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New Insight into Damage-Related Phenomena in Si Implanted under Extreme Conditions

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NEW INSIGHT INTO DAMAGE-RELATED PHENOMENA IN Si IMPLANTED UNDER EXTREME CONDITIONS

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ABSTRACT

New insight into damage formation in Si(100) during self-ion irradiation is gained from processing under extreme conditions. Dislocations form in the near-surface as a result of lattice relaxation in response to strain produced by precursor defects which are shown to be vacancy-type by positron analysis. A model to account for these defects and their distribution is presented. A novel technique is demonstrated which utilizes a subsequent implantation as a depth specific probe to manipulate the vacancy-type defects. Aspects of damage growth which emerge from the probe results are discussed.

INTRODUCTION

Ion-induced damage growth in single-crystal Si at or near room temperature has been widely studied by a number of investigators(1). While it is generally accepted that damage production decreases with increasing temperature, details of the formation mechanism(s) are still lacking for elevated temperature irradiations (≥200°C). Below this temperature range, damage growth is interrupted at moderate fluences by a spontaneous crystalline-to-amorphous transition of the lattice(2), while above the transition temperature, it can be investigated to arbitrarily large fluence. High-temperature processing, therefore, greatly extends the boundary for exploring damage-related phenomena into regimes where new effects may be anticipated. While such prospects are clearly exciting, a better understanding of ion-solid interactions under extreme conditions also serves to underpin evolving ion-beam technologies such as separation by implantation of oxygen (SIMOX); a high-temperature process for synthesis of a silicon-on-insulator (SOI) material by high-dose O^+-implantation(3-8).

Mechanisms responsible for the growth of damage in single-crystal Si during self-ion irradiation at high temperature are investigated. The use of self-ions in the present study allowed the basic mechanisms of damage formation to be investigated without interference from chemical effects associated with a reactive ion specie. The focus of this paper will be on damage accumulation within the superficial layer ahead of the ions' end-of-range (eor), where an accumulation of precursor defects is shown to result in dislocation formation. The precursor defects are shown to be of a vacancy type by positron annihilation spectrometry. A mechanism based solely on the kinematics of the ion-atom interaction (and not the chemistry) is proposed to account for the presence of these vacancy-type defects in the superficial layer. Finally, a technique involving self-ion implantation in the proximity of these vacancy-type defects is shown to reduce their concentration yielding a more defect-free layer. Insight gained from these results into the nature of the ion-induced damage process is discussed. Cross-section transmission electron microscopy (XTEM) and Rutherford backscattering (RBS)/channeling

spectrometry are used to profile the ion-induced damage. The RBS spectra were acquired using 2.3 MeV He^{++}-ions and a detector positioned to intercept backscattered ions at 160°.

RESULTS AND DISCUSSION

XTEM micrographs are shown in Fig. 1 from p-type Si(100) crystals implanted at 450°C with different fluences of 1.25 MeV Si^{+}-ions. The resistivity of the Si crystals was nominally 10 Ω-cm, and the average ion current density during implantation was $\leq 1\ \mu A/cm^2$. Damage formed near the eor is seen to consist of a band of dislocations centered at ~1.5 μm which broadens with fluence. Surprisingly, the 3×10^{17} cm^{-2} implanted sample is seen in Fig. 1(a) to be free of visible defects to a depth of ~1.0 μm. This occurs despite the fact that the average number of displacements per atom (dpa) within this region is calculated at this dose to be ~40 by computer simulation using TRIM(9). Clearly, Frenkel pair recombination dominates at 450°C over those point-defect reactions which result in damage formation. A unique morphology is seen at the higher fluences in Figs. 1(b) and 1(c). A distinct band of dislocations is present within the superficial layer centered near ~0.45 μm. The width of the band increases with fluence and eventually expands to intersect both the surface and the advancing eor damage. Similar results have been reported for O^{+}-implantation under nearly identical conditions(10,11), but the use of self-ions indicates that these effects are intrinsic to these extreme conditions (i.e., high temperature and dose) and are not dependent upon the ion-solid chemistry. In ref. (10), it was shown that these dislocations are formed as a result of yielding of the lattice in response to an accumulation of precursor defects. The similarity of the self-ion results suggests a common mechanism.

