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Investigation of heavily damaged ion implanted Si by atomistic simulation of Rutherford backscattering channeling spectra

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Abstract

Rutherford backscattering channeling (RBS-C) spectra of ion-implanted Si are simulated according to an atomistic model of radiation damage which consists of a distribution of point defects (split-$\langle 1\,1\,0\rangle$ interstitials and vacancies) structurally relaxed by empirical potentials. This model, successfully used to reproduce multiaxial spectra of lightly damaged Si, is applied here to the case of a heavily damaged sample. As a consequence of the increasing strain generated by lattice relaxation, simulations predict a superlinear trend of RBS-C disorder versus defect concentration in the range of intermediate damage density. This contrasts with the linear trend obtained by the usual description of defects as atoms randomly displaced in a rigid lattice. The new approach represents an improvement in the physical description of ion irradiation disorder within RBS-C analysis; however simulation results are found to be in less satisfactory agreement with spectra of a heavily damaged sample than with spectra of lightly damaged material. The description of damage as the result of the accumulation of simple point defects and the use of a static relaxation procedure instead of finite temperature molecular dynamics, are two possible reasons to explain the present limitations in describing the structural properties of heavily damaged, yet not completely amorphized, ion implanted Si.

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1. Introduction

The Rutherford backscattering channeling (RBS-C) technique [1] has been used for decades to characterize damage induced by ion implantation in Si. Simple qualitative inspection of RBS-C spectra is sufficient to compare disorder in different samples or to determine whether an irradiated crystal has been amorphized or has recovered its crystalline structure upon annealing. However, a more quantitative analysis, such as the evaluation of the number of defects introduced by irradiation, requires a microscopic model of damage and of its effect on the dechanneling of analyzing ions [2–4].

In a recently developed approach for the interpretation of RBS-C measurements [5–7], spectra were simulated by the Monte Carlo binary collision approximation (MC-BCA) method and disorder was described by atomic-scale models of defects, structurally relaxed by empirical potentials. It has been shown that distributions of simple self-interstitial defects can account for the anisotropic behavior of damage revealed by multiaxial RBS-C analysis of low-fluence implanted Si, whereas this result cannot be achieved within the usual assumption of randomly distributed defect in a rigid lattice. The experiments analyzed in previous works referred to defect concentrations of the order of a few atomic percent, where the interaction between defects is weak. In this work we have investigated the application of the model to high-fluence implanted Si, where the peak RBS-C signal is close to the random value.

2. Experiment

$\langle 100 \rangle$ Float Zone n-type 500 Ω cm Si was implanted with 180 keV Si^+ ions at fluences of 10^{14} and 10^{15} cm^{-2}. RBS-C measurements were performed using a 2 MeV He^+ beam, and backscattering angle of 170° under different axial and planar alignment conditions. Details of the measurement setup, which includes a Faraday chamber for absolute measurements (uncertainty in the yield ~2%), are reported in [8].

3. Computer modeling

The procedure for generating a computational model of Si containing defects has been reported in details elsewhere [5,7]. A large supercell of crystalline Si ($12 \times 12 \times 1900$ lattice units, the long side corresponding to the [0 0 1] direction perpendicular to the wafer surface), is populated with defects (which can be single interstitials and vacancies or small interstitial clusters) according to a depth distribution profile given in input. An equal profile of vacancies is inserted, to balance the one of interstitials and keep the total number of atoms constant in the supercell. Defects are equally distributed among all possible locations and equivalent orientations. The resulting defect distribution does not include at the moment heterogeneous clusters. The system is then subject to a static energy minimization procedure according to the empirical environment-dependent interatomic potential (EDIP) [9,10], which is known to give a good description of local bonding in bulk defects and disordered phases of Si. The large size of the supercell required for RBS-C simulation [5] does not allow the use of finite temperature, full molecular dynamics (MD) for lattice relaxation. Less computationally expensive static optimization (equivalent to 0 K MD) is therefore applied. We are aware that the disordered phase resulting from static optimization may be energetically and structurally different from the one generated by finite temperature MD.

