle ψ remains less than ψ_F despite possible scattering of the particle by the atoms of the wall. Compared to the spectrum of PXR, the radiation spectrum of CTR is relatively broad, extending up to the cutoff frequency $\omega_{\text{max}} \simeq \omega_p/\psi$.

6.4. Nanotube undulator radiation (NUR)

The idea of using spatially periodic magnetic fields (undulators) for the production of monochromatic radiation belongs to Ginzburg [97]. It was developed by Korkhmazian [98] who analyzed the possibility of undulator radiation by ultra-relativistic particles in the X-ray band and gave the analytical expression for the spectral-angular distribution of radiation in an undulator with a transverse planar sinusoidal magnetic field $\mathbf{H}(z) = H_0 \mathbf{n}_x \sin(2\pi z/\lambda_w)$ which depends on the longitudinal coordinate z . The spectrum of undulator radiation (UR) can be also calculated analytically for the helical magnetic field $\mathbf{H}(z) = H_0[\mathbf{n}_x \sin(2\pi z/\lambda_w) - \mathbf{n}_y \cos(2\pi z/\lambda_w)]$ [99] and for the more complicated case where the helical field is superimposed on a homogeneous longitudinal field [100].

In the theory of the X-ray undulator radiation a fundamental role is played by *the undulator parameter* p which is the ratio of the maximum deviation angle ψ of the electron to the effective angle of the radiation $\theta_{\text{eff}} = E^{-1}$. It is also the amplitude of the transverse momentum oscillation, in units of the electron mass. We recall (see Section 6.2.1) that in the limiting case $p \ll 1$ ($p \gg 1$) the radiation has a dipole (respectively synchrotron-like) character. In the case $p \lesssim 1$ one speaks of a *coherent wiggler*. For the planar sinusoidal magnetic field the undulator parameter can be written as $p = eH_0\lambda_w/2\pi$, where H_0 is the field amplitude and λ_w the undulator period. The calculations [98–100] showed that the spectral-angular energy density of X-ray radiation from an undulator with fixed λ_w and total number of periods N radiation is maximum at $p \simeq 1$. Indeed, at small $p \ll 1$ the amplitude of electron oscillations is too small and at $p \gg 1$ the monochromaticity of the radiation, which is due to the constructive coherence of the different undulator periods, disappears. Besides, the radiation is spread in a larger angular domain and, for the helical undulator, it is no more peaked in the z -direction. This is why it is desirable to hold the undulator parameter near unity. If the magnetic field is measured in Tesla and the undulator period in centimeters, the parameter is given by $p = 0.1 H_0 \lambda_w$. One can see that it is a rather difficult task when λ_w is below 1 cm. On the other hand, because the characteristic wavelength of the undulator radiation is proportional to the undulator period and to the inverse square E^{-2} of the electron energy, shorter periods are desirable, if we want to achieve shorter wavelengths without elevating the electron energy.

It was shown in Section 3.4 that chiral nanotubes bent with the Tsyganov radius are equivalent to a very strong (588 T) magnetic field. By screwing the nanotube rope one may obtain a bunch of spiral nanotubes which obviously act as a spiral magnetic field [46]. Alternatively, periodically curved channels can be produced by an intense ultrasonic plane wave propagating through a crystal [101,102]. As is known, in ordinary crystals charged particles cannot follow the curved channels over long enough path because incoherent multiple scattering is important. However, the results of Section 5.2 give the hope that this is possible at least for positrons in nanotubes. In this subsection we analyze how the *nanocrystal undulator* (NU) can indeed help us to solve the short-period problem. To be more specific, we will consider the case of a helically bent nanotube.

Most of the theoretical results [98–100] for the magnetic undulators can be applied to NU. However, there are several major differences between a magnetic undulator (MU) and NU:

- The helix radius and period of NU cannot be chosen independently since helix curvature radius must be larger than Tsyganov critical radius, otherwise particles cannot follow the helix for long enough time.
- There are short-wave oscillations of the channeled particles in the nanotube continuum potential which may affect the coherence conditions of NUR.
- Since NUR occurs in a medium one should take into account the possible influence of the dielectric polarization of the medium [103].
- In NU, the deviation angle ψ is imposed through the rope helix radius and period, therefore the undulator parameter $p = E\psi$ strongly depends on the particle energy, whereas in MU $\psi \propto E^{-1}$ and p is energy independent.
- The effective NU length is limited by particle dechanneling.

6.4.1. Limitations due to the critical bending and channeling adiabaticity

Let us denote by R_w the radius of the nanotube spiral. In the case of the planar sinusoidal bending of the channel caused by an ultrasonic wave, R_w will mean the amplitude of the sinusoid. From (3.29)

(there R_w was denoted by A) we have

$$\psi = \omega_w R_w, \quad R_b \simeq 1/(\omega_w^2 R_w),$$

where $\omega_w = 2\pi/\lambda_w$. For a given helix radius R_w and curvature radius R_b of the channel the NU period λ_w is determined by the equality

$$\lambda_w = 2\pi(R_b R_w)^{1/2}.$$

The NU period is limited from below by the condition $R_b > R_c$ where $R_c = d/\theta_L^2$ is the Tsyanov critical radius. Thus the period λ_w cannot be shorter than

$$\lambda_w^{(\min)} = \pi \left(\frac{2d R_w E}{U_0} \right)^{1/2}. \quad (6.25)$$

Taking this value for λ_w , the deviation angle ψ is maximum, therefore the largest possible undulator parameter is $p^{(\max)} = (2E U_0 R_w / d)^{1/2}$.

The NU period should be also significantly larger than the periods of channeling oscillations, which is itself larger than $\lambda_{ch} = 2d/\theta_L$. The condition $\lambda_w \gg \lambda_{ch}$ guarantees that the channeling states evolve adiabatically and also that there is no interference between channeling radiation and undulator radiation (the influence of channeling oscillations on the averaged longitudinal velocity and the Doppler shift will be discussed below). This condition can be rewritten in the form

$$\pi \left(\frac{R_b R_w}{d R_c} \right)^{1/2} \gg 1.$$

If the helix curvature radius R_b is equal to R_c (i.e., the period is minimum, $\lambda_w = \lambda_w^{(\min)}$) then the helix radius must be large enough compared to the channel diameter, $R_w \gg \pi^{-2}d$. However, the inequality $R_w \gg d/2$ is also needed to consider channeling oscillations as a small perturbation of a smooth particle trajectory along nanotube deformation. Thus the above condition is satisfied automatically.

6.4.2. Kinematics of NUR

The influence of other factors mentioned above on NUR can be understood from simple considerations of NUR kinematics.

