Atomistic model of defects for the simulation of RBS-channeling measurements in ion irradiated silicon

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Abstract.
In this work, a new method for the atomistic simulation of ion–channeling spectra for ion irradiated Si is reported. The disordered crystal is represented by a supercell populated with point defects and then relaxed through a static energy minimization procedure based on empirical potentials. By including this supercell in a computer code for the simulation of ion–channeling spectra, we try to reproduce multi–axial results in the slightly damaged surface region of high–energy ion implanted Si. In spite of the simple assumptions on the nature of defects, we find that our method substantially improves the multi–axial data fit in comparison with that obtained under the usual assumption of random point defects.

INTRODUCTION
Rutherford backscattering–channeling (RBS–C) has been used for decades to characterize radiation damage in semiconductors [1]. So far, methods to extract quantitative information from the measurements have treated defects as atoms displaced from lattice sites, without taking into account the structural relaxation of the surrounding crystal. Although speculations about this effect were reported in the past [2, 3], a simulation of ion channeling in Si containing relaxed configurations of point defects has been presented only very recently [4]. In that work, we have modeled the relaxation induced by point defects using a static energy minimization procedure based on empirical potentials. This description of defects has been introduced in the computer code BISIC (Binary collision Simulation of Ion Channeling) [5, 6] which is based on the Monte Carlo calculation of ion trajectories in the binary collision approximation (MC–BCA). The simulation work reported in our previous paper [4] has mainly focused on the significant effects expected from this model of disorder on ion–channeling spectra. In the present work we address, in particular, the application of the method to the interpretation of a set of multi–axial RBS–C measurements performed in the slightly damaged surface region of high–energy ion implanted Si, some of which were preliminarily reported in our previous paper [4].

DEFECT MODELING
RBS–C spectra were simulated with the computer code BISIC [5, 6], in which full calculation of incoming ion trajectories is performed according to the MC–BCA method. Using the concept of close encounter probability [7] and approximating the path of a backscattered ion with a straight trajectory, the program calculates the yield at the detector as a function of energy. The standard procedure to describe lattice disorder in the simulation is to shift atoms from their original lattice site, according to a gaussian displacement distribution. The result is a pseudo Frenkel pair, where the self interstitial and the corresponding empty site (vacancy) are separated by a distance which, according to the chosen displacement distribution, is, on average, about 1.44 Å. This procedure leaves the surrounding crystal unperturbed.

The new model of structurally relaxed point defects, may be summarized as follows. Interstitials are put in symmetrical (hexagonal: $I_H$), tetrahedral: $I_T$, split–<110>: $I_{<110>}$ positions of a large Si supercell (size $11\times11\times1900$ lattice units). An equal number of vacancies is also introduced by removing Si atoms from lattice sites. The concentration of symmetrical sites where defects are placed follows a given depth distribution. Sites are chosen at random, according to the constraint that a minimum interstitial–vacancy, interstitial–interstitial and vacancy–vacancy distance is kept. The purpose is to minimize defect interactions, in particular, recombination or clustering during relaxation.
Yield (counts mC^{-1} msr^{-1} keV^{-1})

FIGURE 1. <100> RBS–C spectrum of the sample implanted with a dose of 10^{14} ions cm^{-2} 3 MeV As^{2+} ions, measured with 3 MeV He^{2+} ions and backscattering angle of 170°. Random and virgin spectra are also reported for reference, together with the corresponding simulations (full lines). The double dashed arrow indicates the region of the spectrum which originates from the 1 µm thick surface layer of the material.

A static relaxation procedure at constant volume is therefore performed using periodic boundary conditions. Different empirical interatomic potentials developed for Si may be used for this purpose, but in the present work we will refer only to results obtained with the Tersoff III (TS) [8] one. After energy minimization, the response of RBS–C from the structurally relaxed supercell is simulated. A comprehensive discussion of the method, and of the results observed for a model system composed of a fixed concentration of different kinds of point defects that are relaxed according to different interatomic potentials, has been reported in Ref. [4].

EXPERIMENT

The sample used for RBS–C characterization was (100) Si, implanted with 10^{14} cm^{-2} 3 MeV As^{2+} ions at nominal room temperature. The comparison of simulation and experiment was limited to a surface layer of 1 µm thickness, where the damage level is low and the approximation of dilute, weakly–interacting point defects is better satisfied.

RBS–C measurements were performed under the five axial <100>, <110>, <112>, <012>, <013>, and the (100) planar alignments, with a 3 MeV He^{2+} beam at a backscattering angle of 170°. More details on the experimental setup, which includes a Faraday chamber for absolute yield measurements, are reported in Ref. [6]. For all beam–sample orientations, we measured spectra of reference virgin and deeply amorphized Si samples and verified that they were accurately reproduced by the simulation. Fig. 1 shows the example of the <100>–aligned spectrum of the implanted sample and of the reference (virgin and random) sample, along with the corresponding simulated spectra for the reference sample.

The three damage models used to simulate the surface region of RBS–C spectra of the implanted sample were: i) disordered atom displaced at random in the otherwise unperturbed lattice [5, 6]; ii) a model supercell containing split–<110> interstitials + equal number of vacancies in the otherwise unperturbed lattice; iii) a model supercell populated with the same kinds of defects, but relaxed through the application of the TS potential. The choice of I_d defects is justified by our previous preliminary work [4], where we found that neither I_H nor I_I interstitial defect types, either in unrelaxed or relaxed supercells, could simultaneously reproduce in a satisfactory manner the measurements performed under <100>, <110> and <112> axial alignments.