$\langle 100 \rangle$ RBS-C spectrum of the structurally relaxed supercell is simulated and compared with the experimental one, and the input depth distribution profile of defects is adjusted until a satisfactory agreement is achieved. The defect profile fitted to the $\langle 100 \rangle$ spectrum is then used to simulate spectra under the other alignment conditions. If good overall agreement is found in all directions using the same profile, we can conclude that the damage model describes well the structural properties of ion induced disorder. Using the $\langle 100 \rangle$ spectrum for fitting defect profiles is due to the fact that this geometry is the one mainly used for RBS-C characterization of ion implanted Si. A true best-fit, involving the search for a profile which minimizes the sum of deviations in all the alignment conditions investigated, would be in

principle more satisfactory, but also more difficult to perform in practice. The consideration that the method based on ⟨1 0 0⟩ fitting allows in any way a good test of the structural model of defects, led us to choose this simpler procedure.

For the purposes of the present work only two defect models have been considered, namely the simple split-⟨1 1 0⟩ interstitials (I_S) + vacancies (V) and the standard random defects, the latter consisting of atoms displaced at random from lattice sites, with no distortion induced in the surrounding crystal. The I_S has been previously demonstrated to give a good overall fitting of multiaxial RBS-C spectra in a low fluence implanted sample [6,7], whereas the random defect model is important as a reference, being widely used in data elaboration, and also because its isotropic features are those expected for fully amorphous disorder.

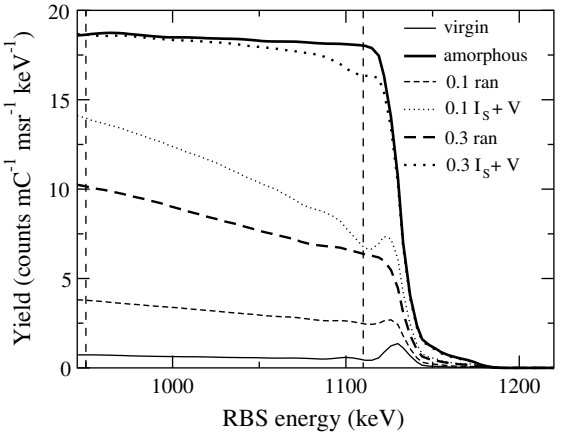

Fig. 1. Simulated ⟨1 0 0⟩ RBS-C spectra of model systems containing uniform distributions of structurally relaxed $I_S + V$ defects or of randomly displaced atoms in a rigid lattice (ran). The reported examples refer to defect concentrations of 0.1 and 0.3 atomic fractions.

4. Results and discussion

4.1. Damage accumulation model

In the low damage concentration regime considered in our previous works [5–7], defect–defect interactions are weak and disorder can be schematized as a distribution of simple defects, each one surrounded by a strained region which does not significantly overlap with the ones generated by the others. With increasing damage concentration the disorder in the originally perfect lattice surrounding defects increases. To investigate this point, we have built a model system containing a uniform concentration of $I_S + V$ and performed RBS-C simulations for increasing concentrations of defects. Simulations using the random model of defects were also performed for comparison. Results of this analysis are reported in Figs. 1 and 2. The former shows examples of RBS-C spectra obtained for two different damage concentrations, the latter reports the normalized RBS-C yield as a function of the concentration of defects. Normalized yield is the integral of the spectrum in the energy interval marked in Fig. 1, divided by the integral of the amorphous spectrum. As expected, the random model shows a trend which is almost linear for low damage concentration, and turns

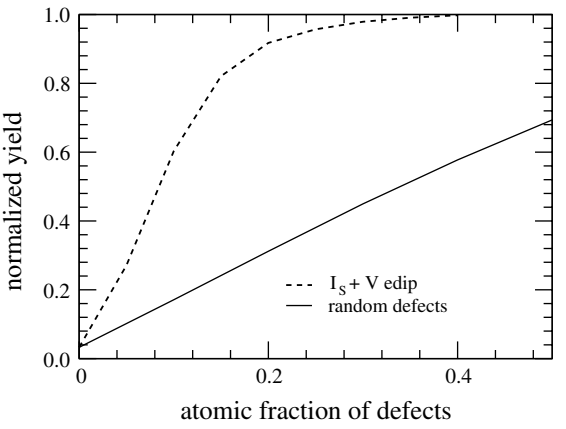

Fig. 2. RBS-C yield (normalized to random) as a function of the defect concentration in the uniformly damaged samples, obtained from spectra simulated according to the defect models under investigation. Normalized yield is calculated in the energy interval marked by dashed lines in Fig. 1.

into sublinear when the RBS-C signal starts to saturate (out of the range shown in Fig. 2). The model of relaxed $I_S + V$ shows instead a superlinear trend at low-intermediate damage concentration. A detailed analysis of the supercell [11] shows that the number of lattice atoms displaced by defect induced strain increases with increasing concentration of

