COLLOQUIA: Channeling 2010

# Simulation of axial channeling radiation on a thin Ge single crystal

B. AZADEGAN(¹), S. B. DABAGOV(²)(³) and W. WAGNER(⁴)(*)

(¹)  *Sabzevar Tarbiat Moallem University - Sabzevar, Iran*
(²)  *INFN, Laboratori Nazionali di Frascati - Via E. Fermi 40, 00044 Frascati (RM), Italy*
(³)  *RAS - P.N. Lebedev Physical Institute - Leninsky Pr. 53, 119991 Moscow, Russia*
(⁴)  *Helmholz-Zentrum Dresden-Rossendorf - POB 510119, 01314 Dresden, Germany*

**Summary.** — Based on classical electrodynamics the radiation emitted by axially channeled electrons has been investigated by means of computer simulations. Using the Doyle-Turner approximation for the atomic scattering factor and taking thermal vibrations of atoms into account, we calculated the two-dimensional continuum potential of the $\langle 110 \rangle$ crystallographic axis of a thin Ge single crystal. The trajectories, velocities and accelerations of electrons are obtained by solving the equations of motion in three dimensions, and the spectral-angular distribution of radiation has been calculated within classical approach.

PACS `61.80.Fe` – Electron and positron radiation effects.
PACS `61.85.+p` – Channeling phenomena (blocking, energy loss, etc.).

## 1. – Introduction

The physics of channeling radiation (CR) has been developed by many authors (see, *e.g.* [1-4]). While the one-dimensional problem of planar CR is well understood, the two-dimensional nature of axial channeling leads to more complicate phenomena. In quantum-mechanical treatment, the channeled charged particle is considered to be bound in the transverse electrostatic potential of the crystal axis or plane, and CR is emitted due to spontaneous transitions between eigenstates of this potential. The classical model considers channeling as coherent scattering by the crystal atoms ordered in strings and planes, what enforces an oscillatory motion of channeled particles along the corresponding string or plane. Since this oscillatory motion is an accelerated one in the rest frame of the channeled particle, it emits electromagnetic CR.

In case of planar channeling at energies of tens of MeV, the number of bound states is usually low, and calculations by means of the so-called many-beam formalism describe

                                                                            149

the experimental results rather accurately. Axial channeling at such energies, however, is characterized by a relatively large number of quantum states of transverse motion. Therefore, a classical approximation is appropriate and less complicate as well.

The present paper deals with the calculation of the two-dimensional continuous potential of $\langle 110 \rangle$ crystallographic axis of a Ge single crystal using a Doyle-Turner approximation with taking the thermal vibrations of the crystal atoms into account. The trajectories, velocities and accelerations of axially channeled electrons are obtained by solving the equations for a 3D motion. In the framework of classical electrodynamics, spectral-angular distributions of CR are obtained from Fourier transforms of real trajectories, velocities and accelerations of the particles within the 3D crystal.

## 2. – Theory

Former computer simulations of CR from axially channeled electrons based on the binary-collision approximation and classical electrodynamics [5, 6]. The electron trajectories were assumed to be spiral windings around an atomic string. Then the equations of motion in the transverse plane read

$$(1) \qquad \frac{m}{2}\dot{\rho}^2 + w(\rho) = E_\perp, \qquad m\dot{\phi}\rho^2 = L_z,$$

where $\rho$ and $\phi$ are the polar coordinates of the particle with respect to the atomic string, $m$ is the relativistic mass, $E_\perp$ is the transverse energy, $L_z$ is the angular momentum, $w(\rho)$ is the effective potential

$$(2) \qquad w(\rho) = u(\rho) + \frac{L_z^2}{2m\rho^2},$$

and $u(\rho)$ is the continuous potential of the atomic string (axis). Refering to [7], in first approximation it may be written

$$(3) \qquad u(\rho) = \frac{1}{d} \int_{-d/2}^{d/2} V(\sqrt{\rho^2 + z^2})\mathrm{d}z,$$

where $V$ is the potential of interaction of the particle with a crystal atom, $d$ is the spacing of atoms in the row, and the $z$-axis is directed along the atomic string. The transverse energy and angular momentum determined at the crystal entrance read

$$(4) \qquad E_\perp = u(\rho_{in}) + \frac{p_{\perp in}^2}{2m}, \qquad L_z = p_{\perp in}\rho_{in},$$

where $p_{\perp in}$ and $\rho_{in}$ are the initial transverse momentum and the radius vector of the entrance point. In this model, the continuous potential is approximated by a term $u(\rho) \propto 1/\rho$.

