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THE DISTRIBUTION OF SHORT-WAVE RADIATION IN AN INTERNAL HOLE OF NANOTUBE

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Abstract. Spectral dependences and distributions of diffraction intensity of short-wave radiation (X-ray, particles of corresponding energies) by non-chiral, chiral, spiral and radial lattices in the internal hole of nanotube are calculated. The significant increase of intensity, diffracted by some kinds of nanotubes at characteristic lengths of waves, is shown. Differences and abnormal character of radiation propagation through the hole are determined.

Keywords: nanotube, short-wave radiation, internal hole, spectral dependence.

1. Introduction

One of the unique properties of nanotubes is the presence of internal cylindrical hole, not having a crystal lattice, but being an integral part of the cylindrical crystal. The problem of radiation diffraction in such a hole by cylindrical structure, surrounding it, is of fundamental interest and can enable for new applied developments.

Experimental researches have allowed distinguishing three types of nanotubes, having non-chiral, chiral and spiral (roll and cone) structures, as a whole called layered [1]. The fourth type – radial structure – can arise at sorption atoms by internal hole or an external surface of a nanotube [2].

With the purpose of revealing the basic features and distinctions between scatterings by cylindrical crystals of various types we shall consider a case of their lattices. As the distance up to observing point is comparable with the distances between the scattering centers, the general Fresnel's approach is used, that is why we shall consider diffraction of spherical waves.

The amplitude of Fresnel diffraction by cylindrical lattice in case of direct passage looks like:

$$A(r,j,z)=\sum_{n=-N+1}^{N-1}\sum_{m=0}^{M-1}\sum_{n=0}^{p_m-1}\exp\left(\frac{2p\,i}{l}z_{mnn}\right)\cdot$$

$$\cdot\frac{\exp\left[\frac{2p\,i}{l}\sqrt{r^2+r_m^2-2rr_m\cos\left(j_{mnn}-j\right)+\left(z_{mnn}-z\right)^2}\right]}{\sqrt{r^2+r_m^2-2rr_m\cos\left(j_{mnn}-j\right)+\left(z_{mnn}-z\right)^2}} \quad (1)$$

where m = 0–(M-1) – number of the site cylinder or of the turn of a site spiral, n = 0–(N-1) – number of a site circle (or a turn of the helix) on the cylinder or number of a site spiral, n = 0–(p_m-1) – number of a site on the circle (or on the turn of the helix) of the cylinder or on the turn of a site spiral, p_m – number of sites on the circle or on the turn of helix of m-th cylinder, or on the m-th turn of spiral, l – a wavelength, ρ, φ and z – radial, circular and longitudinal coordinate of observing point. Values $\rho_{mn\nu}$, $\varphi_{mn\nu}$ and $z_{mn\nu}$ generally present the cylindrical components of lattice vector, in special cases the number of interlinear indexes can be less.

Let's perform the analysis of spectral dependence of scattered intensity and its spatial distribution by the direct numerical calculation of all lattice sums, having place in (1). We shall take cylindrical components of the radial lattice in the form, corresponding to cylindrical analogue of a body-centered bulk crystal:

$$\begin{cases} r_{m+1}\approx r_m+\frac{1}{2}\sqrt{3d^2-\left(\frac{2p\,r_m}{n_B}\right)^2} \\ j_{mn}=e_m+\frac{2p}{n_B}n \\ z_{mn}=na+\Delta z_m=na+\left[1-(-1)^m\right]\frac{a}{4} \end{cases} \qquad e_m=\left[1-(-1)^m\right]\frac{p}{2n_B} \quad (2)$$

where d – diameter of atom, n_B – quantity of atoms on an internal circle, other designations correspond to layer structures [1]. By default for calculations the following values of lattice parameters were used: $a = 5$ Å, $d = 7$ Å, $b = 2\pi d/g$, $g = 5$, $\Delta z = a/13$; besides in radial lattices: $d = a$, $r_0 = n_B d/2\pi$.

2. The Spectral Dependence of Diffraction Intensity

The mathematical analysis of amplitude (1) for non-chiral lattice has shown [3], that corresponding intensity should have essential increase at

$$l = \frac{2a}{h}, \quad h = 1; 2; 3;\ldots \tag{3}$$

where a – lattice parameter in direction of the nanotube's axis. We shall name such wavelengths "characteristic".

In Fig. 1 the spectral dependences of scattered intensity in the center of nanotube by h as continuous variable (its integer values number the characteristic wave modes according to (3)), calculated from (1) are presented. In Fig. 2 a comparison of spectral characteristics of non-chiral and radial lattices, where argument is a wavelength of radiation, is shown.