The polarization effect in the X-ray region was first considered in [79] for the case of channeling radiation (see Section 6.2. Note that classical channeling can be treated as a kind of electric undulator) and then in [104] for the gas-filled magnetic undulators. Let us first show how the polarization and channeling effects influence the X-ray energy, using the conservation laws during the radiation. Ignoring the relatively rapid (if $2R_w \gg d$) oscillations of the channeling motion we may consider the channel curvature as an equivalent magnetic field. Since a magnetic field does not change the total particle energy by itself, the latter changes only due to the radiation of the photon with energy ω and we may write the conservation of energy as

$$E_1 - E_2 = \omega, \quad (6.26)$$

where E_1 and E_2 are the particle energy before and after the radiation of the photon, respectively. Since the equivalent magnetic field is periodical along z , the particle has a quasi-momentum p_z which conserves

modulo the reciprocal vector $\omega_w = 2\pi/\lambda_w$ of the magnetic lattice, therefore we may write the conservation of longitudinal quasi-momentum as

$$\Delta p_z = p_{z1} - p_{z2} = k_z + \frac{2\pi}{\lambda_w} n, \quad (6.27)$$

where k_z is z -component of the photon momentum and n denotes the integer *harmonic number* of NUR. Since $\omega \ll E$ (we do not consider the possibility of quantum recoil effects), the energy difference can be presented as

$$E_1 - E_2 \simeq \frac{\partial E}{\partial p_z} \Delta p_z, \quad (6.28)$$

where $\partial E/\partial p_z = \langle v_z \rangle$ is the mean (over the period) particle velocity along the NU axis. The substitution of $E_1 - E_2$ in (6.28) by ω , and Δp_z by the right-hand side of (6.27) gives for the frequencies of NUR the following result

$$\omega \simeq \frac{2\pi n \langle v_z \rangle}{\lambda_w} \frac{1}{1 - \langle v_z \rangle \sqrt{\epsilon'(\omega)} \cos \theta}, \quad (6.29)$$

where θ is the angle of NUR with respect to the axis of the undulations. The influence of the polarization is taken into account through the relation $k = \omega \sqrt{\epsilon'(\omega)}$ where $\epsilon'(\omega)$ is the real part of the dielectric permeability of the medium. For the first harmonic $n = 1$ the denominator in (6.29) express the Doppler shift of the radiation frequency ω from the oscillation frequency $2\pi \langle v_z \rangle / \lambda_w \simeq \omega_w$ of the particle in NU.

According to the standard theory of helical magnetic undulators [98–100], in the ultrarelativistic limit the mean longitudinal velocity can be written as

$$\langle v_z \rangle \simeq 1 - (E^{-2}/2)(1 + p^2). \quad (6.30)$$

For an ordinary (magnetic) helical undulator, $p = E\psi = E\omega_w R_w$. As expected, the larger is the transverse velocity $v_T = \psi$, the slower is the longitudinal one. In the nanotube undulator case, as noted in Section 3.4, we have also the short-wave oscillations of the channeling motion, which are superimposed on the long-wave oscillations of the periodically bent nanotube axis. These channeling oscillations increase $\langle v_T^2 \rangle$, therefore make a further decrease of $\langle v_z \rangle$. The effective value of p^2 is then

$$p^2 = \langle \mathbf{p}_T^2 \rangle \simeq (E\omega_w R_w)^2 + 2E\epsilon_{\text{kin}}, \quad (6.31)$$

where $\mathbf{p}_T(t) = E\mathbf{v}_T(t)$ is the time-dependent transverse momentum with respect to the undulator axis and ϵ_{kin} is the averaged (over the short-wave oscillations) kinetic part of the transverse energy ϵ in channeling motion. One may equally consider the channeled electron or positron as a particle of effective mass squared $m_{\text{eff}}^2 = m^2 + 2\epsilon_{\text{kin}}E$. Due to the flatness of the continuum potential for positrons in nanotubes (except the vicinity of the wall), most of channeled positrons have $\epsilon_{\text{kin}} \approx \epsilon$.

At frequencies above the binding energy of K -shell electrons (which is about 284 eV for carbon) the real part of the dielectric permeability $\epsilon'(\omega)$ is determined by the “plasma formula” $\epsilon'(\omega) = 1 - \omega_p^2/\omega^2$, therefore Eq. (6.29), connecting the frequency and the angle of NUR, can be represented as

$$\theta^2 = \frac{2n\omega_w}{\omega} - \omega_p^2/\omega^2 - E^{-2}(1 + p^2) \quad (6.32)$$

in the small-angle approximation (the big Doppler shift requires $\theta \ll 1$). In p^2 , let us forget temporarily the term $2E\varepsilon_{\text{kin}}$, which is small for energies $E \lesssim E_{\text{cr}}^{(1)} = 1/U_0$ determining the applicability of the dipole approximation to CR (as shown in 6.2.1 for chiral nanotubes $E_{\text{cr}}^{(1)} = 4.3$ GeV). Note that for a given spirally bent nanotube R_w and ψ are fixed, therefore the NU parameter $p = E\psi$ is energy dependent. This is in contrast to the case of a magnetic undulator, where $\psi \propto E^{-1}$ and p occurs to be independent of energy. Eq. (6.32) has solutions for real θ and ω only if E is higher than the threshold (called critical energy in [77])

$$E_c^{(n)} = \frac{\omega_p}{\omega_w [n^2 - (\omega_p R_w)^2]^{1/2}}. \quad (6.33)$$

Taking into account the “channeling term” $2E\varepsilon_{\text{kin}}$ in p^2 makes this threshold still higher. In the dipole approximation ($p \ll 1$) we omit the R_w term in Eq. (6.33) and obtain a threshold energy similar to (6.4) for the case of quantum channeling radiation.¹

If the particle energy is below $E_c^{(n)}$, then all radiation up to n th harmonic is totally suppressed by the polarization effect. The critical energy $E_c^{(n)}$ tends to infinity when the helix radius R_w tends to $R_w^{(\text{max})}(n) = n\lambda_p$, where $\lambda_p = 1/\omega_p$ is the plasma wavelength which, as noted in Section 4.2, is about 85 Å for a rope of (11, 9) SWNTs (λ_p increases with the diameter of the nanotube like $(d + g)d^{-1/2}$ where the inter-tube gap g is about 3.15 Å). Let us estimate now the lowest possible value of the critical energy, $\inf E_c^{(n)}$. For this purpose we should take for ω_w in (6.33) the largest possible value $\omega_w^{(\text{max})} = 2\pi/\lambda_w^{(\text{min})}$, which is fixed by (6.25). We find

$$\inf E_c^{(n)} = \frac{1}{2U_0} \frac{dR_w}{\lambda_p^2} \frac{1}{[n^2 - (\omega_p R_w)^2]}. \quad (6.34)$$

For chiral (11, 9) nanotube according to (2.1) $d = 13.4$ Å, $U_0 = 60$ eV (Fig. 3) and supposing $R_w = 50$ Å we find $\inf E_c^{(1)} = 307$ MeV.

For electrons instead of the nanotube diameter d we should use the width of the potential well which according to Fig. 4 is about 2 Å. The critical energy (6.33) for electrons happens to be one order of magnitude lower than for positrons. Unfortunately, as shown in Section 5.2.1, electrons have much shorter dechanneling length than positrons and their ability to pass lots of NU periods is rather questionable.

The band of X-ray emission at n th harmonic is determined by the condition that the right side of (6.32) be positive:

$$\begin{aligned} \omega_n^{(\text{min})} &\leq \omega \leq \omega_n^{(\text{max})}, \\ \omega_n^{(\text{max})/(\text{min})} &= \gamma_z^2 \{ n\omega_w \pm [(n\omega_w)^2 - \omega_p^2 \gamma_z^{-2}]^{1/2} \}. \end{aligned} \quad (6.35)$$

Here $\gamma_z \equiv E(1 + p^2)^{-1/2}$ with p^2 given by (6.31). The extreme frequencies $\omega_n^{(\text{min})}$ and $\omega_n^{(\text{max})}$ are always radiated at zero angle θ . The maximum possible angle of X-ray emission at n th harmonic is

$$\theta_n^{(\text{max})} = [(n\omega_w/\omega_p)^2 - E^{-2}(1 + p^2)]^{1/2}. \quad (6.36)$$

¹ Similar threshold effects also exist for radiation in a medium with dielectric permeability varying periodically in space (*resonance transition radiation*) [80].