$I_S + V$. At low concentration the amount of induced displacements is relatively small, and so is their contribution to the RBS-C yield. For a concentration of $I_S + V$ above ~4% the defect induced deformation begins to push lattice atoms far from their lattice positions. The contribution of these largely displaced (LD) atoms to the RBS-C yield rapidly increases, generating the superlinear trend observed in Fig. 2. From Fig. 2 it is also possible to deduce that, when lattice relaxation is taken into account, the contribution of each defect to the RBS-C disorder is larger than the one expected from the model of randomly distributed defects in a rigid lattice. As already discussed [12,13,5–7], this has important consequences on the quantitative evaluation of RBS-C data.

4.2. Analysis of heavily damaged Si^+ implanted Si

Following the same procedure used for the analysis of the sample implanted at ten times lower fluence [7], we have measured RBS-C spectra of the sample implanted at the fluence of 10^{15} Si^+ cm^{-2} under seven axial and two planar alignment conditions. Defect distribution profiles were obtained by fitting the ⟨100⟩ spectrum according to both relaxed $I_S + V$ and random defect models. These two profiles were then used to simulate RBS-C spectra in the other alignment conditions. Fig. 3 shows simulated and experimental spectra of samples implanted at 10^{14} and 10^{15} Si^+ cm^{-2} and analyzed under ⟨100⟩ and ⟨120⟩ axial alignments. The latter orientation has been taken as an example because it was found to be very sensitive to the difference between the two defect models. Dashed lines refer to the relaxed $I_S + V$ model, full lines to the random defect model. Virgin and random spectra are reported for comparison. Fig. 4 reports the defect distribution profiles (fitted to the ⟨100⟩ spectra) corresponding to the two models and fluences considered. Fig. 5 summarizes, for the case of the sample implanted at the fluence of 10^{15} Si^+ cm^{-2}, the deviations of the two defect models from the experiment for all the alignment conditions investigated. The deviation is calculated as the difference between the yields of the simulated and experimental spectra in the region of the RBS-C peak (corresponding

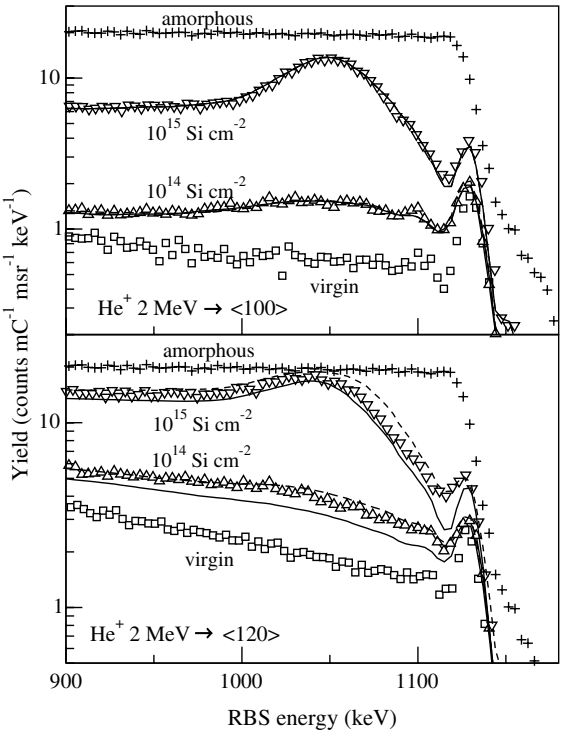

Fig. 3. Simulated (lines) and experimental (symbols) spectra of samples implanted at 10^{14} and 10^{15} Si^+ cm^{-2} and analyzed under ⟨100⟩ (upper figure) and ⟨120⟩ (lower figure) axial alignments. Full continuous lines refer to simulations performed according to the random defect model, dashed ones to simulations performed according to the model of structurally relaxed $I_S + V$ (in the ⟨100⟩ alignment full and dashed lines are not distinguishable, as they overlap almost perfectly).

