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RBS simulations studies of SIMOX structure

Jerzy Czerbniak[ab*], Krzysztof Pudłowski[b], Marek Moneta[a], Tomasz Gwizdałła[a]

[a]*Institute of Physics, University of Łódź, ul. Pomorska 149, 90-236 Łódź, Poland*
[b]*The College of Computer Science, ul. Rzgowska 17a, 91-408 Łódź, Poland*

Abstract

In the paper we present the short description of physical phenomena related to the motion of ion inside the crystal. The form of this description makes it possible and easy to construct the calculation procedures. The final results are the simulation and experimental data for the Si(001)-SiO_2-Si(001 (SIMOX) structure. The comparison of the results obtained shows that the problem of energy losses of fast ion moving inside such well ordered structure like single crystal is the fundamental one in order to good understand the quality of Si-SiO_2 interface and its location under the surface of sample. Only for a very thin amorphous layers thickness' and for the energies of incident ion close to the maximum of energy losses the assumption about the linear dependence between the energy loss and the penetration depth is right. If the direction of incidence of ion lies along one of main crystallographic directions the analytical models proposed in literature give results, which are in bad agreement with experimental data. The correct results were, however, obtained using simulation of successive collisions with the nearest atom of crystallographic lattice with impact parameter dependent energy losses and helium ion charge state taken into consideration. This attempt significantly lengthened simulation time but allowed for good reconstruction of the shape of energetic spectra as to show slight perturbations of SIMOX structure.

1. SIMOX technology

There is a great demand for defect free single crystals with precisely known impurity concentration. The silicon technology requires also good insulating layers, like SiO_2. One of the methods used is to create the silicon oxide layer just below the surface of silicon. The main stages of SIMOX process [1] (Separation by Implantation of Oxygen) are:

a. Implantation of (001) Si with oxygen 0^+ ions at temperatures 800-900 K. In order to produce the 400 nm thick oxide layer the dose $2*10^{18}$ ions/cm^2 is needed. This is a relatively slow process in which conventional implantators are

*Corresponding author: *e-mail address*: jerzy_czerbniak@wsinf.edu.pl

used (forming of 1cm^3 SIMOX requires the ion beam current 1mA/cm^2 and a time about 5 min).

b. Thermal treatment of the sample at temperatures 1600-1650 K under the pressure of 10^5 Pa during approximately 5 hours. The final effect depends on the implantation profile, and as a result on the energy of implanted oxygen ions. High temperature reduces radiation damages, the initial structure of crystal recovers and the chemical bonds between Si and O atoms are formed. These structures are studied using many different experimental techniques (SIMS[2], TEM[3], FTIR[4], X-ray[5], ellipsometry[6]) and also Rutherford Back Scattering. This technique allows to study the distribution of scattering centres in a non-destructive way. In the case of a single crystal the channelling effect, which makes it possible to determine the perfection of the crystalline structure is used.

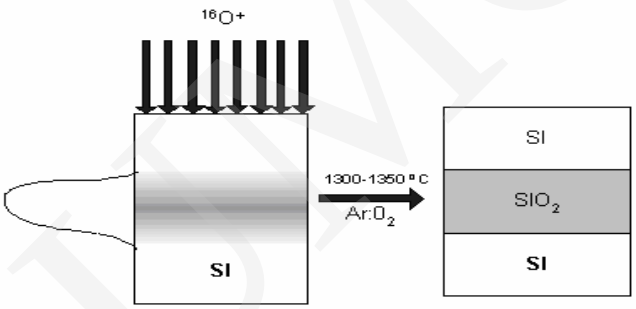

Fig. 1. High temperature implantation in connection with thermal treatment leads to sharp interfaces of SiO_2 layer

2. Simulation program

He-ion collisions are considered according to the binary collision model. In the simulation procedure the crystal is divided into cuboidal cells containing the minimal number of atoms required to construct the whole crystal as well along as perpendicular to the direction of movement. The division is made in this way that the full crystal should be built only using the operations of translation and/or reflection. The efficiency of computer code depends on the correct choice of the single collision cell, allowing for fast choice of the atom, which is the closest to the impinging particle path. In Fig.2 the scheme of choice for the (001) direction is shown. During the simulation the virtual crystal is built along the ion direction. The ion always collides with each nearest atom whose local position depends on the crystallographic structure studied and the temperature. The sampling of thermal displacement of atom from the equilibrium position is realised in accordance with the normal distribution *P(x)*. Optionally, it is also

possible to take into account the correlations of thermal vibrations of surface atoms

$$P(x) = \frac{\exp\left(-\frac{1}{2}x^2 / u_1^2\right)}{\left(2p\,u_1^2\right)^{1/2}}, \qquad (1)$$

where

$$u_1 = \left\langle x^2 \right\rangle^{1/2} = \left\langle y^2 \right\rangle^{1/2} = \left\langle z^2 \right\rangle^{1/2},$$

$$\left\langle u^2 \right\rangle = \frac{3\mathbf{h}^2}{MkT_D}\left[\frac{T^2}{T_D{}^2}\int_0^{q/T}\frac{x\,dx}{e^x - 1} + \frac{1}{4}\right],$$

T_D – Debye temperature.