A single (for a fixed harmonic) frequency $\omega_n(\theta_n^{(\max)}) = \omega_p^2/(n\omega_w)$ is emitted at this angle. Corresponding to each fixed emission angle $\theta < \theta_n^{(\max)}$, there are two different frequencies, determined by (6.32), in the allowed X-ray frequency band.

6.4.3. Intensity of spontaneous NUR

Assuming $\lambda_w \gg \lambda_{ch}$, the undulator radiation emitted in a periodically bent nanotube is not sensitive to the channeling oscillations, except that the longitudinal motion is slower due to the effective mass squared $m_{\text{eff}}^2 = m^2 + 2\varepsilon_{\text{kin}}E$. We can therefore use the general formulae for the radiation from the helical undulator in a medium [99], which at small polar angles $\theta \ll 1$ and X-ray frequencies give the spectral-angular distribution of NUR energy

$$\frac{d^2 W}{d\omega d\Omega} = \frac{e^2 \omega^2}{\omega_w^2} \sum_{n=1}^{\infty} \left\{ \left[\psi \frac{dJ_n(\eta)}{d\eta} \right]^2 + \left| \theta - \frac{n\omega_w}{\omega\theta} \right|^2 J_n^2(\eta) \right\} \frac{\sin^2(N\xi_n)}{\xi_n^2}, \quad (6.37)$$

where $N \gg 1$ is the total number of NU periods, J_n is the Bessel function of $\eta = \omega\theta R_w$ and

$$\xi_n = \frac{\pi\omega}{2\omega_w} \left(\theta^2 + \frac{\omega_p^2}{\omega^2} + E^{-2} + \omega_w^2 R_w^2 + \frac{2\varepsilon_{\text{kin}}}{E} \right) - n\pi. \quad (6.38)$$

The function

$$S_n(\omega) = \frac{\sin^2(N\xi_n)}{\xi_n^2} \quad (6.39)$$

describes the shape of the spectral line radiated at fixed θ . It has a sharp maximum equal to N^2 at $\xi_n = 0$ which corresponds to a totally constructive interference between the radiations from the NU oscillations, and a width $\Delta\xi_n = \pi/N$. The natural spectral width of the line is

$$\Gamma_n = \left(\frac{\partial \xi_n}{\partial \omega} \right)^{-1} \Delta\xi_n = \frac{\omega}{nN} \left(1 - \frac{\omega_p^2}{n\omega\omega_w} \right)^{-1}. \quad (6.40)$$

For an infinite undulator we have

$$\lim_{N \rightarrow \infty} S_n(\omega) \rightarrow \pi N \delta(\xi_n),$$

where $\delta(\xi_n)$ is the Dirac delta-function, i.e. the frequency and polar angle θ of the radiation are indeed connected by the relation (6.32) which gives the zeros of ξ_n . The effective number of NU periods N_{eff} is limited by the ratio of the dechanneling length l_{dc} , for the estimation of which we can use (5.5), to the NU period $\lambda_w^{(\min)}$ (6.25).

The line-shape function (6.39) refers to a particle with definite total E and transverse channeling energy ϵ . For a particle beam we should take into account the spread of E and ε_{kin} . The spread of E consists of the primarily spread (which may be very low) and the spread attained due to the energy loss in the medium. The spread of ε_{kin} cannot be eliminated in principle and is always of the order of the depth U_0 of the continuum potential (see Figs. 3 and 4). It gives a so-called *inhomogeneous broadening* of the radiation line $\Delta\omega_{\text{inh}} = 2\omega E U_0 / (1 + p^2)$, which adds to inhomogeneous broadening coming from the spread of other parameters determining ξ_n , like R_w , λ_w and NU axis direction.

For example, in the case of a twisted nanotube rope, the helix radius is not the same for all nanotubes, but has relatively large spread. Inhomogeneous broadening can be much higher than the natural width (6.40), thus changing the line shape (6.39) and reducing the peak value of spectral-angular density (6.35) proportionally to $\Gamma/\Delta\omega_{\text{inh}}$.

As follows from (6.37), in forward direction ($\theta = 0$) only the first circularly polarized [99] harmonic can be emitted, with the spectral-angular density

$$\frac{d^2 W_0}{d\omega d\Omega} = \frac{e^2 \omega^2 R_w^2}{2} \frac{\sin^2(N\xi_1)}{\xi_1^2} . \quad (6.41)$$

In this case the peak (or resonance) radiation frequencies are equal to $\omega_1^{(\text{max})}$ and $\omega_1^{(\text{min})}$ in (6.35).

An interesting situation occurs at $E = E_c^{(1)}$. Here the two frequencies come to a common value $\omega_c = n\omega_w \gamma_z^2 = \gamma_z \omega_p$ and (6.36) gives $\theta_1^{(\text{max})} = 0$. It means that the X-ray photons are emitted in a very narrow forward cone and are nearly monochromatic. The group velocity of the photon (which has an effective mass ω_p) is equal to $\langle v_z \rangle$, i.e. we are at the kinematical (photon + final electron) threshold. The half-aperture $\Delta\theta$ of the cone can be defined as the angle θ where ξ_1 attains its half-width value $\pi/(2N)$ (for $\omega = \omega_c$). This gives

$$\Delta\theta = (1/E_c^{(1)}) \left[\frac{1 + p^2}{N} \right]^{1/2} .$$

The half-width $\Delta\omega/2$ in frequency at $\theta = 0$ can be defined similarly. Expanding ξ_1 up to second order in $\omega - \omega_c$, one gets

$$\Delta\omega = 2\omega_c N^{-1/2} .$$

Note that expression (6.40) for the width goes to infinity and cannot be applied in this case (more generally, when $\theta \simeq \theta_n^{(\text{max})}$). Integrating over ω one obtains an angular intensity $dW_0/d\Omega$ at $\theta = 0$ larger than usual by a factor $\sim N^{1/2}$.

The spectral-angular density (6.41) at a fixed ξ_1 is proportional to the squared helix radius which, as shown above, is limited by λ_p . Thus the maximum spectral-angular density of NUR is $e^2 \omega^2 N^2 / (2\omega_p^2)$ multiplied by the factor $\Gamma/\Delta\omega_{\text{inh}}$ describing the influence of the inhomogeneous broadening of the line. The effective number of periods N_{eff} is limited by the ratio of the dechanneling length (5.5) to $\lambda_w^{(\text{min})}$ (6.25). One can see that N_{eff} is proportional to $E^{1/2}$. Besides dechanneling, the X-ray absorption length may be the main factor limiting N_{eff} .

At non-zero polar angles $\theta \neq 0$ the higher harmonics $n \geq 2$ can be also emitted. They have significant spectral-angular density if $p \gtrsim 1$.