Since the longitudinal component of the velocity of relativistic electrons approaches the speed of light, a crystallografic plane may assumed to be charged continuously. In the axial continuum model, taking the direction $\hat{z}$ along the channeling axis, the relativistic equations of motion read

$$(5) \qquad \gamma m\ddot{x} = -\frac{\partial U(x,y)}{\partial x}, \qquad \gamma m\ddot{y} = -\frac{\partial U(x,y)}{\partial y}, \qquad \gamma m\ddot{z} = 0,$$

where $\vec{r}_\perp = x\hat{x} + y\hat{y}$ and $z$ are the transversal and longitudinal coordinates, respectively, of the instantaneous particle position $\vec{r} = \vec{r}_\perp + z\hat{z}$, $\gamma$ is the Lorentz factor, $m$ is the rest mass of the electron, and $U(x, y)$ is the continuous potential. The initial conditions are: point of incidence $\vec{r}_{\perp 0} = x_0\hat{x} + y_0\hat{y}$, transverse momentum $\vec{p}_\perp = \gamma m(\dot{x}_0\hat{x} + \dot{y}_0\hat{y})$ with $|\vec{p}_\perp| = p\theta_0$ and $\theta_0$ being the angle of incidence with respect to the axis. The transverse energy is defined by

$$(6) \qquad E_\perp = \frac{1}{2}\gamma m(\dot{x}^2 + \dot{y}^2) + U(x_0, y_0) = \frac{p_\perp^2}{2\gamma m} + U(x_0, y_0).$$

The expansion of the periodic potential into a Fourier series represents the most general form of the continuous potential. It reads

$$(7) \qquad U(x, y) = \sum \nu_{\vec{g}_m} e^{i\vec{g}_m \vec{r}_\perp},$$

where the sum is taken over all reciprocal lattice vectors $\vec{g}_m$ normal to $\hat{z}$. Using the Doyle-Turner approach [8] for the electron-atom interaction, the Fourier coefficients $\nu_{\vec{g}_m}$ may be written [9]

$$(8) \qquad \nu_{\vec{g}_m} = -\frac{2\pi a_0^2}{V_c}\frac{e^2}{a_0}\sum a_i \exp\left[-\frac{1}{4}\left(\frac{b_i}{4\pi^2} + 2\rho_{th}^2\right)|\vec{g}_m|^2\right], \quad i = 1, 2, 3, 4,$$

where $V_c$ is the volume of unit cell, $a_0$ is the Bohr radius, $e$ is the electron charge, $a_i$ and $b_i$ are tabulated coefficients [8], and $\rho_{th}$ is the one-dimensional thermal vibration amplitude. The accuracy and convergence of the potential depends on the number of reciprocal lattice vectors normal to the axis considered.

Classical electrodynamics can be applied to calculate the CR spectrum, if the energy of emitted photons is small compared to the primary electron energy. Then the spectral-angular distribution of CR has the following form [3]:

$$(9) \qquad \frac{d^2 E}{d\omega d\Omega} = \frac{e^2}{4\pi^2 c}\left|\int_0^\tau e^{i(\omega t - \vec{k}\cdot\vec{r})}\frac{\vec{n}\times\left((\vec{n} - \vec{\beta})\times\vec{\dot{\beta}}\right)}{(1 - \vec{\beta}\cdot\vec{n})^2}dt\right|^2,$$

where $c\vec{\beta} = \dot{\vec{r}}(t)$ is the velocity of the particle, $\vec{r}(t) = \vec{v}_z t + \vec{r}_\perp(t)$ is its trajectory, $\vec{k} = \omega\vec{n}/c$ is the wave vector, $\vec{n}$ is the unit vector defining the direction of photon emission, and $\tau$ is the time the particle needs to pass through the crystal. In order to obtain the CR spectrum, one only has to substitute into eq. (9) the trajectories, velocities and accelerations of the electrons which may be obtained by solving eq. (5) numerically. Since in a real experiment, a large number of particles enters the crystal at different points of incidence, the total CR spectrum represents an average of the spectral-angular distribution of radiation over all possible trajectories, *i.e.*, over all points of incidence.