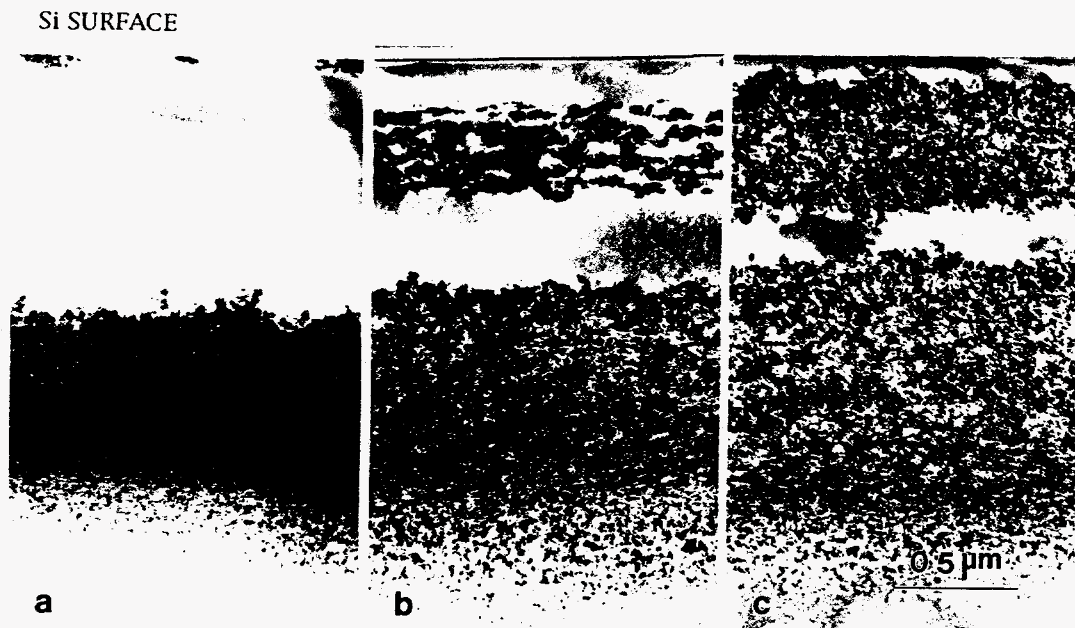

Fig. 1. XTEM micrographs from Si(100) crystals implanted at 450°C with 1.25 MeV self-ions to a fluence of (a) 2×10^{17} cm^{-2}, (b) 3×10^{17} cm^{-2}, and (c) 5×10^{17} cm^{-2}.

Identification of the precursor defects within the superficial layer prior to dislocation formation was done using positron annihilation techniques which are very sensitive to open volume defects in solids(12). The sensitivity of positrons to lattice defects is reflected in a quantity called the S-parameter which measures the Doppler broadening of the 511 keV photon annihilation peak. The S-parameter is calculated by dividing the area of a fixed region in the center of the annihilation peak by the total peak area. Since a positron trapped within an open-volume defect interacts less frequently with the higher momentum, inner shell electrons, the width of the annihilation spectrum from such defects will be narrower (and the S-parameter larger) than from sites in undamaged crystal. The dependence of the S-parameter on the incident positron energy (depth) is shown in Fig. 2 for samples implanted with (a) 2×10^{17} and (b) 5×10^{17} cm^{-2}; a dose range which spans the onset of dislocation growth within the superficial layer. At the lower dose, the S-parameter is seen to change rapidly over the ions' range with a peak value near ~0.4 μm much greater than S_b=1 for the bulk. This signifies the presence of open-volume defects within the superficial layer far in excess of the bulk concentration prior to dislocation formation. A much smaller S-parameter was measured in the sample implanted at the higher fluence of 5×10^{17} cm^{-2}. It is clear that dislocation formation during yielding reduces the concentration of vacancy-type defects within the superficial region.

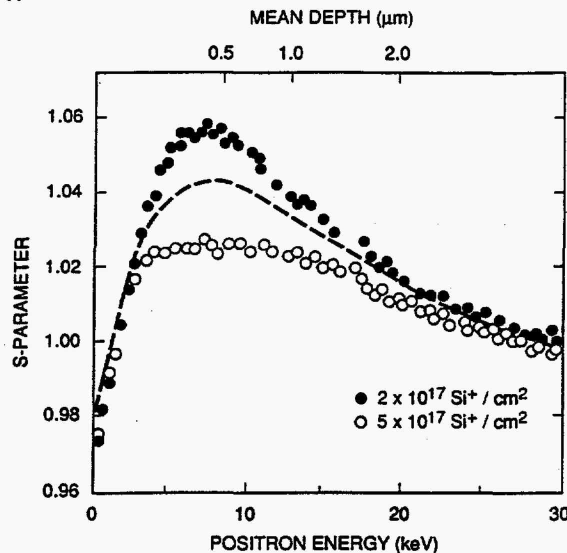

Fig. 2. S-parameter verses positron energy after implantation at 450°C with 1.25 MeV self-ions to a dose of 2×10^{17} and 5×10^{17} cm^{-2}. The dashed spectrum is from a sample dual implanted at 450°C with self-ions at 1.25 MeV (2×10^{17} cm^{-2}) and 300 keV (2×10^{15} cm^{-2}). The depth scale at the top of the figure corresponds to the average annihilation depth of the positrons.