6.4.4. Induced NUR as X-ray amplifier

It is well known that the stimulated undulator radiation is used in the so-called *free-electron lasers* (FEL) for the generation of intense coherent microwave or even ultraviolet radiation. The principles of FEL action can be understood from the following semi-classical consideration. Let $w^{(\text{sp})}(E, \omega, \mathbf{n}) = d^3 N_{\text{phot}} / (dt d\omega d\Omega)$ be the differential spectrum of spontaneous NUR photons per unit of time, i.e. expression (6.37) divided by the photon energy ω and by the NU length $L = N\lambda_w$. The argument E is the *initial* charged particle energy and $\mathbf{n}$ is the unit vector in the photon direction. When an external beam

of photons propagates in this direction it can either stimulate the radiation or be absorbed by the beam. The cross section of the induced radiation $\sigma^{(\text{ind})}(E, \omega, \mathbf{n})$ and the cross section of photon absorption $\sigma^{(\text{abs})}(E, \omega, \mathbf{n})$ are connected to $w^{(\text{sp})}(E, \omega, \mathbf{n})$ through the relations

$$\sigma^{(\text{ind})}(E, \omega, \mathbf{n}) = \sigma^{(\text{abs})}(E - \omega, \omega, \mathbf{n}) = 2\pi\lambda^2 w^{(\text{sp})}(E, \omega, \mathbf{n}) . \quad (6.42)$$

Note that these equalities relate transitions between the same upper and lower energy levels of the particle, E and $E - \omega$. Besides, due to the natural width of NUR, ω may not exactly equal to the *resonance frequency* ω_{res} which satisfies (6.32). The photon beam is amplified if the induced cross section is larger than the absorption one for the *same initial* particle energy E . In the small-signal ($G \lesssim 1$), cold-beam (no energy or angular spread of the beam is taken into account) approximation, the *gain coefficient* G is given by

$$\begin{aligned} G &= \rho_e [\sigma^{(\text{ind})}(E, \omega, \mathbf{n}) - \sigma^{(\text{abs})}(E, \omega, \mathbf{n})] \\ &= 2\pi\lambda^2 \rho_e [w^{(\text{sp})}(E, \omega, \mathbf{n}) - w^{(\text{sp})}(E + \omega, \omega, \mathbf{n})] , \end{aligned} \quad (6.43)$$

where $\rho_e = IL/(eS)$ is the number of beam particles per unit transverse area which are inside the undulator at a given time, I and S are the current and cross section of the charged particle beam, respectively.

Due to the smallness of ω/E , the gain is usually small, except near the resonance where $w^{(\text{sp})}(E, \omega, \mathbf{n})$ is rapidly varying with E . In (6.37) we may neglect the E dependence of all factors except the last one. This gives

$$\begin{aligned} &w^{(\text{sp})}(E, \omega, \mathbf{n}) - w^{(\text{sp})}(E + \omega, \omega, \mathbf{n}) \\ &\simeq -L^{-1} N^{-2} \frac{d^2 W(\omega = \omega_{\text{res}})}{d\omega d\Omega} \frac{d}{d\xi_n} \left[\frac{\sin^2(N\xi_n)}{\xi_n^2} \right] \frac{d\xi_n}{dE} . \end{aligned} \quad (6.44)$$

For a photon beam propagating along the axis ($\theta = 0$), if one ignores the variation of $\varepsilon_{\text{kin}}/E$ in expression (6.38) for ξ_1 , we have

$$\frac{d\xi_1}{dE} = -\frac{\omega\lambda_w}{2m\gamma^3} \quad (6.45)$$

and gathering (6.41), (6.44) and (6.45), we obtain the gain

$$\begin{aligned} G &= \frac{\pi}{2} \frac{I}{I_0 S} \omega p^2 N^3 \lambda_w^3 \gamma^{-5} f(\varsigma) , \\ f(\varsigma) &= \frac{d}{d\xi} \frac{\sin^2 \varsigma}{\varsigma^2}, \quad \varsigma = N\xi_1 , \end{aligned} \quad (6.46)$$

where $I_0 = mc^3/e$ and $\gamma = E/(mc^2)$. If in addition we ignore the polarization effect ($E \gg E_c^{(1)}$), we may replace γ by $[(1 + p^2)\lambda_w/(2\lambda)]^{1/2}$ and recover the well-known result for the helical undulator [105,106]

$$G = \frac{I\pi^2}{I_0 S} N^3 \lambda_w^{1/2} \lambda^{3/2} \frac{p^2}{(1 + p^2)^{5/2}} f(\varsigma) , \quad (6.47)$$

except for an additional power of $(1 + p^2)$ in the denominator of (6.47). This difference is due to dependence of the NU parameter $p = ER\omega_w$ (or the invariance of ψ) with respect to the particle energy E .

The gain is positive in the region $-\pi < \varsigma < 0$ where the frequency is slightly below ω_{res} , which is the maximum of the spontaneous emission line. Above this maximum the external radiation is preferably absorbed by the beam, giving rise to particle acceleration. The maximum of $f(\varsigma)$ corresponds to $\varsigma \simeq -1.30$ and is equal to 0.54. The values of p optimal for the gain are close to unity, therefore to obtain an optimal gain for the shorter wavelengths at a fixed particle energy E , one should decrease simultaneously the undulator period λ_w and the helix radius R_w , to preserve the value of $p = E\omega_w R_w$ close to unity. It should be noted that (6.47) gives an upper limit of the gain since it does not take into account inhomogeneous broadening discussed above. Inhomogeneous broadening reduces the gain approximately by a factor $(\Delta\omega_{\text{inh}}/\Gamma)^2 \approx (\Delta\omega_{\text{inh}}N/\omega)^2$ if $\Delta\omega_{\text{inh}}/\omega \gtrsim 1/N$. Thus the effective for NUR FEL number of periods is limited above by $\omega/\Delta\omega_{\text{inh}}$.

Noteworthy, since NUR takes place in condensed medium the gain should be large enough compared to the X-ray absorption coefficient, which demands high enough current. As mentioned above, electron beams are probably not suitable for NUR due to their very short dechanneling length, whereas available currents of positron beams are usually much lower than for electrons.

7. Miscellaneous effects

Besides CR, CB, PXR and NUR other types of X-ray electromagnetic radiation from ultra-relativistic particles can exist in carbon nanotubes and fullerenes. As shown in [107] theoretically and measured in [108], near the K-edge of carbon there is a relatively narrow frequency interval where the dielectric susceptibility is positive and Cherenkov X-ray radiation (CXR) can be emitted by fast enough charged particles. Cherenkov X-ray radiation was detected at normal [109] and grazing [110] incidence of electron beam on carbon materials. Due to the high monochromaticity and narrow angular distribution CXR was considered [111] as a candidate for soft X-ray free-electron laser (FEL), however since the particle beam must move inside a dense medium, multiple scattering substantially reduces the beam quality (angular divergence) needed for any kind of FEL. In this connection for this purpose it may be interesting to use particle beam channeled in nanotubes. From the results of Section 5.2 it follows that the angular divergence of the channeled beam stays within the limits of the Lindhard angle over a long distance (dechanneling length), thus the influence of multiple scattering can be substantially reduced.

Another interesting type of radiation arises when a laser beam collides with a beam of channeled particles [112,113]. The backward Compton scattering of light on ultra-relativistic electron beams is well known as a source of polarized γ -quanta. The resonance scattering of light on channeled particles have much higher cross section $\sigma(\omega, \mathbf{n}, \omega', \mathbf{n}')$ than the Compton scattering. On the resonance condition $\omega - \mathbf{k} \cdot \mathbf{v} = \omega_{if}$ it can be presented by the Breit–Wigner formula

$$\sigma(\omega, \mathbf{n}, \omega', \mathbf{n}') = \sigma^{(c)}(\omega, \mathbf{n}) \frac{w(\omega', \mathbf{n}')}{\Gamma_f},$$

where $\sigma^{(c)}(\omega, \mathbf{n})$ is the cross section of the initial photon capture resulting in the transition of channeled particle from the initial transverse energy level i to the higher final one f , $\omega_{if} = \varepsilon_i - \varepsilon_f$, $\mathbf{n} = \mathbf{k}/k$ is the unit vector in the direction of the initial photon beam, $w(\omega', \mathbf{n}')$ is probability (6.1) of the spontaneous radiation of a photon with energy ω' per unit of time in the direction of $\mathbf{n}'$, Γ_f is the total width of level f determined mostly by non-radiative (dechanneling) processes. Cross section $\sigma^{(c)}(\omega, \mathbf{n})$ is connected with

the spontaneous radiation probability $w(\omega, \mathbf{n})$ in the direction $\mathbf{n}$ by the Einstein relation

$$\sigma^{(c)}(\omega, \mathbf{n}) = 2\pi\lambda^2 w(\omega, \mathbf{n}) .$$

Since the level width Γ_f for positrons in nanotubes is much less than that in ordinary crystals, the backward resonance scattering is easier to observe in nanotubes, however they must be transparent for the initial photons, like diamond.