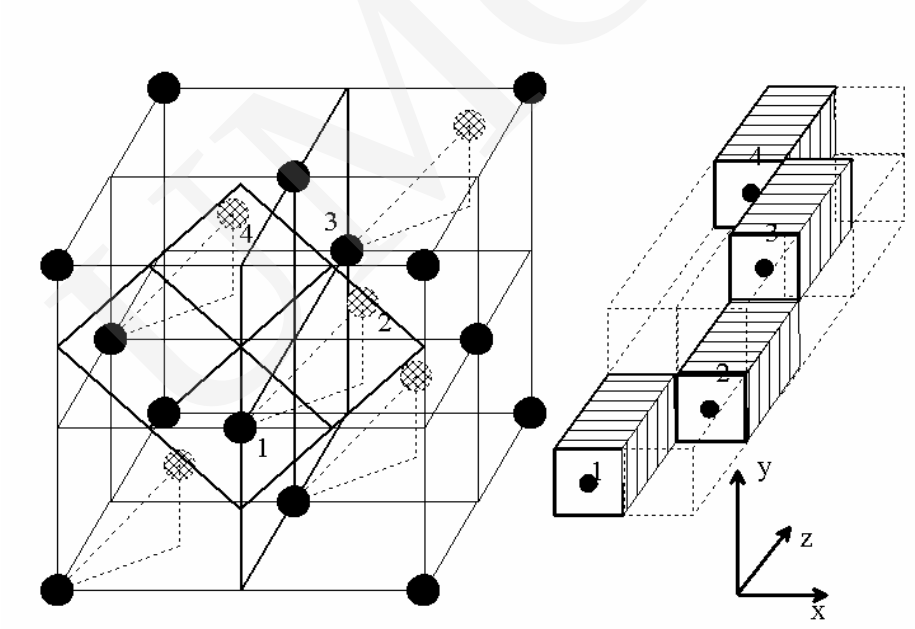

Fig. 2. The scheme of choice of collision cell for diamond structure and (001) surface. The ion trajectory is calculated with the step equal to the distance between the successive positions of scattering centres

After calculating the temporary position of scattering centre there were determined: the impact parameter **s**, the deflection angle, and the new position of ion after scattering and passing the path $\Delta z = z_{i+1} - z_i$. Also the translation of scattering cell was performed. Optionally, it is also possible to change the equilibrium positions of scattering centres caused by linear dislocations [7-9].

The scattering angle is determined using the "magic formula" for the screened Coulomb potential. In the code there was used the screening function in the Moliere approximation of Thomas-Fermi potential

$$f\left(r/a\right)=\sum_i a_i \exp\left(-b_i r/a\right), \tag{2}$$

where a_i={1,0.55,0.3}, b_i={6.0, 1.2,0.3}, $a = 0.8853 a_0 (Z_1^{1/2} + Z_2^{1/2})^{-2/3}$.

Then the physical characteristics of single scattering event was calculated:

1) ion energy losses in the function of impact parameter [10] and dependently on the temporary ion charge state. In every step of calculations the atoms nearest to the current scattering centre were taken into account. Such atoms don't have a significant influence on the change of trajectory but are very important due to total energy loss up to the distance of about lattice constant.
2) probability of backscattering (nuclear encounter probability) $NEP = \frac{A_0}{p r^2} e^{-\left(\frac{u_0^2}{r^2}\right)}$ where A_0 is the surface on which the ion falls [11] ,
3) fluctuations of shape of trajectory due to collisions with electrons they are determined from the normal distribution N(Θ,ΔΘ) $\Delta\Theta = \sqrt{\left(\frac{1}{2}\frac{m_e}{m_1}\frac{\Delta E}{E}\right)}$ where m_1 – mass of ion, m_e – mass of electron, ΔΘ – energy loss due to close collisions with electrons [12],
4) outgoing path in the direction into the detector,
5) ion energy straggling on the outgoing path with energetic resolution of detector considered $\Omega_{TOT}^2 = \Omega_{FWHM}^2 + \Omega_{STRAGGLING}^2 + \Omega_{BEAM}^2$,
6) energy of ion registered by the detector with the given solid angle. The energy losses on the outgoing path were calculated with the assumption that the trajectory is a straight line in a not ordered structure. The procedures compatible with the TRIM standard were used.

The calculated physical values were saved as a function of depth of penetration of ion and also as a function of total energy losses (this part of code was performed using parallel computations MPI). Then the position of crystal with respect to the impinging ion flux was changed (the rotation around the chosen rotation axis) and the calculations were repeated leading to the full angularly–energetical spectra of scattered ions.

The direct result of simulations is the value of relative probability of ion scattering, NEP, in the function of penetration depth and the energy of ion as registered by the detector for the given value of energy of incoming particles and the geometry of simulation experiment being in agreement with the real

geometry of measurement. The results can be directly compared with the experimental data with the known value of flux density of ions and the value of Rutherford's scattering cross section. It is also possible to calculate the average energy losses of incoming ions along the chosen segment of trajectory with fixed geometry of experiment. It is typically physical aspect of studying the problem of energy losses especially important for the partially ionized ions.

