ECHARM - A SOFTWARE FOR CALCULATION OF PHYSICAL QUANTITIES OF INTEREST IN COHERENT INTERACTION OF RELATIVISTIC PARTICLES WITH CRYSTALS

E. Bagli, INFN, Ferrara, Italy

V. Guidi, Università di Ferrara and INFN, Ferrara, Italy

V. Maisheev, IHEP, Protvino, Russia

Abstract

We present an analytical model to calculate the physical quantities of interest experienced by relativistic particles in their motion aligned with periodic complex atomic structure. Classical physics equations and the expansion of periodic functions as a Fourier series have been used for the calculation. This method allows to calculate the contribution from all the planes and axes inside the crystal, in contrast to other simulation codes for which the motion is evaluated only on nearest neighbors atomic strings. Based on the calculation technique we have developed the "ECHARM" program, which allows to calculate one- and two- dimensional averaged physical quantities of interest. The calculation holds for the main axes of any orthorhombic and tetragonal structures and for any orientation in the cubic structure. To underline the capability of the program, complex structures such as zeolites have been worked out. Based on the "ECHARM" code, simulation of the relativistic particle motion within complex structures has been developed. With this code it is possible to simulate the motion in bent crystal to study planar and axial channeling volume reflection.

INTRODUCTION

In the last decades interaction of particles with matter was a widely explored area. Particular attention have to be paid to particle interaction with aligned matter, such as crystals: indeed, new effects have been studied, spanning from plasma etching [1] and plasma surface interaction in nuclear fusion facilities [2] to emission of many types of coherent radiation [3] and particle steering in bent crystals [4-6] via either channeling or volume reflection [7,8]. For most experiments and applications, especially those pertaining to radiation emission and particle steering, silicon has been the base material because of the high perfection and ease of availability of currently produced monocrystals as wafers or ingots. Indeed, experiments have been made with other monocrystalline materials, such as Ge [9] and W [10]. In the last year new experiment with lithium niobate crystal was made. Lithium niobato possess two peculiar characteristic which make it unique, it could be produced with high crystalline quality and it is a piezoelectric material. As an example of application it could emulate the action of a synchrotron magnet on a charged beam, due to the modifying of its bending radius via electric signal. The discovery of novel effects is strongly related to simulate the behavior of charged particles motion. First simulation step is the evaluation of crystal potential and related quantities. For cubic and orthorhombic structures, a program based on their Fourier expansion has been developed [11]. In this paper we propose the extension of the calculation program to any structure under the planar condition for the main planes and the calculation results for three crystals, i.e. silicon, boggsite and lithium niobate.
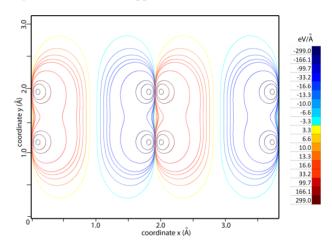

Figure 1: x-component of the electric field in the axial case along the [112] axis for a Si crystal at T=297 K.

CALCULATION METHOD

Lindhard [12] showed that the motion of relativistic charged particles under channeling condition is well approximated with classical physics equations. A traditional approach for the calculation of the potential felt by the particles relies on the analytical representation of the screened Coulomb potential [13]. Another more flexible approach is based on the expansion in Fourier series of the potential and the related quantities of interest. This method allows one to determine averaged one- and two-dimensional potential. First we briefly review of the calculation method of the "ECHARM" program, based on the Fourier expansion. Secondly we show the simplification adopted to evaluate the physical quantities of interest under the channeling condition in the planes for any crystal.

General Case

Crystals are solid materials with atoms arranged in periodic structures. To study the potential and related quantities inside a crystal we can treat it as an infinitely periodic structure. As a consequence, we expand the crystal potential as a Fourier series and we integrate over the whole space

$$\varphi(\mathbf{r}) = \frac{4\pi e}{\Delta} \sum_{g\neq 0} \sum_{l=1}^{N} Z_l S(Z_l, \mathbf{g}) \frac{[1-F(Z_l,g)]}{g^2} e^{-i\mathbf{g}\cdot\mathbf{r}} \quad (1)$$

where $S(Z_l, \mathbf{g})$, Z_l, $F(Z_l,g)$ are structure factors, atomic numbers and atomic form factors; $\mathbf{r_{j,l}}$ and N_l are the corresponding coordinates and number of atoms of the l--th species; $\mathbf{g}$ is the reciprocal vector and Δ is the volume of the primitive cell.