The most essential feature of these spectral characteristics is the presence of sharp splashes of intensity on a nanotube's axis at the integer values of h that is at characteristic wavelengths. Maxima in these points have been theoretically predicted for a non-chiral lattice, but they also take place in spiral and radial cases and absent – in the chiral one. Comparison of curves shows, that relative intensity of splashes increases in a line: the chiral, spiral, non-chiral and radial lattice, and that intensity of splashes in the first case is equal to zero, and in the last one – is especially great. It is interesting, that the general monotonous rise of background intensity with increasing λ is the same for all lattices.

This distinction in scattering by chiral and non-chiral lattices is of fundamental type and has analogy in various character of Fraunhofer diffraction regarding these structures [4, 5]. It is a question of so-called "pseudo-orthogonality effect" [4], which means formation, side by side with the full set of reflexes from a cylindrical lattice, the narrow and intensive additional maxima in the positions, corresponding to reflexes $h00$ of orthogonal polytypes at the total absence of their other reflexes. The pseudo-orthogonality effect is peculiar to non-chiral cylindrical structures, somewhat – to spiral and is completely absent for chiral cylindrical structures.

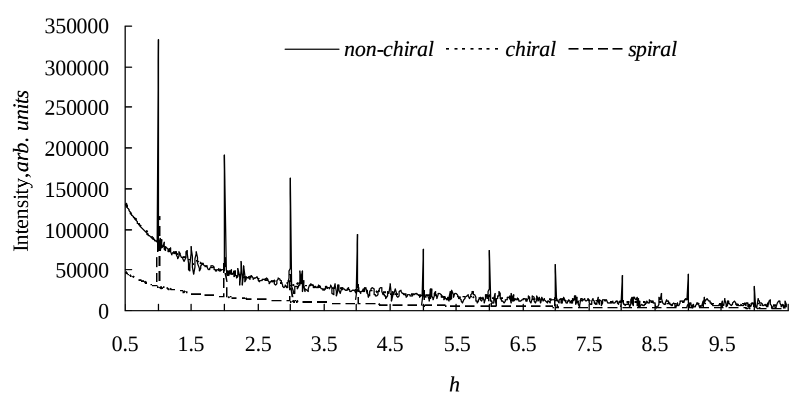

Fig. 1. Spectral dependences of intensity, diffracted by different lattices in the point $\rho = 0$, $\varphi = 0$, $z = 0$

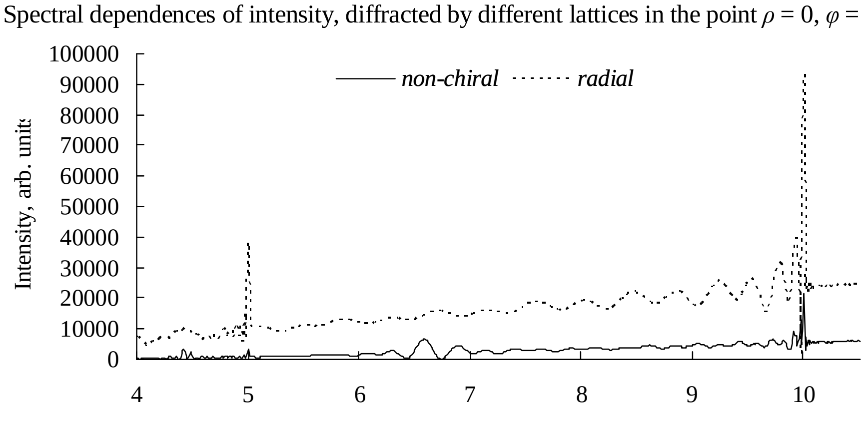

Fig. 2. Spectral dependences of intensity, diffracted by non-chiral and radial lattices in the point $\rho = 0$, $\varphi = 0$, $z = 0$

When $\lambda\to\infty$ ($h\to0$) the scattered waves in amplitude (1) lose the phase difference and the corresponding intensity turns into the sum of inverse values of squares of distances up to all sites of a lattice. In Fig. 1 this corresponds to continuous rise of intensity at $h\to0$. This computing effect is connected with inadequacy of the diffraction mathematical theory outside a range of the possible diffraction phenomena.

3. The Longitudinal and Cross-Section Distributions of Diffraction Intensity

In Fig. 3 the profiles of diffraction by a non-chiral lattice along z and at various values of a number of a wave mode h are presented. It is clear visible, that when h increases an appreciable reduction of intensity takes place and that the longitudinal intensity distribution has a harmonious character. In Fig. 4 the profiles of diffraction by orthogonal (*Or*) and monoclinic (*M*) polytypes of a non-chiral lattice along z within the unit cell at $h = 1$ are presented. The profile from a chiral lattice differs from non-chiral and spiral cases. In fact it is a constant that, in combination with a kind of spectral functions in Fig. 1, allows speaking about rather various character of longitudinal propagation of waves through chiral and non-chiral nanotubes.