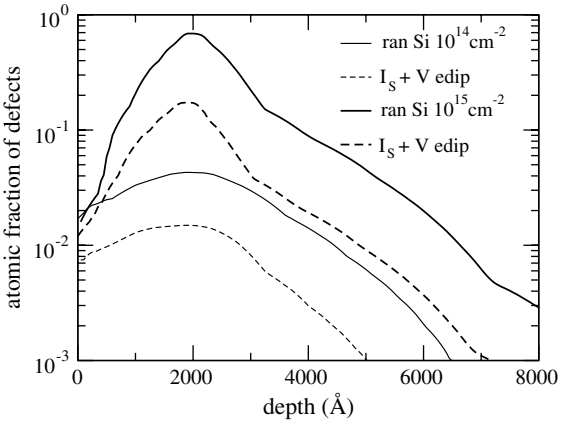

Fig. 4. Defect depth distribution profiles fitted to the ⟨100⟩ spectra, corresponding to the two models and fluences reported in Fig. 3.

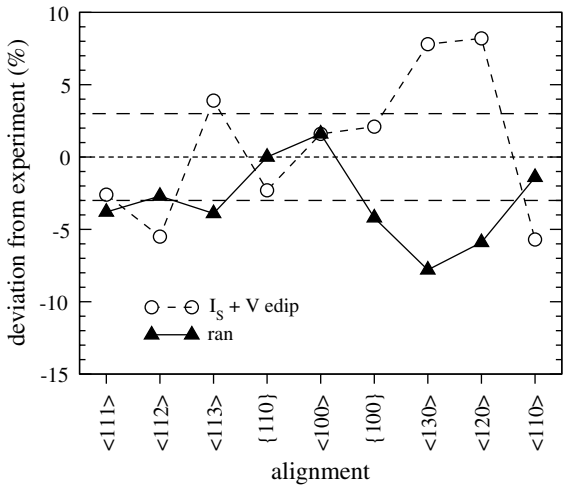

Fig. 5. Deviations of the two defect models from the experiment for all the alignment conditions investigated, measured as the difference between the yields of the simulated and experimental spectra in the region of the RBS-C peak.

in Fig. 3 to an energy of ~1050 keV). Dashed horizontal lines indicate the band of estimated experimental error in the yield.

The agreement between simulations and experiments in the upper part of Fig. 3 is the obvious consequence of the fact that defect profiles (Fig. 4) have been fitted to the ⟨100⟩ RBS-C spectra. As concerns the ⟨120⟩ alignment, we observe that for the lower implantation fluence the model of relaxed $I_S + V$ shows a satisfactory agreement with experiment, whereas the random model largely underestimates it. The situation changes for the higher fluence. As can be seen also in Fig. 5, in most cases the measured RBS-C spectra fall in between spectra calculated according to the two models and sometimes, such as in the ⟨120⟩ alignment, both simulations fall out of the estimated error. The comparison with results of low-fluence implanted sample, reported in [7,11], shows that experimental disorder becomes more isotropic with increasing fluence, but not enough to be described by the fully random model of damage. Actually, due to the increasing effect of lattice induced strain, the model of relaxed defects naturally predicts a more isotropic RBS-C response with increasing concentration of disorder. However, this is not sufficient to reproduce the experimental spectrum within the estimated accuracy. The first possible explanation of this result is that the absence of defect clusters or agglomerates may prevent a detailed description of the heterogeneous nature of heavily ion-damaged Si, where, according to electron paramagnetic resonance (EPR) measurements [14], both fully incoherent (amorphous) and heavily damaged regions, coexist. The second hypothesis is that the structure relaxed by static minimization may preserve too much the memory of the I_S configuration. To clarify these points work is in progress to (a) allow the introduction of heterogeneous distributions of damage in the model supercell, (b) perform finite temperature MD to investigate the stability and structural evolution of the heavily disordered phase.

5. Conclusions

In comparison with the model of randomly displaced atoms in a rigid lattice, the model of structurally relaxed point defects significantly improves the physical description of damage used to interpret RBS-C spectra of ion implanted Si. The strain induced by lattice relaxation increases its contribution to disorder with increasing concentration of defects, thus predicting a superlinear increase of RBS-C disorder versus fluence in the low-intermediate damage concentration regime. Moreover, this description allows good simulation of the anisotropic behavior of damage in low-fluence implanted Si, where the random model fails. With increasing damage concentration the model accounts only partially for the reduced anisotropy of damage. In this regime experimental RBS-C spectra fall in between spectra simulated according to the atomistic model of interstitials and spectra simulated under the assumption of fully incoherent damage. Possible reasons of this result are: (a) the spatially continuous distribution of point defects assumed in the model, which contrasts with the possible presence of both heavily defective and fully incoherent (amorphous) regions in the sample; (b) the limitation of the static optimization method (as opposed to finite temperature MD) which could preserve too much the memory of

the configuration of point defects originally introduced in the model supercell.

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