Eq 1. Represent the potential of an ideal structure, but for our purpose a fundamental role is played by thermal vibrations: as a consequence we approximate the potential by averaging over time and spatial isotropic and independent fluctuations as suggested in the literature. Our method does not consideration the delocalization of electrons among neighbouring atoms, because there is no need for a more precise description of the potential for relativistic particles. To evaluate the atom vibration displacement we take the assumption that the amplitudes are the same for each atom of a given species. Under this assumption we obtain the three-dimensional potential averaged over thermal fluctuations:

$$\varphi(\mathbf{r}) = \frac{4\pi e}{\Delta} \sum_{g\neq 0} \frac{\langle Y(\mathbf{g})\rangle}{g^2} e^{-i\mathbf{g}\cdot\mathbf{r}} \quad (2)$$

where

$$\langle Y(\mathbf{g})\rangle = \sum_{l=1}^{N} Z_l S(Z_l, \mathbf{g})[1-F(Z_l,g)]e^{-\frac{A_l g^2}{2}}$$

Planar Potential for the Main Planes

The classical ideal of interaction of particles with ordered media is that a particle does not feel the scattering kick of an individual atom, but many small-angle scatterings by a plane or a row of atoms. Under this condition the potential could be treat as continuous, i.e. the continuous potential approximation.

When a particle hits a crystal parallel to a crystal plane, we can replace the analytic potential by a potential averaged over a direction parallel to the crystal planes:

$$\varphi_p(x) = \frac{1}{S_p} \iint_0^{S_p} \varphi(x,y,z)\,dy\,dz \quad (3)$$

Substituting Eq. (2) into Eq. (3) and using the crystal system coordinates we obtain for the (100) plane:

$$\varphi_p(x') = \frac{1}{S_p} \iint_0^{S_p} \frac{4\pi e}{\Delta} \sum_{\mathbf{g}\neq 0} \frac{\langle Y(\mathbf{g})\rangle}{g^2} e^{-i\mathbf{g}\cdot(x\mathbf{e_1}+y\mathbf{e_2}+z\mathbf{e_3})}\,dy'\,dz'$$

Where $\mathbf{e_i}$ are the base vectors. As a result we reach the equation for the potential averaged over the (100) plane, in which $\mathbf{r'} = \mathbf{r}$, :

$$\varphi_p(x) = \frac{4\pi e}{\Delta} \sum_{n_1} \frac{\langle Y(\mathbf{g})\rangle}{g^2} e^{-i\frac{2\pi}{a_1}n_1}$$

It is easy to reproduce this result for the (010) and the (001) planes.

CALCULATION EXAMPLES

Silicon

Silicon is the most used crystal for channeling experiment, because of the low number of imperfection in its structure and its low price in the global market. It shows diamond structure and it was test both in planar and axial case with positive and negative particles [8,14-16].

We determine the axial potential depths for [011] (U_0=152 eV) direction, which is in good agreement with the estimates in Ref. [3] (U_0=140 eV), and in fair agreement with Ref. [4] (U_0=114 eV. In Fig. 1 we show the axial [112] electric field both for x and y components to demonstrate the capability of the program.
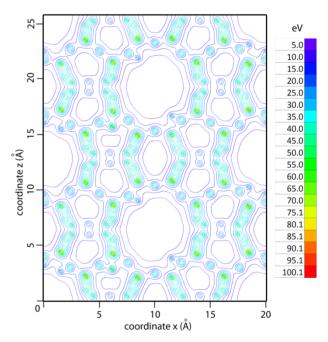

Figure 2: countour plot of potential averaged along [010] axis of the Boggsite at T=300 K.