In Fig. 5 the radial profiles of diffraction by various lattices at $h = 1$ are presented. It is obvious, that diffracted intensity concentrates both in an internal cavity of a nanotube, and in its structure, practically not spreading for its limits in a radial direction. The basic maxima of intensity from non-chiral and spiral lattices are located on the nanotube's axis (axial maximum) while in a case of chiral lattice the unique maximum is by the average radius of the lattice (additional maximum). Summarizing results, presented in Figs. 3 and 4, it is possible to make conclusion, that intensity, scattered by the non-chiral or spiral lattice, concentrates in the form of standing wave both on the axis of the nanotube, and by its average radius. In a chiral case almost all intensity is concentrated within the lattice, where the standing wave also takes place.

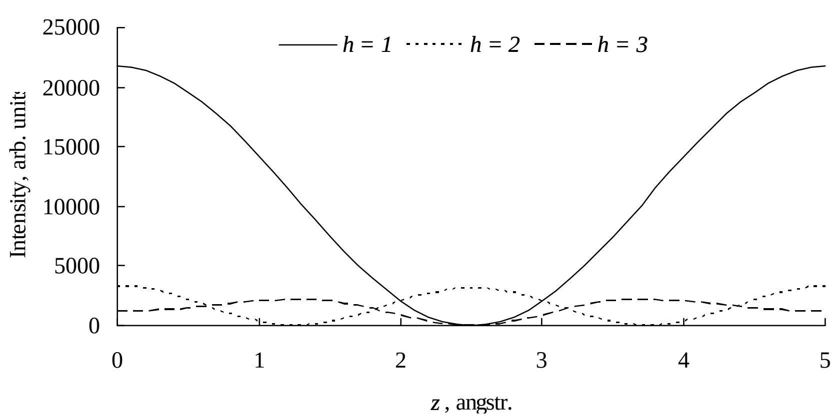

Fig. 3. Profiles of intensity from a non-chiral lattice at $z = 0 \div a$, $\rho = 0$, $\varphi = 0$

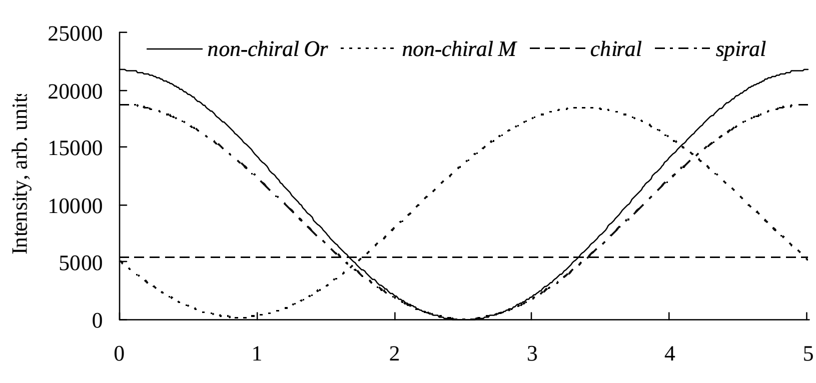

Fig. 4. Profiles of intensity from different lattices at $h = 1$ and $z = 0 \div a$, $\rho = 0$, $\varphi = 0$

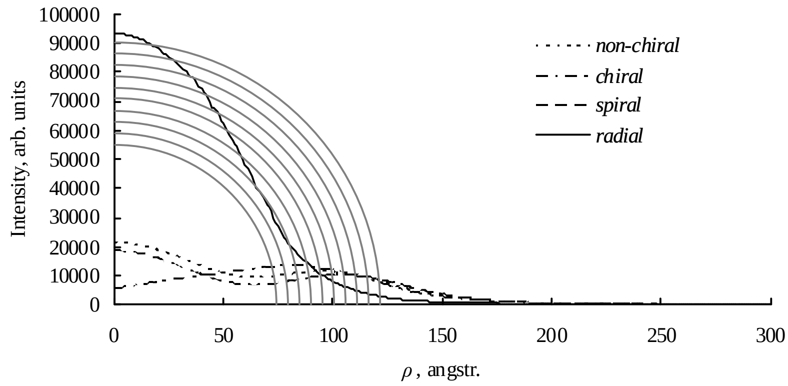

Fig. 5. Radial distribution of intensity, diffracted in the hole of various nanotubes at $h = 1$, $z = 0$, $\varphi = 0$ (nanotube's layers are drawn by grey lines)