## 3. – Results of calculation

The present paper considers channeling of electrons of energy 119 MeV along the $\langle 110 \rangle$ crystallographic axis of a $1\,\mu$m thick Ge single crystal. The continuous potential viewed in this direction is shown in fig. 1. It is composed of two families of minima.
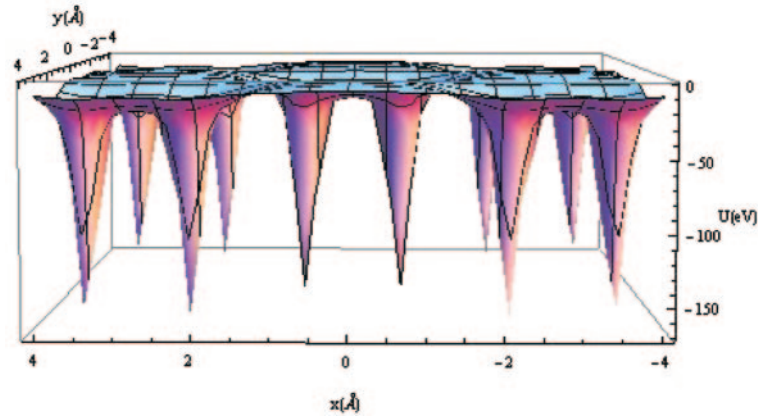
Fig. 1. – Three-dimensional continuous potential in direction of the $\langle 110 \rangle$ crystallographic axis of a Ge single crystal.

The spiraling motion of electrons entering the Ge crystal at different points of incidence and channeling around the $\langle 110 \rangle$ axis can be seen in fig. 2. An example of transverse trajectories, *i.e.*, of the functions $x(t)$ and $y(t)$, for given initial conditions is displayed in fig. 3.

The scatter plots presented in fig. 4 demonstrate the evolution of the angular distribution of the electrons during their passage through a $10\,\mu$m thick Ge crystal along two atomic strings of the $\langle 110 \rangle$ axis.

The CR photon spectra emitted by the channeled electrons are strongly determined by the angular momenta characterizing their trajectories. To illustrate this fact, two-dimensional projections of the trajectories of channeled electrons are faced with the associated photon spectra. If the electron trajectory is associated with a small angular momentum, as demonstrated in fig. 5, the electron is deeply trapped within the axial potential and performs a rosette-like motion. The corresponding photon spectrum consists of two sharp and relatively intense peaks at dedicated energies. The case of medium angular momentum is shown in fig. 6. Here the electron is successively scattered down into the potential of a major axis, and, consequently, the emitted photon spectrum has many peaks. The opposite case of large angular momentum in demonstrated in fig. 7. The CR spectrum of such electrons is characterized by a broad and smooth distribution.

Since channeling may occur as for different points of incidence of the electrons into the crystal as for a finite interval of angular momenta, the resulting spectrum of axial CR may be simulated as an average over a sufficiently large number of different electron trajectories (see fig. 8).

## 4. – Conclusions

Instead of the binary collision approximation adopted in previous works, the calculation of the spectral-angular distribution of axial channeling radiation presented in this paper is based upon the Doyle-Turner formalism and an expansion of the real two-dimensional continuous potential of the $\langle 110 \rangle$ axis of a thin Ge single crystal into a Fourier series. The trajectories, velocities and accelerations of electrons channeled along this axis have been obtained from numerical solutions of the equations of motion in three
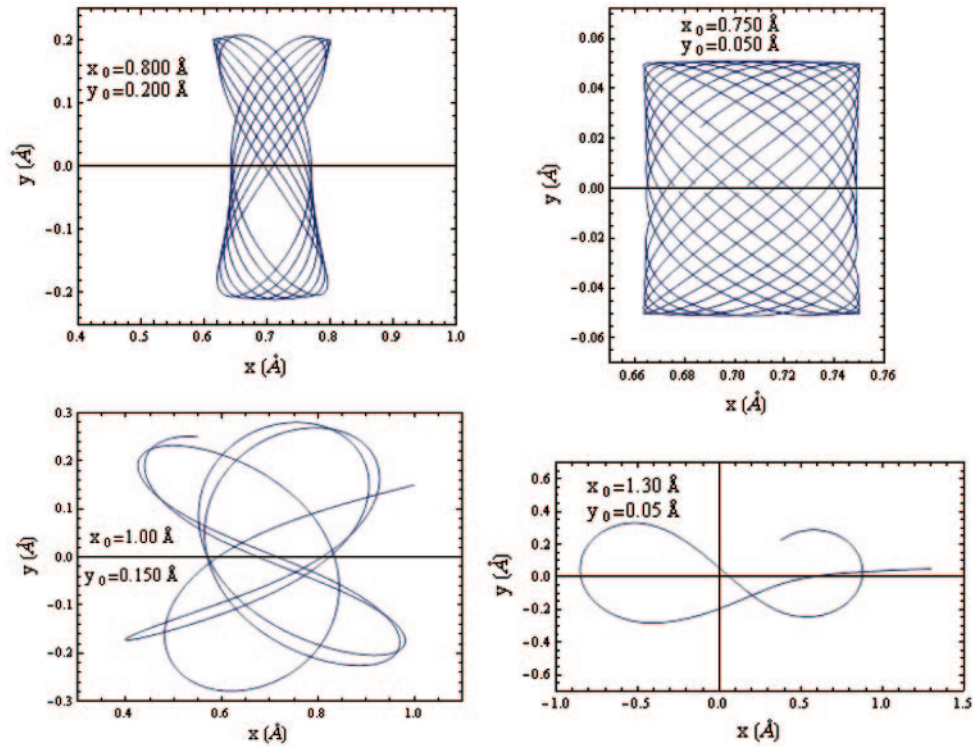
Fig. 2. – Parametric plots of trajectories of channeled electrons for different points of incidence into a $1\,\mu$m thick Ge crystal.

