Electron exchange influence on the energy loss of ions in SIMOX structure

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Abstract

In this research report we analyse Rutherford back scattering (RBS) measurements with SIMOX structure and transmission experiments with Si single crystals by means of Monte Carlo simulation code with explicit implementation of impact parameter dependence of the electron transfer and the electronic energy loss processes. Although all the basic experimental characteristics of the ion channelling have been successively reproduced, effects related to the charge pre-equilibrium region turned out to be much smaller than these determined from experiment.

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1. Introduction

The electronic energy loss of ions channelled in single crystal has long been a theoretical and experimental problem with application consequences. The loss in the subsurface region is mainly determined by initial ion beam charge. It is clear that the electron exchange between ion and the target is a continuous process during the ion motion in the crystal and thus modifying the energy loss. Another important feature of ion beam interaction with crystals is dependence of elementary processes on impact parameter with respect to scattering centres. The simplest transmission experiments, which make use of channelling effect, require relatively thick crystals and thus high ion energy. At lower energy one can use RBS geometry with large angle scattering and single crystals formed in SIMOX structure. In the latter case the extraction of information about fundamental process of the energy transfer is more cumbersome Czerbniak et al. (2002). The hypothesis on

\begin{equation}
\frac{\partial\sigma}{\partial R} \propto Z^2
\end{equation}

anomalies in stopping power Bridwell et al. (1986) or back-scattering yield Schiedeskamp et al. (1986) due to pre-equilibrium charge state effect just after crossing the crystal surface were previously studied and rather not solved definitely, as being behind the experimental resolution. Recently however, it was reported measurement on differences in the energy loss of He\textsuperscript{+} and He\textsuperscript{2+} ions channelled in Si single crystal (SIMOX) (Azevedo de et al., 2001; Lulli et al., 2002). Also, models for impact parameter treatment of the electron exchange and the electronic energy loss were published (Smulders and Boerma, 1987; Grande and Schiwietz, 1998; Schiwietz and Grande, 1999) allowing for quantitative analysis of the channelling effect.

For swift ions the electronic stopping $S_e$ described by the Bethe theory, is proportional to the square of effective charge $Z^*$. $S_e \propto Z^{*2}$ (Lindhard, 1954; Ziegler et al., 1985). In general the effective charge of ions in matter (and also the average equilibrium charge) is different from the ion atomic number. The energy losses along the main crystallographic directions, in channelling conditions, are much smaller than the energy losses in disordered structures due to the lowering of the probability excitation and charge exchange (Azevedo de et al., 2000). The
characteristic distance for reaching the equilibrium charge distribution for 0.38 MeV He⁺ and He⁺² ions is about 2 nm, i.e. several lattice constants (dos Santos et al., 1995). It is difficult to estimate the contribution to the energy loss from the first atomic layers and relate it to the contribution that comes from the ion motion in the bulk lattice. A possible experimental method to find the relation is a detailed analysis of the RBS-transmission energy spectra in SIMOX-like structures (Azévedo de et al., 2001). Also, it is commonly known the sensitivity of the angular RBS spectra to the angle of ions incidence in respect to crystallographic axis and planes. The initial ion beam divergence and the surface structure strongly modify the measured spectra. It is expected that the analysis of angular RBS spectra measured as functions of the initial charge state of the incident ion beam enables getting information on the process of equilibration of the charge state distribution in the subsurface regions for medium energy ions.

2. Theory

The charge distribution of an ion beam proceeding through random solid is determined by the differential propagation equations (Moneta and Czerbniak, 1989). After relatively short distance which depends on the ion charge, its energy and material the distribution reaches the equilibrium form. If \( \phi_i \) is defined as \( i \)th charge fraction and \( \sigma_{ij} \) is defined as cross-section for capture \( \sigma_{1-j} \) and loss \( \sigma_{j+1,j} \) of an electron by an ion of \( j \)th initial charge (for higher ion energy the double electron transfer can be neglected), then the equilibrium charge distribution can be determined from the asymptotic equations:

\[
\sigma_{ji} = \phi_{j+1} - \phi_{j+1}, \quad \sum \phi_i = 1. \quad (1)
\]

\( \phi_0 \) is got from the normalisation condition. From Eq. (1) in the case of He ions the equilibrium fractions are:

\[
\phi_0 = \left( 1 + \frac{\sigma_{1,0}}{\sigma_{0,1}} \right) ^{-1} \quad (2)
\]