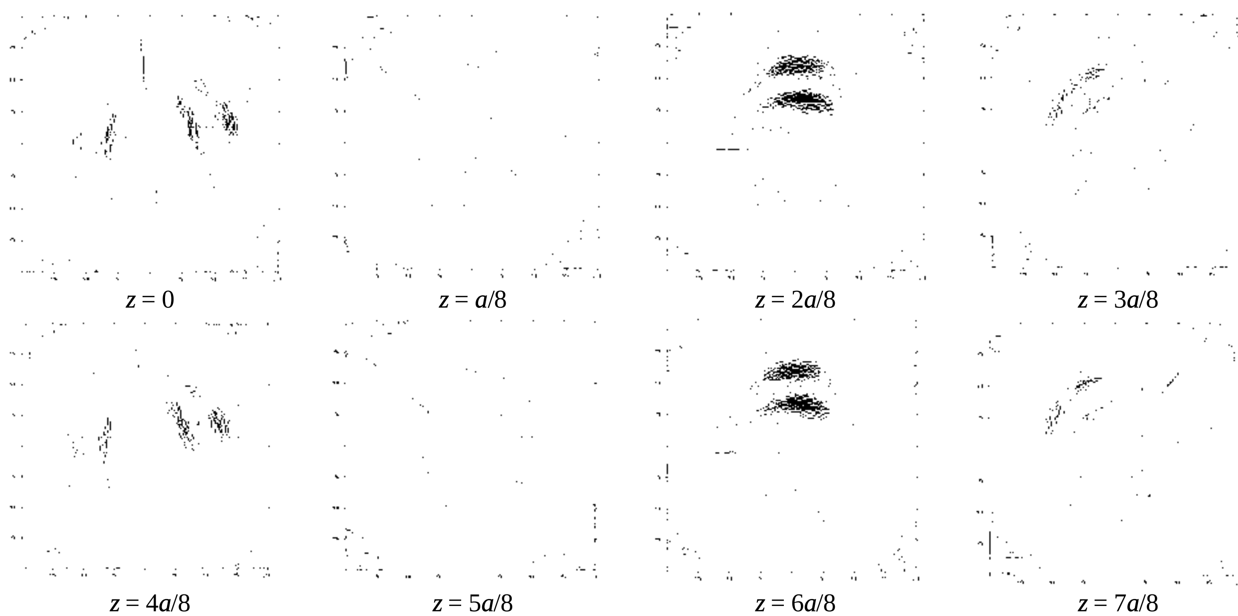

Fig. 6. Distributions of diffraction intensity in the cross-sections of chiral lattice at $h = 2$ and various values of z

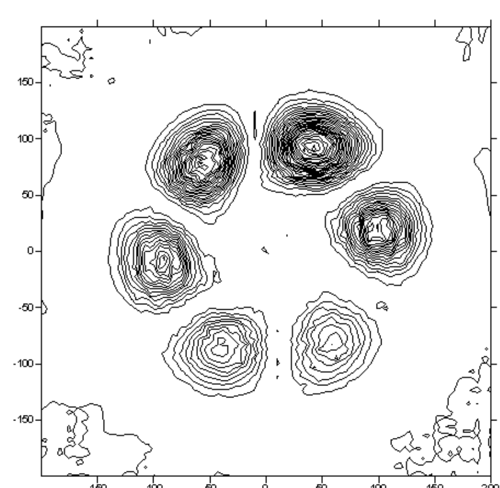

Fig. 7. Distribution of diffraction intensity in cross-section of the chiral lattice at $h = 6$, $z = 0$