dimensions. Classical electrodynamics has been used to simulate the forward-directed radiation from axially channeled electrons of energy 119 MeV. Typical spectral distributions of radiation contributions, which result from different types of electron trajectories, are separately examined. The applied method is well suited for simulations of axial channeling radiation spectra for moderate energies of channeled electrons and positrons.
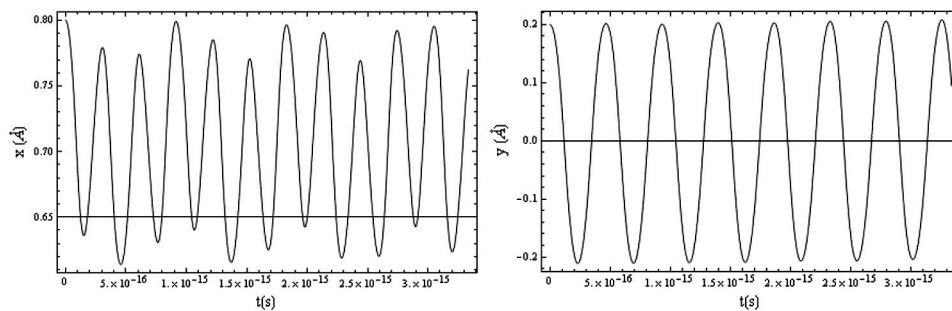