or single crystals the Monte-Carlo simulation must be used. Principles of the present model were presented elsewhere (Czerbniak et al., 2002). In brief, the projectile trajectory was determined on the basis of binary collision model. The scattering angle was calculated from the magic formula (Ziegler et al., 1985) using the Ziegler Biersack Littmark (ZBL) potential with respect to the nearest atom. The temporary position of the atom was determined in each step of calculation from the 3-dimensional normal distribution with the bulk Debye temperature. For a given charge state the energy loss due to interaction with atomic electrons were determined for each collision by using table of impact parameter dependent energy loss produced by CASP code (with PCA option) (Schwiertz and Grande, 1999). Additionally, four atoms closest to the scattering centre were taken into account in calculation of the scattering angle and the energy loss. The ion charge state after each collision was sampled from the charge distribution which was constructed from Eq. (1) under assumption of one electron exchange. The exchange cross-sections were determined from fitting of the solution of the propagation equations to the experimental date along the \( ETACHA \) procedure (Rozet et al., 1996). The nuclear energy probability (NEP) (Barret, 1979) was calculated for each scattering event and stored as a function of the collision number and separately as a function of the energy loss. After scattering the straight line trajectory of ion from the point of scattering to the crystal surface (and to the detector) were assumed. The energy losses per unit path length with step of 10 keV were calculated with \( SRIM2003 \) according to Ziegler et al. (1985). The energy straggling on the outgoing path was calculated according to Bohr (1948) with Chu (1976) correction. The angular straggling path was calculated as suggested by Smulders and Boerma (1987) and the energy resolution of the detector were taken into account. The structure of crystal surface was taken into account by generating random positions of Si and O atoms for the first and subsequent layers of the selected channelling cell.

On the basis of calculated NEP(E) the average values of NEP for the energy region corresponding to the energy resolution of spectrometric set up and for the subsequent values of the rotation angle \( \omega \) for a given tilt angle \( \theta \) it were determined. In this manner, the code generated results correspond exactly to the geometry and experimental conditions.

3. Results and data analysis

Typical fragments of experimental and simulated RBS energy spectra for 2 MeV He⁺ and He⁺² particle beam incident on Si(001) SIMOX membrane of 1023 nm thickness are shown in Fig. 1. Points are the experimental data by Luli et al. (2002), whereas lines come from the present simulation. The lower spectrum was determined for (001) channelling direction and the upper spectrum was for so-called random direction. The simulated spectra for He⁺ and He⁺² are indistinguishable each from the other, but they fairly reproduce the experimental spectrum. This is first of all due to the fact that at this relatively high energy the cross-sections for electron capture and loss are low and thus path for reaching equilibrium charge distribution is very short, of the order of few atomic layers. The average charge state is close to 2 and for relatively thick targets the He⁺² contribution is low. Also the energy loss straggling, included in the simulation and the energy resolution of the spectrometric arrangement, remove dependence of the energy loss spectra on the initial charge state. Particularly, edges of the energy spectra for...
both, random and channelling direction are identical with these determined from experiment (Lulli et al., 2002) and independent of the initial charge. For lower energy the situation changes.

The complementary simulation of RBS spectra from SIMOX structure was performed also for 1 MeV He\(^+\) and He\(^{2+}\) initial charge states. The results for 70° scattering angle and for the energy resolution of the data acquisition system FWHM = 10 keV are shown in Fig. 2. For this energy the average equilibrium charge, coming from the solution of the charge distribution propagation equation, was 1.7, which means 30% He\(^+\). For 1 MeV He\(^+\) ions the cross-sections for charge exchange were determined as: for loss $\sigma_{21} = 0.323$ A\(^{-2}\) and for capture $\sigma_{12} = 0.123$ A\(^{-2}\). Consequently, from the simulation, for He\(^{2+}\) the average charge was 1.71 after passage of 200 nm in random direction. However, in the (001) channelling direction of Si the average charge was 1.92 for He\(^{2+}\) incidence and much lower 1.84 for He\(^+\) incidence. The depth of 200 nm is then, by no means, the equilibrium depth for stabilisation of charge distribution in channelling direction.

From analysis of the energy loss we can get information on the effective charge of ion beam. The average energy loss (which incorporates the electron exchange procedure) calculated along the path of ion movement in random direction is 31.5 eV/A, the same for He\(^+\) incidence and for He\(^{2+}\) incidence. In (001) channelling direction we get 24.6 eV/A for He\(^{2+}\) and 23.45 eV/A and for He\(^+\). The spectra simulated along (001) channelling direction are shifted in respect to each other by 2 keV, as shown in Fig. 2, which gives the energy loss difference of approximately 1 eV/A. According to CASP, the difference of the energy loss for He\(^+\) and He\(^{2+}\) in this direction is 15.1 eV/A. Then the edge shift in (001) direction yields the charge pre-equilibrium depth of 13 nm. This is much larger than 4.5 nm calculated in random direction from Eq. (1) with the accepted electron exchange cross-sections.

### 4. Conclusions

In the presented report the RBS experiments with SIMOX structure were analysed numerically in order to get information from subsurface region. We also tested the basic characteristics of ion-atom interaction in solid, like the impact parameter dependent electronic energy loss or the electron exchange. In the region the charge distribution and energy loss distribution are far from equilibrium. It may result in change of some RBS characteristics, e.g. shift of the RBS edge. Channelling direction allows us to additionally extend this region deeply in the solid, comparing to the random incidence. This is due to domination of distant collisions and suppression of close collision in this regime. The edge shift becomes measurable allowing for estimation of the pre-equilibrium region size and it influence on the average charge or on the effective charge in ion beam.

### References


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