Zeolites

Zeolites are alumina-silicate crystals, whose structure forms cavities filled with water and exchangeable cations [17]. Under some circumstances, neighboring cavities merge to form long channels, which are periodically repeated over the whole structure. These channels form a bundle of parallel nanotubes, which represent ideal structure for particle capture via axial channeling. Due to their complex framework a large zeolite assortment exists: among them we chose the Boggsite crystal, that hold broad channels, good thermal stability.

Boggsite owns orthorhombic lattice, with a base formed from Si, O and Al. We exposed Boggsite potential along the [010] axis in Fig. 2. The profile of the potential is very similar to the structure of the zeolite. It show s a field-free 14 eV deep channel, extending roughly 4.5 Å in diameter.

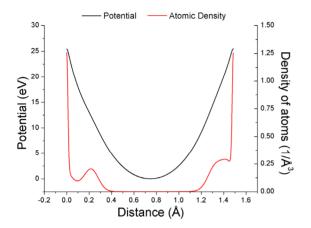The channel shaped out embodies a perfect arrangement for axial channeling.

Figure 3: calculation of potential and density of atoms between (010) planes in lithium niobate crystal at the room temperature (T= 300 K). The form factor used was the Moliere form factor.

Lithium Niobate

Lithium Niobate is a synthetic crystal which exhibits extraordinary characteristics, such as piezoelectricity, ferroelectricity and pyroelectricity [18]. Its possible usages spread out from acousto-optic filters to amplitude modulator.

Lithium niobate possess hexagonal structure. Its base is composed by one lithium atom, one niobato atom and three oxygen atoms. We use the extension of the ECHARM program to evaluate its potential along the major planar orientation.

In Fig. 3 we expose the potential, the electric field, the density of atoms and the density of electrons felt by a particle hitting the crystal parallel to the (010) plane. It is necessary to underline that, instead the depth of the

potential well (U_0=25.49 eV), the channeling efficiency in this peculiar crystal is affected by the multiple scattering. As a result this crystal appears a perfect aspirant to apply the volume reflection effect for charged particle beam deflection.

REFERENCES

[1] M. Sugawara, *Plasma Etching: Fundamentals and Applications.* New York : Oxford University Press Inc., 1998.

[2] Eliezer, Y. E. Shalom, *Plasma Physics and Fusion Energy.* Cambridge : Cambridge University Press, 2008.

[3] V. Baier, V. Katkov, and V. Strakhovenko, *Electromagnetic Processes at High Energies in Oriented Single Crystals.* Singapore : World, 1998.

[4] V. Biryukov, Y. Chesnekov, and V. Kotov, *Crystal Channeling and Its Applications at High-Energy Accelerators.* New York : Springer, 1996.

[5] V. I. Kuz'min, R. N. Vysotskii, Sov. Phys. Usp. 35 (1992) 725.

[6] U. I. Uggerhøj, Rev. Mod. Phys. 77 (2005) 1131.

[7] W. Scandale et al., Phys. Rev. Lett. 98 (2007) 154801.

[8] W. Scandale, Phys. Rev. Lett. 101 (2008) 164801.

[9] C. Biino et al., Phys. Lett. B. 403 (1997) 163.

[10] T. Suwada et al., Phys. Rev. ST Accel. Beams 10 (2007) 073501.

[11] E. Bagli, V. Guidi, V. Maisheev, Hysicla Review E 81 (2010) 026708.

[12] J. Lindhard, "Influence of crystal lattice on motion of energetic charged particles", Matematisk-fysiske meddelelser 34 (1965) 63.

[13] Gemmell, D. S. *Rev. Mod. Phys.* 1974, 46, p. 129.

[14] W. Scandale et al., Phys. Lett. B 680 (2009) 301.

[15] W. Scandale et al., Phys. Lett. B 681 (2009) 233.

[16] W. Scandale, Phys. Rev. ST Accel. Beams 11 (2008) 063501.

[17] G. Gottardi, *Natural Zeolites*, Berlin : Springer-Verlag, 1985.

[18] R. S. Weis, T. K. Gaylord, Applied Physics A: Materials Science & Processing 37 (1985) 191.