Fig. 3. – Transverse trajectories $x(t)$ and $y(t)$ of channeled electrons entering the crystal at $x_0 = 0.8\,$Å, $y_0 = 0.2\,$Å.
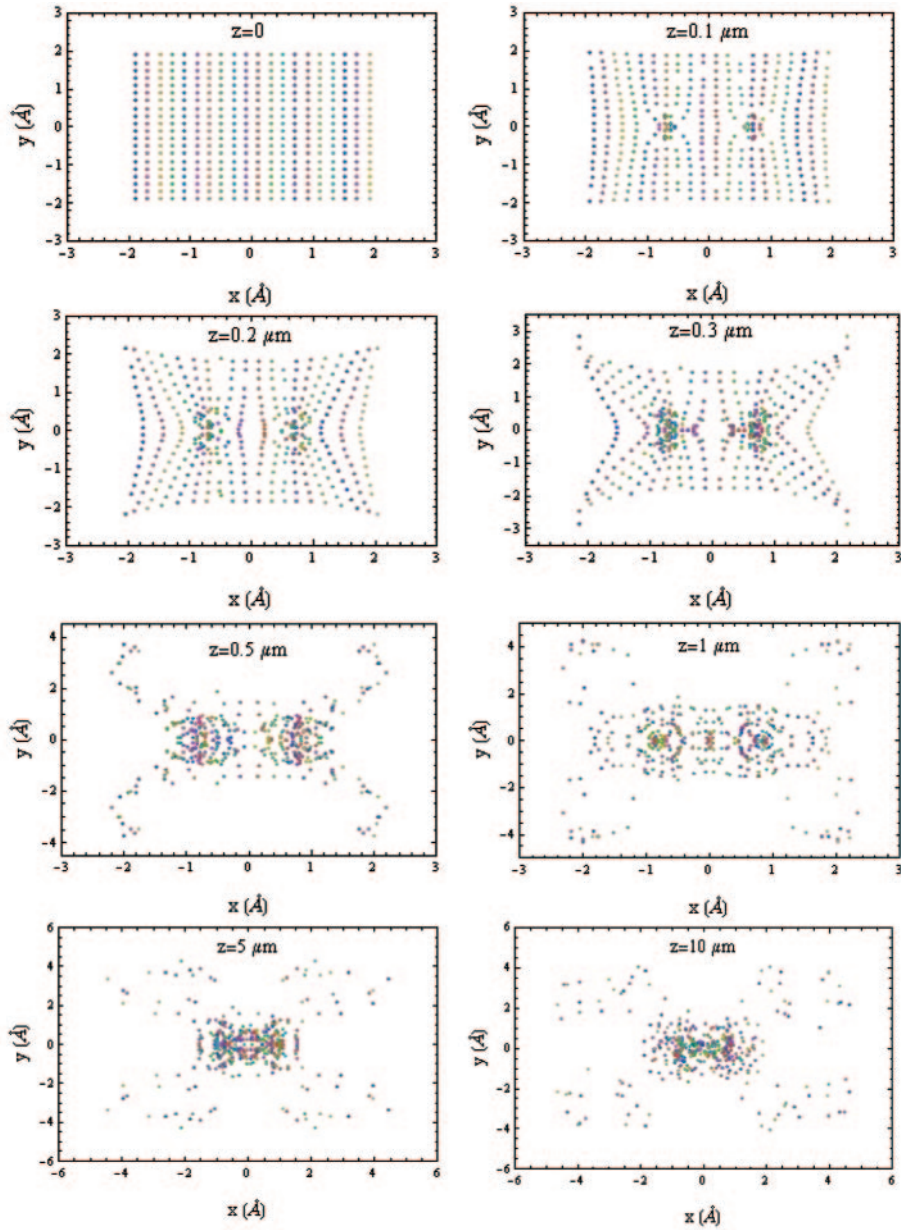
Fig. 4. – Evolution of the angular distribution of axially channeled electrons on their path through a $10\,\mu$m thick Ge crystal.
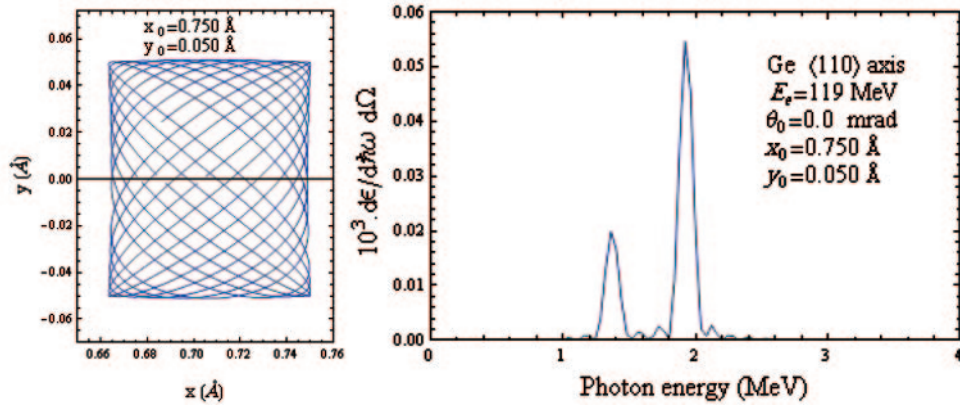
Fig. 5. – Electron trajectory and associated CR intensity spectrum of forward-emitted photons by electrons of energy 119 MeV at small angular momentum.
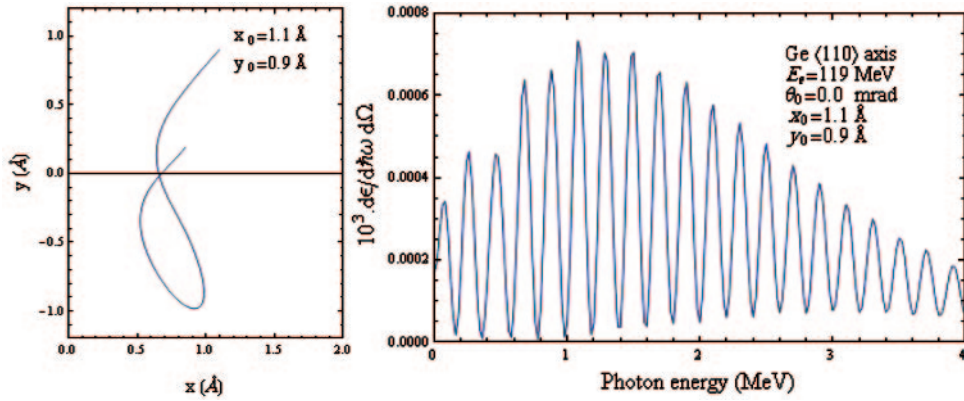