Since the usual geometry for RBS–C characterization in Si is the <100> alignment, we decided to determine first the defect distributions which reproduces the <100> RBS–C spectrum for each of the three models. These distributions were therefore used to simulate RBS–C spectra collected under the other alignment conditions.

RESULTS AND DISCUSSION

In Fig. 2 the results of the simulations performed with the different damage models and for the different measurement geometries, are compared with experiments. For each of the damage models investigated, the disorder distributions have been chosen to give a similar good fit (deviation ≤ 1 %) of the <100> RBS–C spectrum. These depth profiles are shown in Fig. 3. Small differences with results reported in previous Ref. [4] are due to some aging of the implanted samples which have been re–measured for the purposes of the present work. The larger amount of defects needed to fit the <100> RBS–C spectrum when an unrelaxed lattice is assumed, is due to the absence of strain, which develops as a consequence of the relaxation procedure and adds a significant contribution to the backscattering yield. The largest amount of displaced atoms required by the random defect model is due also to the procedure used for positioning disordered atoms. In fact, their displacement from lattice sites, chosen according to a random distribution, is, on average, lower than the one characteristic of the open volume symmetrical interstitial sites. For this reason they give a smaller contribution to the increase of backscattering yield than unrelaxed I_d defects. So, the first observation is that the quantitative information that is extracted from the elaboration of an RBS–C spectrum is model–
dependent. It must be stressed that it depends also on the definition of "point defect". If we count point defects as the Wigner–Seitz cells with occupation numbers zero (vacancies) and two (interstitials), we find that their number does not change upon relaxation, while on the other hand the overall disorder increases as a result of the high number of small displacements induced in the lattice surrounding each point defect. In our previous work we have shown that a more useful criterion to quantify disorder in RBS–C characterization is the number of atoms which are located outside the spheres of radius 0.45 Å (known as Lindemann spheres) centered around the original lattice sites. In fact a monotonic, nearly linear correlation exists between this number and the simulated backscattering yield.

Table 1 reports the deviations of the integrals of simulated spectra from experimental spectra (Fig. 2), calculated in the energy window corresponding to the 1 µm thick surface layer. First of all, we observe that the application of the random defect model, which is an isotropic representation of disorder, produces, except for two cases (<112> axis and (100) plane), rather large differences with experiments. Moreover, these discrepancies change their sign depending on the measurement geometry. This means that decreasing or increasing the disorder level in order to improve the overall multi-axial fit, would im-

![FIGURE 2. Comparison of RBS–C spectra simulated according to different damage models, and experimental spectra, under the different beam lattice alignment conditions investigated.](image)

prove results under some conditions, but would at the same time produce larger discrepancies under others. Since the damage present in the sample is anisotropic to reproduce RBS–C spectra an anisotropic model of defects is necessary.

The model of split–<110> interstitial defects in their unrelaxed highly-symmetrical configuration, does not
lead to any improvement. In fact, this model significantly increases the yield for all alignment conditions, especially in the <110> orientation [4]. A difference from the random damage model is that the deviations from experiments are positive for all alignment conditions.

By adding the step of lattice relaxation, things change quite dramatically. The data fit improves substantially in comparison with those obtained by the previous models, giving a maximum discrepancy below 10%. Moreover the deviations observed are systematically positive for all geometries. This means that it is possible to obtain a better overall agreement with experiments, decreasing the disorder distribution which fits the <100> axial measurement. This would produce some underestimation for the case of <100> alignment, with the advantage of reducing the overestimation in all the others.

Unrelaxed split–<110> interstitials display a significant projection in the wide <110> axial channel of Si, and this is the reason of the high backscattering yield they produce when the beam is aligned along this axis. Upon relaxation, their projection reduces substantially. As shown in our previous work [4], relaxation leads to a relative yield increase (due to defects + surrounding atoms that move out of perfect lattice sites) which is anisotropic, and is in general the lowest for the <110> alignment. This seems to be the key feature which allows a better fit of experiments.

It must be stressed that, at the present level of experimental knowledge, very little can be said about the atomic–scale configuration of small defects which are not resolved by Transmission Electron Microscopy techniques. There are plenty of theoretical calculations proposing many different configurations of small interstitial clusters, the so called "precursors" of larger and better characterized interstitial defects ([311], dislocation loops). In our work we have just pointed out that multi–axial RBS–C analysis, interpreted with the aid of simulation and of a physically–based model of disorder, can be one of the best methods to select among different approaches. In this first modeling we have done an assumption on as–implanted damage which is certainly too simple for Si, where isolated point defects are known to be unstable at room temperature. The present approach, beside its interest as a refinement of the treatment of ion–channeling from point defects, has to be considered as a first step towards the introduction of more complex configurations of defects in the simulation of ion–channeling.

### CONCLUSIONS

The damage in the slightly damaged surface region of high–energy ion implanted Si is expected to be more complex than a simple distribution of point defects. Nevertheless, we have shown that the RBS–C spectra simulation based on structurally relaxed, weakly–interacting point defects, allows a significant improvement of the multi–axial data fit in comparison to the results of the models which describe damage as displaced atoms (either randomly or to symmetrical lattice positions) in an unstrained lattice. This may be considered as an indication that lattice relaxation, even if applied in the framework of a simple point–defect model, gives a microscopic description of a slightly disordered Si lattice which better accounts for the anisotropy of irradiation induced defects.

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