Results

The spectra of backscattered He ions with energy 1.0 MeV incident on the SIMOX structure are presented in Fig.3. The flux of ions hit perpendicularly the Si(001) crystal surface. Detector was placed at a scattering angle of 175 degree and the energetic resolution (Full Width at Half Maximum) was 18 keV.

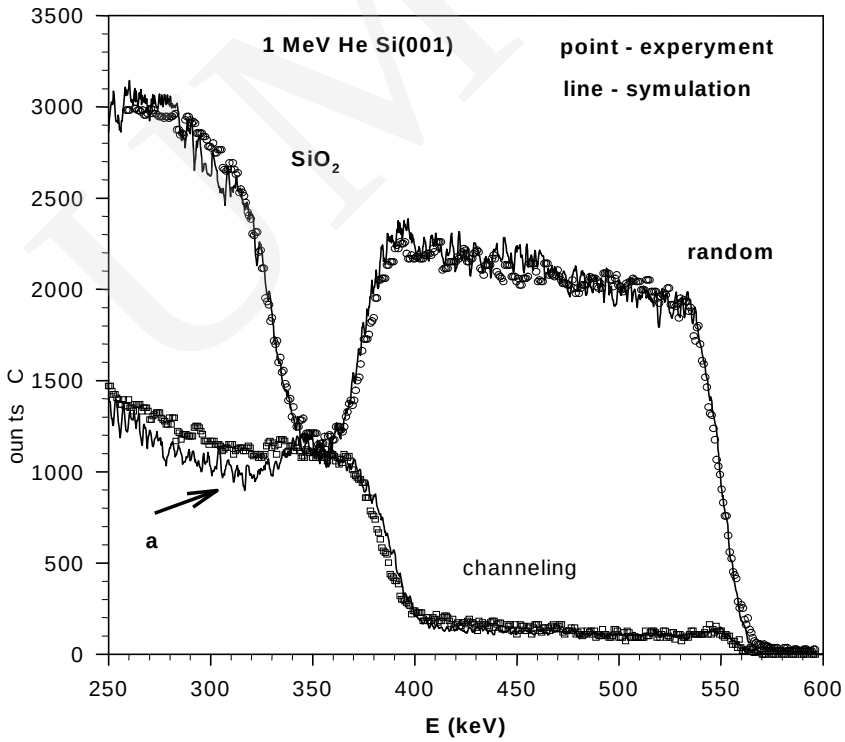

Fig. 3. Experimental [13] and simulation RBS energy spectra for SIMOX structure

The structure was composed of three layers: the surface layer Si(100) of thickness 316 nm, intermediate layer of $Si0_2$ 88 nm thick and the crystalline Si(001) substrate. For every kind of atoms the energy loss in single scattering in

the function of energy and helium atom charge state was determined. Because the outgoing path of backscattered ion in the direction of detector is treated as a "random" the energy losses was determined on the basis of continuous loss model [13]. It was assumed in the simulation that the silicon oxide layer is made of randomly distributed atoms with stoichiometric composition. The validity of this assumption was checked as follows: the RBS spectra were simulated for the [001] direction with the assumption that all the atoms in the sample are distributed randomly and then compared to the spectra simulated for random direction. Both spectra were identical, it means that there is no channelling effect and the energy losses are the same. The $Si0_2$ layer lying under the crystal surface layer contains oxygen atoms. Reduced Rutherford cross section for He+O scattering causes the reduction of number of counts in this region proportional to the concentration of oxygen atoms. Great mass difference between Si and O (kinematic factor) is the reason why helium ions scattered on oxygen have smaller energies when compared to those scattered on silicon and the maximum corresponding to them lies on the energetic spectrum in the vicinity of 200 keV. The spectra presented correspond to the scattering only on the silicon atoms. The part of spectrum obtained under channelling conditions (a) corresponds to the scattering in the intermediate layer, the base Si(001). Experimental values of counts are greater then simulation results. It means that in this region the Si(001) structure is distorted. The width of this distortion is about 30 nm. Significant differences in the volume of elementary cell for silicon and silicon dioxide lead to strong stresses and finally to emergence of closed dislocation loops. The presence of dislocations perturbs the trajectory of channelled ion and additional, when compared to ideal crystal structure, scattering events are generated [14]. The shapes of energetic spectra in the channelling regime show their very good agreement. There were made the calculations for other models describing the energy losses in the function of impact parameter [15-16]. For these models the results being in agreement with the data presented in [17] was obtained.

Conclusion

Presented here model of simulation calculations of process of atomic collisions in crystalline structures allows to reproduce exactly the experimental data using only well documented description of physical processes. A lot of other simulation works didn't take into account the process of charge exchange and related to it differences in the description of energy losses. The phenomenological parameters of energy loss models [18] were determined on the base of a rich experimental material. Such an attempt significantly decreases the time of performing calculations but considering the motion of ion in the channelling regime in presence of impurity atoms or structure deformations leads to distinct differences between the results of experiment and simulation.

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