It is known that rough metal surfaces can emit ultraviolet radiation under electron bombardment at grazing incidence. The reason for such radiation is the excitation of local plasmons (oscillations of the substance electron density) in small metal particles representing the roughness [114]. These particles act like the resonators for the electromagnetic waves with resonance frequencies depending on their shape and size (if this size is larger than the wavelength of radiation). The local plasmons are instantaneous sources of electromagnetic radiation with resonance frequencies. The condition for the excitation of local plasmons is a negative value of the real part of the dielectric permittivity $\varepsilon(\omega)$ which can be satisfied for metals in UV and visible range. The excitation of the local plasmons by electrons or an external electromagnetic radiation with the resonance frequency gives rise to a significant enhancement of the local electric field near the roughness and consequently to the enhancement of all electromagnetic processes depending on the local field strength, particularly surface enhanced Raman scattering (SERS) [115] by adsorbed molecules. On the surfaces with broad randomly distributed shapes and sizes of roughness the resonance frequencies occur to have relatively broad distribution too. Nanotube films represent the better surface for the local plasmons due to the uniform shapes of the structures (cylinders with or without hemisphere caps). The field enhancement near the nanotube tips due to the local plasmon excitation can be superimposed on the spike effect (see below) and used for the enhancement of the electron emission from nanotube films under the electromagnetic radiation with the resonance frequency. This possibility should be considered elsewhere with more details.

Let us say some more words about the field emission (FE) from nanotubes and other related phenomena, such as photoemission (PhE) and secondary electron emission (SEE), in conjunction with possible applications of these phenomena in devices for high-energy physics.

Due to the very small curvature radius of nanotube tips very strong electric field (up to 10^7 V/cm) can be produced near the tips using the well known effect of the enhancement of external electric field near spikes. This effect can give rise to much higher yield of electrons from the tips of single- and multi-wall nanotubes (SWNT and MWNT) compared with other substances used as electron emitters. The FE properties of nanotubes were first discussed in [116]. At present the electron field-emission (FE) experiments have been carried out with both single nanotubes and arrays of many aligned nanotubes (SWNT or MWNT), nanotubes with tips capped by fullerene hemisphere or opened nanotube tips. Stable in time FE electron current was observed from pure, preheated nanotubes free of any adsorbates. There are review articles [117,118] and some articles containing new interesting results [119] devoted to FE from nanotubes.

Summarizing these results, we can formulate the main features of FE from nanotubes as follows: (1) The Fowler–Nordheim law for current–voltage curves of all nanotube emitters holds only at voltages much lower than those in other metallic and semiconductor emitters. With growing voltages this law is violated, and at further rising of the voltage the emission stops with sudden electric breakdown of nanotubes. (2) The maximum FE current which can be obtained from a single MWNT tip is extremely high (about 0.2 mA) and close to the value at which nanotube can be damaged by the thermal effect of the current (Joule heating). On the other hand, the current density from an array of MWNTs occurs to

Fig. 53. Schematic view of electron tunneling through the potential barrier near a nanotube cap.

be relatively low (probably due to insufficient alignment and packing of nanotubes used in experiments). (3) Higher and more stable currents were observed from MWNTs with closed tips rather than opened. (4) The width of the energy distributions of the emitted electrons occur to be about 0.2 eV, that is substantially less than for metal emitters. Furthermore, sometimes several relatively narrow peaks in the energy spectra were observed. (5) High Joule heating up to 2000 K was observed along the whole length of nanotubes. (6) It was detected that FE can produce a luminescence the spectrum of which is the superposition of a wide incandescence and a narrow peak in the vicinity of 1.77 eV with 0.022 eV FWHM. Only a few luminescence photons are emitted per million electrons.

In order to explain theoretically the above mentioned features, particularly (3), Ispirian and Melikian [120] suggested the resonance tunneling model which was successfully applied previously [121] for the description of FE from metal–semiconductor compounds. According to this model (Fig. 53) the field repels electrons from nanotube metallic body (region I) through the semiconductor tip (region II) into vacuum (region III). When an external field is applied, a one-dimensional double-barrier potential well is formed where substance electrons are in metastable states with energy below Fermi level. The tunneling of electrons through the potential barrier into vacuum is assumed to take place via resonance energy levels and thus have a transmission coefficient D close to unity. Solving Schroedinger equation for electrons in potential well and taking into account the equality $D \simeq 1$, one can find the expressions for the energy levels of electrons, the widths of the resonance levels and the current density. This model quantitatively (and in definite cases qualitatively) can explain most of the mentioned features of FE from nanotubes. Unfortunately, some of the parameters used in this model, particularly the width of the conductivity and forbidden zones and the work of exit from the metallic nanotube bodies (well known for other materials) have not been measured yet for nanotubes.

As mentioned in [121], when the external electric field has a pulsed character, FE from nanotubes may attain some new features which facilitate production of intense electron beams with low angular divergence. This is important for advanced charged particle beam acceleration using radio-frequency electron guns.

Fig. 54. Photocurrent excitation spectrum for an individual (18, 10) SWNT.

Let us say some words about other possible applications of nanotubes which has not been studied yet. To our knowledge, there are only a few scientific publications devoted to the very close to FE process of photoelectron emission (PhE). Particularly, in [122] PhE from SWNTs and the influence of Cs-intercalation on PhE was investigated. The photocurrent from an individual (18, 10) semiconducting SWNT was recently measured in [123] using Ti/Sapphire laser as photon source with tunable photon energy (and polarization parallel to the nanotube axis). The photocurrent against photon energy is shown in Fig. 54. It is almost a linear function, but with a peak at 1.73 eV which was attributed to the van Hove singularity of the electron state density of the SWNT. For the development of various kinds of particle detectors using PhE, e.g. ring imaging Cherenkov detectors, a good sensitivity to the entrance point of a single photon into a detector is required. The detector sensitivity is strongly dependent on the quantum efficiency of the medium used and since the latter is expected to be relatively high for nanotubes, these objects are good candidates for this purpose.

Another electromagnetic process closely connected with PhE and FE is secondary electron emission (SEE). The structure of nanotubes is similar to the structure of micro-channel plates, commonly used in particle detectors as signal amplifiers. We can hope that some kinds of nanotube structures will have SEE characteristics appropriate for using them in this field.

8. Conclusion

It is well known that the unique properties of fullerite crystals and nanotubes can be used in various fields of industry, medicine and science [124]. As shown above, fullerite single crystals and aligned nanotubes [14,125,126] can also find various applications in such fields as: production of X-rays with high-energy particle beams, Bragg mirrors for X-rays down to nanometer wavelength which are probably more resistant to extreme irradiation and heating than other soft X-ray mirrors, steering of charged and

neutral particle beams, etc. Recently, some of the discussed possibilities of using nanotubes in high-energy physics were reconsidered in [127–129].