Fig. 6. – Electron trajectory and associated CR intensity spectrum of forward-emitted photons by electrons of energy 119 MeV at medium angular momentum.
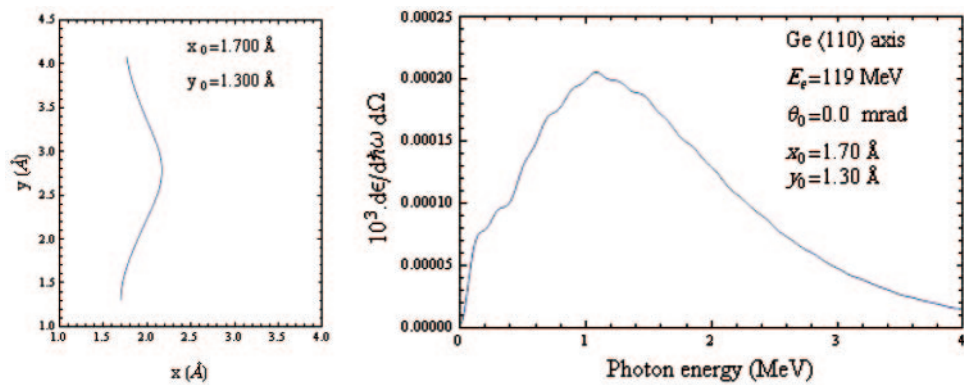


Fig. 7. – Electron trajectory and associated CR intensity spectrum of forward-emitted photons by electrons of energy 119 MeV at large angular momentum.
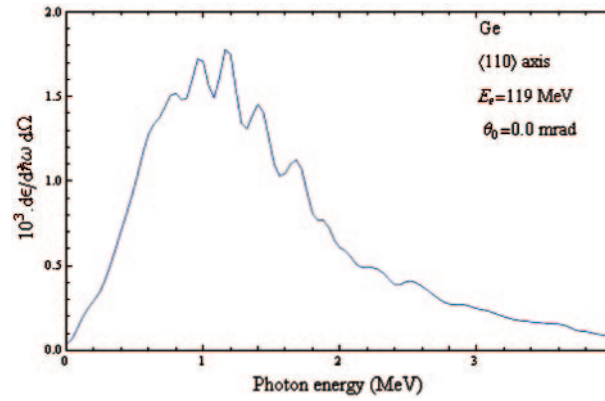
Fig. 8. – Spectral-angular distribution of axial CR from electrons of energy 119 MeV channeled along the $\langle 110 \rangle$ axis of a $1\,\mu$m thick Ge crystal.

REFERENCES

[1]  ANDERSEN J. U. and LAEGSGAARD E., *Phys. Rev. Lett.*, **44** (1980) 1079.
[2]  ANDERSEN J. U., BONDERUP E., LAEGSGAARD E. and SOERENSEN A. H., *Phys. Scr.*, **28** (1983) 308.
[3]  KUMAKHOV M. A. and WEDELL R., *Radiation of Relativistic Light Particles during Interaction with Single Crystals* (Spektrum Akademischer Verlag, Heidelberg) 1991.
[4]  DABAGOV S. B. and ZHEVAGO N. K., *Riv. Nuovo Cimento*, **31** (2008) 491.
[5]  YAMAMURA Y. and OHTSUKI Y. H., *Phys. Rev. B*, **24** (1981) 3430.
[6]  OHTSUKI Y. H. and YAMAMURA Y., *Phys. Rev. B*, **28** (1983) 3718.
[7]  LINDHARD J., *K. Dan. Vidensk. Selsk., Mat. Fys. Medd.*, **14** (1965) 34.
[8]  DOYLE P. A. and TURNER P. S., *Acta Crystallogr., Sect. A*, **24** (1968) 390.
[9]  AZADEGAN B., WAGNER W. and PAWELKE J., *Phys. Rev. B*, **74** (2006) 045209.