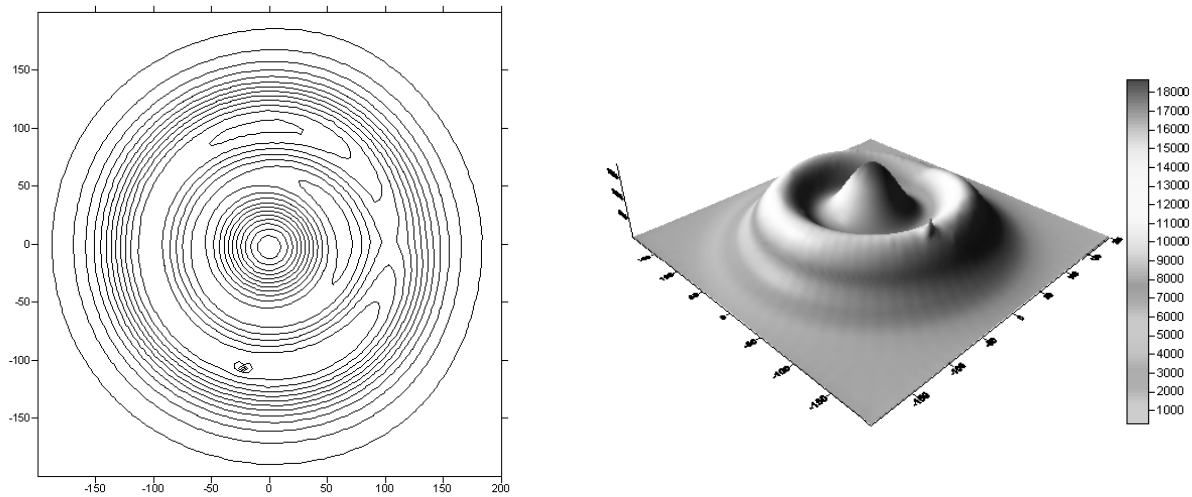

Fig. 8. Distribution of diffraction intensity in cross-section of the spiral lattice at $h = 1$, $z = 0$

In Fig. 6 the distributions of diffraction intensity in a cross-section of the chiral lattice, calculated at $h = 2$ and values of z, changing within the limits 0–a with the step $a/8$, are presented. It is obvious, that the geometrical place of intensity maxima is the h-fold helical line with the step a. A case $h = 6$ in Fig. 7 confirms this.

The distribution of intensity in the cross-section of a spiral lattice is presented in Fig. 8 for $h = 1$. The shape of distribution means that the case of a spiral lattice differs from a non-chiral one only in the quantitative aspect.

4. Conclusions

The analysis of intensity distribution of short-wave radiation's Fresnel diffraction in a hole of various type nanotube's lattices, performed by direct numerical calculation, has shown, that at longitudinal propagation of radiation and under diffraction condition (3) the radiation concentrates with forming the standing wave: in a case of radial lattice – on the axis of nanotube, in non-chiral and spiral cases – on the axis of nanotube and by its average radius. In a case of chiral nanotube radiation concentrates by the h-fold helical line with the radius, equal to average radius of lattice, and the step, equal to longitudinal parameter a, where h is the number of characteristic wave mode. The degree of concentration of diffraction intensity on the tube's axis is maximal for radial lattice and minimal for a chiral one, for non-chiral and spiral lattices it has an intermediate character. In a case of radial lattice practically all scattered radiation concentrates in an internal hole of nanotube.

This phenomenon can have various areas of practical application. Concentration of X-ray radiation in the certain area of nanotube can be used for determination of chemical composition of that area by a secondary X-ray spectrum. It is possible to realize the so-called "star detectors" in X-ray range on the basis of non-chiral, spiral and radial lattices. The estimation of the angular selectivity of such a system gives value $\sim 10^{-8}$ radian, thus the detector can be rather compact and have greater relative aperture in case of using the natural parallel blocks of chrysotile nanotubes.

It is possible to approve, that in the case of longitudinal propagation of charged particles, for example electrons, through nanotube's hole the discussed phenomena will take place side by side with the effects, connected with the behavior of electron in a cylindrical potential well. In this case the electron, having the wavelength (3) and scattered in an internal hole of non-chiral, spiral or radial nanotube, should form a longitudinal standing wave in vacuum of the hole. This effect can explain the known phenomenon of quantum conductivity, observed for carbon nanotubes.

The discussed phenomenon has the obvious analogy with the area of waveguide effects. Not concerning the terminological part of a question, authors, on the basis of obtained results, assume, that in nanotubes (excepting the chiral ones) it is possible to realize the longitudinal propagation of radiation with characteristic wavelength (3) regardless to the physical nature of particles (X-ray quantum, fundamental particles with nonzero rest mass, atoms).

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РОЗПОДІЛ КОРОТКОХВИЛЬОВОГО ВИПРОМІНЕННЯ У ВНУТРІШНІЙ ПОРОЖНИНІ НАНОТРУБОК

Анотація. *Розраховані спектральні залежності і розподіл інтенсивності дифракції короткохвильового випромінювання (рентгенівські кванти, частинки відповідної енергії) на ахіральній, хіральній, спіральній та радіальній решітках у внутрішній порожнині нанотрубки. Показане суттєве збільшення інтенсивності, дифрагованої деякими видами нанотрубок, при характеристичних довжинах хвиль. Визначено відмінності і аномальний характер проходження випромінювання внутрішньою порожниною нанотрубки.*

Ключові слова: *нанотрубка, короткохвильове випромінення, внутрішня порожнина, спектральна залежність.*