Theoretical calculations and computer simulations clearly indicate that nanocrystals are comparable to or even go beyond the regular targets (crystals) for the production of intense quasi-monochromatic X-ray photons of parametric X-ray radiation (PXR), coherent bremsstrahlung (CB), channeling radiation (ChR), and other types of emission. The intensity of PXR from nanocrystals can be up to three orders higher than in ordinary crystals like diamond; moreover, it becomes possible to extend the PXR spectrum to the soft X-ray region where ordinary crystals cannot emit this type of radiation at all.

Besides PXR, a specific channeled transition radiation (CTR) can arise at grazing incidence of electrons to MWNT axis which is less monochromatic, but more intense than PXR. All these features make PXR a very promising portable source of radiation in various technological and scientific fields wherever monochromatic and wavelength tunable X-ray radiation is needed, while CTR may be used in lithography and X-ray imaging.

Using channeling of high-energy particles in nanotubes it is possible to deflect and focus charged particles more effectively than in ordinary single crystals and maybe even accelerate them using external electromagnetic waves. Moreover, long and wide enough MWNTs can act like waveguides for X-rays and thermal neutrons. On the other hand, like with ordinary crystals, one can use soft X-ray diffraction, PXR and especially ChR in fullerites and nanotube ropes for the determination of the structural parameters of the fullerene and nanotube targets themselves. These possibilities should be analyzed more carefully in the case of relatively thin MWNT films.

Most of the theoretical predictions reviewed above have been discussed at a number of International Symposia, e.g. “Radiation of Relativistic Electrons in Periodical Structures (RREPS)”, Baikal 1999 and Altai 2001, Russia; NATO sponsored Workshop “Interaction of Electrons and Photons in Dense Media”, Nor-Hamberd, Armenia, 2001; Workshop “Application of Carbon Nanotubes and Fullerites in High Energy Physics, X-ray and Neutron Optics”, IASA, Athens, Greece, 2002, International Workshop on Interactions between Nano-structure and Particle Beams, Shanghai, China, 2004, Workshop on Charged and Neutral Particles “Channelling 2004”, Frascati, Italy. The discussions indicated the evident need for the experimental study of the high-energy beam interactions with nanocrystals in order to verify these predictions and thus to give the stimulus to the further development of this field of science which represents an interplay between nanotechnology, X-ray optics and high-energy physics.

The preparation of perfect enough fullerites and aligned nanotubes arrays is crucial for the kinds of experiments mentioned above. Concerning fullerites, they can be probably produced, using the existing methods [130], in sample suitable for all kinds of experiments with high-energy electrons and X-rays mentioned above. However, for experiments at very high energies of the beam particles (say > 1 GeV) it may become necessary to improve these methods for producing better fullerite single crystals with controllable mosaic spread, dislocations and impurities. More difficult task is the production of films of aligned nanotubes. For this purpose various methods are rapidly developing. Among them the most promising are the catalytic vapor deposition method (CVD) of growth of nanotubes from hydrocarbons on surfaces of porous substrates or crystal surfaces [123,131,132] and the method of extraction of carbon nanotube targets from cathode deposits formed in arc evaporation of graphite rods [133]. At present the CVD method is developed better for MWNT than for SWNT production. The achieved angular spread (15° or worse) of nanotubes in grown films is unsatisfactory for the channeling experiments mentioned, since it is two orders above the Lindhard critical angle, even in the case of moderate (20 MeV) electron energies. Fortunately, PXR and CB are less sensitive to the nanotube alignment, but 15° misalignment is

still too large. Recently, a spinning process was developed [134] at Centre de Recherche Paul-Pascal, in Bordeaux, to assemble SWNTs into macroscopic fibers, with diameters ranging from 10 to 100 μm and lengths up to several tens of cm. MWNTs with wall thickness from several to more than 100 regularly spaced carbon layers, which was about 10% of the large inner diameter of 20–800 nm, were produced using alternative method of hydrothermal synthesis [135]. This kind of MWNTs is very promising for experiments with X-ray channeling.

Hence, the existing methods of nanotube alignment should be improved to the degree at which at least the study of PXR (and probably ChR) becomes possible, using electron beams of low energy (up to 10 MeV). Foreseeing the difficulties in the preparations of perfect enough structures, it becomes necessary to modify the already developed theory in order to estimate the influence of imperfections of the targets and electron beam quality on the electromagnetic processes mentioned above.

The investigations of soft X-ray diffraction, channeling of high-energy charged particles, different kinds of electromagnetic radiation accompanying the passage of the particles through nanocrystals, and other low-energy electromagnetic processes taking place in FC, SWNTs and MWNTs are innovative since they bring together the problems of chemical physics, solid state physics and high-energy physics. They will lead to a further development of the theory of electromagnetic interactions of X-rays and electrons with nanocrystals, and help to test the theoretical predictions of promising new sources of intense monochromatic X-ray radiation with photon energies from 0.1 to 30 keV, which can be used in industry, science and medicine. The experimental and theoretical investigations of FE, PhE and SEE from nanotubes may result in the production of novel pulsed electron emitters which will provide short electron pulses with low emittance for radio-frequency guns and in the construction of nanotube-based photo-detectors comparable to or even better than the existing micro-channel plate (MCP) detectors. At the same time, the investigations of fast particle interactions with nanocrystals and associated phenomena may give rise to new methods of structure analysis of nanotubes and fullerenes themselves. The expected results will promote advances in many interdisciplinary fields of science and may have industrial applications.

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Appendix A

Here we give the analytical representation of the exact (not averaged along the axis) nanotube potential based on Doyle–Turner approximation to the atomic potential. Let (r, φ, z) denote the cylinder coordinates attached to the nanotube. Since unit cell of a graphite plane shown in Fig. 1a contains two carbon atoms,

we present the total potential of a nanotube $U(r, \varphi, z)$ as a sum $U(r, \varphi, z) = U^{(1)}(r, \varphi, z) + U^{(2)}(r, \varphi, z)$, where $U^{(1)}$ and $U^{(2)}$ are the potentials generated by all the atoms which are in the positions $(\mathbf{a} + \mathbf{b})/3$ and $2(\mathbf{a} + \mathbf{b})/3$ of a graphite unit cell, respectively. Since the exact nanotube potential is a periodical function of z with period $d_R = (3l/q)(n^2 + nm + m^2)^{1/2}$ we may expand it in the following series:

$$U(r, \varphi, z) = \sum_{v=-\infty}^{\infty} \sum_{\mu=-\infty}^{\infty} \mathfrak{U}(r, v, \mu) \exp \left[i v \varphi + i \frac{2\pi\mu}{d_R} z \right]. \quad (\text{A.1})$$

The expansion coefficients is determined by equalities $\mathfrak{U}(r, v, \mu) = \mathfrak{U}^{(1)}(r, v, \mu) + \mathfrak{U}^{(2)}(r, v, \mu)$

$$\mathfrak{U}^{(1)}(r, v, \mu) = (2\pi d_R)^{-1} \int_0^{2\pi} \int_0^{d_R} U^{(1)}(r, \varphi, z) \exp \left[-i v \varphi - i \frac{2\pi\mu}{d_R} z \right] dz d\varphi \quad (\text{A.2})$$

and similar for $\mathfrak{U}^{(2)}(r, v, \mu)$.

Integration in (A.2) is performed over the unit cell of a nanotube considered as 1D crystal. It is not difficult to see that the number of atoms $N' = r_0 d_R \sigma$ in such a cell coincides with the number $2N$ of atomic rows (N given by (2.6)). Expansion coefficients $\mathfrak{U}^{(1)}(r, v, \mu)$ may be written as a product $\mathfrak{U}^{(1)}(r, v, \mu) = u(r, v, \mu) S^{(1)}(v, \mu)$ (and similar for $\mathfrak{U}^{(2)}(r, v, \mu)$), where

$$u(r, v, \mu) = (4Ze^2/d_R) \sum_{j=1}^4 a_j b_j^2 \exp[-b_j^2(r^2 + R^2)] I_v(2b_j^2 R r) \exp \left[-\left(\frac{\pi\mu}{d_R b_j} \right)^2 \right] \quad (\text{A.3})$$

refers to a single carbon atom with Fourier transformed potential (2.12) and

$$S^{(1,2)}(v, \mu) = \sum_{k=0}^{N-1} \exp \left[-i v \varphi_k - i \frac{2\pi\mu}{d_R} z_k \right] \quad (\text{A.4})$$

is the geometrical structure factor, which is determined by coordinates φ_k, z_k , ($\varphi_0 = z_0 = 0$) of N carbon atoms belonging to the first (second) sequence of rows. $S^{(1)}$ and $S^{(2)}$ are related by the following relation:

$$S^{(2)}(v, \mu) = S^{(1)}(v, \mu) \exp \left[\frac{2\pi i}{N} \left(\frac{n+m}{q} v + \frac{n-m}{3} \mu \right) \right]. \quad (\text{A.5})$$

Thermal vibrations may be taken into account by inserting the Debye–Waller factor e^{-W} , with

$$W = (1/2)(k_r^2 u_r^2 + k_\tau^2 u_\tau^2 + k_z^2 u_z^2),$$

in (A.3). As further calculations show, $S^{(1)}(v, \mu)$ is either N or zero depending upon the relations between nanotube indices n, m and harmonics v and μ . Particularly, in two specific cases:

$$S^{(1)}(v, 0) = N \delta_{v, sN}, \quad S^{(1)}(0, \mu) = N \delta_{v, sN^*}.$$

Here δ is the Kronecker symbol, $N^* = N/q^*$, q^* is the largest common denominator of n and m , and $s=0, \pm 1, \pm 2, \dots$. The case where $\mu=0$ corresponds to continuum potential (2.14), and $v=0$ corresponds to the actual potential of a nanotube averaged over the azimuthal angle φ . The above results may be useful, for example, in calculations of resonant excitation of channeled ions (Okorokov effect) or electron density in nanotubes in the next approximation.

Appendix B

The solution $\Psi(x)$ of the Dirac equation for an electron in an external field can be presented in the form

$$\Psi(x) = (\gamma^\mu P_\mu + m)F(x) , \quad (\text{B.1})$$

where we use the relativistic units, γ^μ are the Dirac matrices, $P_\mu = -i\partial/\partial x_\mu - eA_\mu$, and $x = \{x, y, z, t\}$ denote space and time coordinates of an electron. Particularly, when particle moves in the continuum potential of a nanotube, only the scalar component of the 4-potential A_μ is non-zero, therefore we obtain the following equation for $F(x)$:

$$\left[\left(i \frac{\partial}{\partial t} - U(\mathbf{r}) \right)^2 + \Delta - m^2 + i\alpha \cdot \nabla U(\mathbf{r}) \right] F(x) = 0 . \quad (\text{B.2})$$

Let E be the energy of the relativistic particle and U_0 the characteristic potential energy of the particle, then we may neglect the terms U^2 and $\alpha \cdot \nabla U$ (the latter describes the interaction of the electron spin with the continuum potential) as small compared to $U\partial/\partial t \sim UE$. Representing $F(x)$ as

$$F(x) = \exp[i(p_z z - Et)]\psi(\mathbf{r}) \begin{pmatrix} \phi \\ 0 \end{pmatrix} , \quad (\text{B.3})$$

where p_z is the longitudinal momentum and ϕ is the Pauli spinor describing the spin state of the electron, we find the equation for the scalar transverse wave function ψ

$$\left[-\frac{1}{2E_\parallel} \Delta + U(\mathbf{r}) \right] \psi(\mathbf{r}) = \varepsilon \psi(\mathbf{r}) . \quad (\text{B.4})$$

Here we have introduced the following notations: $E_\parallel = (p_z^2 + m^2)^{1/2}$, $\varepsilon = E - E_\parallel$ is the so-called transverse energy. Substitution of (B.3) into (B.1) gives

$$\Psi(x) = \left(\frac{2E_\parallel}{E_\parallel + m} \right)^{-1/2} \begin{pmatrix} \phi \\ -i\sigma_j \phi \nabla_j / (E_\parallel + m) \end{pmatrix} \exp[i(p_z z - Et)]\psi(\mathbf{r}) , \quad (\text{B.5})$$

where σ are the Pauli matrices. The spinor structure of electron wave function (B.5) may be of importance only if radiation of hard photon (with energy ω comparable to E) by the electron is under consideration. In this case we must take into account the spin flip effects. In other cases the more simple scalar function (B.3) is sufficient.

In the case of a curved channel the above equations should be modified in the following way. We choose orthogonal curvilinear spatial coordinates (x', y', s) , s being the curvilinear abscissa along the axis of one particular channel (in a family of neighboring channels) and the (x', y') surface being orthogonal to the channel axes and write $F(x, y, z, t) = F'(x', y', s, t)$. We have approximately

$$\Delta F(x, y, z, t) = \Delta_\perp F'(x', y', s, t) + (1 + 2\mathbf{C} \cdot \mathbf{X}') \frac{\partial^2}{\partial s^2} F'(x', y', s, t) ,$$

where $\mathbf{C}$ is the curvature vector and $\mathbf{X}' = (x', y')$ is the particle location vector in the transverse plane. Writing, instead of (B.3),

$$F'(x', y', s, t) = \exp(iPs - iEt)\psi(x', y', s) ,$$

where $P = \sqrt{E^2 - m^2}$ and keeping the dependence in s , instead of (B.4) one gets

$$i \frac{\partial}{\partial s} \psi(x', y', s) = \left[-\frac{1}{2P} \Delta_{\perp} + U(x', y') + P \mathbf{C} \cdot \mathbf{X}' \right] \psi(x', y', s) . \quad (\text{B.6})$$

Appendix C

Gauged with zero scalar potential φ the electric field $\mathbf{E}(\mathbf{r}, t)$ in a non-magnetic medium is connected with the vector potential $\mathbf{A}(\mathbf{r}, t)$ by the relation

$$\mathbf{E}(\mathbf{r}, t) = -\partial \mathbf{A}(\mathbf{r}, t) / \partial t . \quad (\text{C.1})$$

Using (C.1) for the corresponding Fourier time expansion coefficients we find

$$\mathbf{E}(\mathbf{r}, \omega) = i\omega \mathbf{A}(\mathbf{r}, \omega) . \quad (\text{C.2})$$

From the Maxwell equations it follows the wave equation for $\mathbf{A}(\mathbf{r}, \omega)$:

$$[\varepsilon(\mathbf{r}, \omega)\omega^2 - \nabla \times \nabla] \mathbf{A}(\mathbf{r}, \omega) = -4\pi \mathbf{j}(\mathbf{r}, \omega) , \quad (\text{C.3})$$

where $\varepsilon(\mathbf{r}, \omega) = 1 + \chi(\mathbf{r}, \omega)$ and $\mathbf{j}(\mathbf{r}, \omega)$ are the dielectric permittivity of the inhomogeneous medium and the Fourier expansion coefficient of the current created by a charged particle.

Appendix D

It is well known [81] that the spectral-angular distribution of the electromagnetic energy W radiated by a particle with charge e over the total time of its motion with velocity $\mathbf{v}(t)$ along a trajectory $\mathbf{r}(t)$ in vacuum can be presented as

$$\frac{d^2 W}{d\omega d\Omega} = \frac{\omega^2}{(2\pi)^2} |\mathbf{e} \cdot \mathbf{j}(\mathbf{k}, \omega)|^2 , \quad (\text{D.1})$$

where ω and $\mathbf{k}$ is the radiation frequency and the wavevector respectively, $\mathbf{e}$ is the orthogonal to $\mathbf{k}$ unit vector which determines the radiation polarization (direction of the electric field in the electromagnetic wave), Ω is the solid angle,

$$\mathbf{j}(\mathbf{k}, \omega) = e \int_{-\infty}^{\infty} \mathbf{v}(t) \exp[i(\omega t - \mathbf{k} \cdot \mathbf{r}(t))] dt \quad (\text{D.2})$$

is the Fourier expansion of the electric current created by the charged particle. The summation over all possible polarizations $\mathbf{e}$ in (D.1) gives the following result

$$\frac{d^2 W}{d\omega d\Omega} = \frac{\omega^2}{(2\pi)^2} |\mathbf{n} \times \mathbf{j}(\mathbf{k}, \omega)|^2 , \quad (\text{D.3})$$

where $\mathbf{n} = \mathbf{k}/k$ is the unit vector along the radiation direction. Usually, the above formulae are derived as a result of the calculation of the electromagnetic energy flux through an infinitely distant sphere surrounding particle trajectory. Practically the distance must be much greater than the coherence length of radiation.

The standard formulae (D.1)–(D.3) should be modified in the case of radiation in a medium. Furthermore, in an absorptive medium the flux turns to zero. In the general case of radiation in a media with the complex dielectric permittivity $\varepsilon(\omega) = 1 + \chi(\omega)$ it is more reasonable to calculate the total electromagnetic energy loss of the particle which coincides with the work of the electromagnetic field generated by the particle upon the particle itself

$$W = - \int \int_{-\infty}^{\infty} \mathbf{j}^*(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) dt d\mathbf{r} , \quad (\text{D.4})$$

where $\mathbf{j}(\mathbf{r}, t) = ev(t)\delta(\mathbf{r} - \mathbf{r}(t))$ and $\mathbf{E}(\mathbf{r}, t)$ are the electric current of the particle and the strength of the electric field at particle locus, respectively. Using the Fourier expansion of the kind

$$\mathbf{E}(\mathbf{r}, t) = (2\pi)^{-4} \int \int_{-\infty}^{\infty} \mathbf{E}(\mathbf{k}, \omega) \exp[i(\mathbf{k}\mathbf{r} - \omega t)] d\omega d^3k \quad (\text{D.5})$$

and relations $\mathbf{j}^*(-\mathbf{k}, -\omega) = \mathbf{j}(\mathbf{k}, \omega)$, $\mathbf{E}(-\mathbf{k}, -\omega) = \mathbf{E}^*(\mathbf{k}, \omega)$, we can rewrite (D.4) as

$$W = -\frac{1}{8\pi^4} \text{Re} \int_0^\infty \int \mathbf{j}^*(\mathbf{k}, \omega) \cdot \mathbf{E}(\mathbf{k}, \omega) d\omega d^3k . \quad (\text{D.6})$$

Then from the Maxwell equations (Appendix C) we find the three Cartesian components ($i = 1, 2, 3$) of the electric field generated by the particle

$$E_i(\mathbf{k}, \omega) = i\omega \frac{4\pi}{k^2 - \omega^2\varepsilon(\omega)} \sum_{l=1}^3 \left(\delta_{il} - \frac{k_i k_l}{\omega^2\varepsilon(\omega)} \right) j_l(\mathbf{k}, \omega) . \quad (\text{D.7})$$

Substitution of (D.7) into (D.6) gives us the spectral-angular distribution of the energy loss in the form

$$W = \frac{\omega}{2\pi^3} \text{Im} \int \int_0^\infty \left[|\mathbf{j}(\mathbf{k}, \omega)|^2 - \frac{|\mathbf{k} \cdot \mathbf{j}(\mathbf{k}, \omega)|^2}{\omega^2\varepsilon(\omega)} \right] \frac{d\omega d^3k}{k^2 - \omega^2\varepsilon(\omega)} . \quad (\text{D.8})$$

For a transparent medium $\varepsilon''(\omega) = 0$ we can use the relation

$$\lim_{\varepsilon''(\omega) \rightarrow 0} \text{Im} \frac{1}{k^2 - \omega^2\varepsilon(\omega)} = \frac{\pi}{2k} \delta(k - \omega\sqrt{\varepsilon'(\omega)}) .$$

Then the integration in (D.8) over the wavevector modulus k gives the spectral-angular distribution of radiation

$$\frac{d^2W}{d\omega d\Omega} = \frac{\omega k}{(2\pi)^2} |\mathbf{n} \times \mathbf{j}(\mathbf{k}, \omega)|^2 , \quad (\text{D.9})$$

where $k = \omega\sqrt{\varepsilon'(\omega)}$. For vacuum $\varepsilon'(\omega) = 1$ (D.9) coincides with the standard expression (D.3).

Noteworthy that even in a transparent dielectric medium ($\varepsilon''(\omega) = 0$) the particle can also loose energy due to the radiation of longitudinally polarized waves (plasmon excitation). This becomes possible at frequencies ω where the real part of $\varepsilon(\omega)$ tends to zero, e.g. in the optical region in metals. Moreover, in absorptive media ($\varepsilon''(\omega) \neq 0$) the particle can loose energy without any real electromagnetic radiation at all. For example, in the ω -region where $\varepsilon''(\omega)$ is determined by the photo production of e^+e^- pairs, (D.8) describes the energy loss due to the direct production of e^+e^- pairs by the charged particle.

In all cases (except PXR) considered in this Report where ultrarelativistic particle moves predominantly along z -direction and radiates X-rays ($|\chi| \ll 1$) at low polar angles, the *phase angle* $\phi = \omega t - \mathbf{k}\mathbf{r}(t)$ in (D.2) can be rewritten as

$$\phi \simeq \omega \theta \mathbf{n}_\perp \cdot \boldsymbol{\rho}(t) - (\omega/2) \left[[\theta^2 + E^{-2} - \chi(\omega)]t + \int_0^t \mathbf{v}_\rho^2(\tau) d\tau \right], \quad (\text{D.10})$$

where $\mathbf{n}_\perp = \{\cos \varphi, \sin \varphi\}$ is the unit vector of the radiation azimuth, $\boldsymbol{\rho}(t)$ and $\mathbf{v}_\rho$ are the transverse components of the corresponding vectors. The presence of $\chi(\omega)$ in the phase angle reflects possible influence of the polarization of the medium on the radiation spectrum. Furthermore, in the region where $\chi(\omega)$ is positive this term gives the Cherenkov radiation mentioned in Section 7. In order of magnitude $\mathbf{n}_\perp \cdot \boldsymbol{\rho}(t)$ is proportional to the deviation angle of the particle from z -direction, while the integrand in the brackets is the squared deviation angle. If the deviation angle is smaller than the effective angle of radiation $\theta_{\text{eff}} \sim E^{-1}$, then $\phi \approx -(\omega/2)[\theta^2 + E^{-2} - \chi(\omega)]t$. This is the case of *the dipole radiation*.

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