The preponderance of vacancy-type defects within the superficial layer can be accounted for by a mechanism involving the spatial separation of Frenkel defects(13,14). Momentum transfer to an interstitial, during Frenkel pair formation, will on average produce a spatial separation of the pair such that the interstitials are distributed to greater depths. TRIM calculations in Fig. 3 reveal that the vacancy excess produced at 1.25 MeV by a self-ion fluence of 2×10^{17} cm^{-2} persists over the top micron at a nominal value of 1 at. % (followed by a much narrower distribution of excess interstitials). This

closely matches the distribution of the vacancy-type defects within the sample, as well as yielding a reasonable value for their concentration. Thermal interdiffusion of defects may reduce the excess concentrations, especially near the boundary (between the excess vacancies and interstitials); but the excess distributions are preserved, in part, by interactions such as vacancy clustering which form less mobile defects.

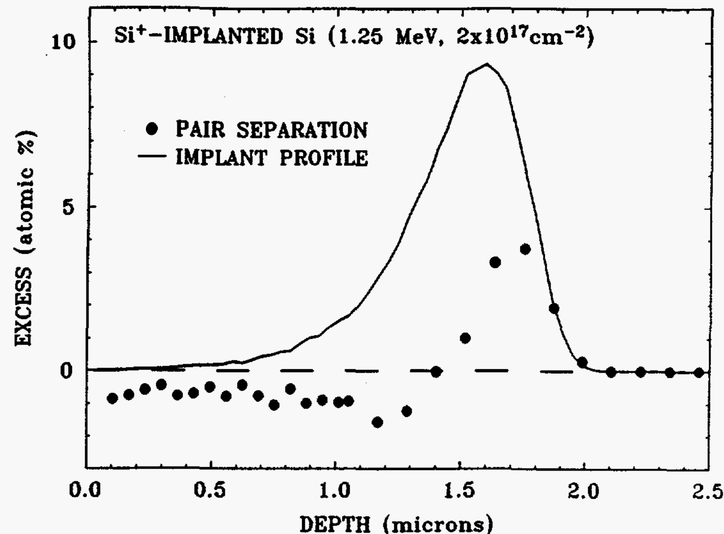

Fig. 3. TRIM calculations of 1.25 MeV self-ion implantation in Si normalized to a fluence of $2 \times 10^{17}\ cm^{-2}$. The uncorrelated pairs, defined as the difference between the interstitial and vacancy distributions, is given by the solid circles. The distribution of the implanted self-ions is shown for reference.

While the focus to this point has clearly been upon ion-induced damage growth within the superficial layer, a more complete understanding of high-temperature effects must include some explanation for the damage behavior near the eor. Unlike the long incubation period within the superficial layer, dislocations form readily near the eor and, if anything, derive from an excess interstitial concentration. A strain-management technique developed to suppress dislocation formation during SIMOX processing(15), yielded insight into the nature of the damage process near the eor. This technique utilizes a self-ion beam as a spatially specific probe to manipulate pre-existing lattice defects. In particular, the beam was used to probe the vacancy-rich superficial layer formed by implanting 1.25 MeV self-ions at 450°C to a fluence of $2 \times 10^{17}\ cm^{-2}$. The energy of the probe beam was set to 300 keV so that the range of the ions (~0.4 μm) would match the depth of the maximum vacancy concentration. RBS spectra in Fig. 4 compare the aligned yield, before and after application of the probe, in a virgin lattice (Δ and −, respectively); and in one previously implanted at 1.25 MeV (• and +, respectively). In particular, attention should be focused within the superficial layer (over a depth of ~0.5 μm) where any damage produced by this 300 keV beam would be seen as an incremental change in the aligned yield. It is clear that the damage produced by the 300 keV ions causes a marked increase in the aligned yield from the virgin crystal. This contrasts with the behavior in the 1.25 MeV implanted sample where the aligned yield is unchanged indicating no additional accumulation of damage due to the probe irradiation. In fact, positron analysis in Fig. 2 (dashed curve) demonstrates that

the 300 keV beam actually reduced the concentration of vacancy-type defects formed by 1.25 MeV self-ions. Presumably, this occurs as a result of an attraction between the atomic excess introduced by the beam and the vacancies resulting in mutial annihilation. (It is interesting to note the difference in sensitivity to vacancies between the two characterization techniques. While these defects are easily detected using positrons, the spectra in Fig. 4 show the RBS technique to be relatively insensitive.)

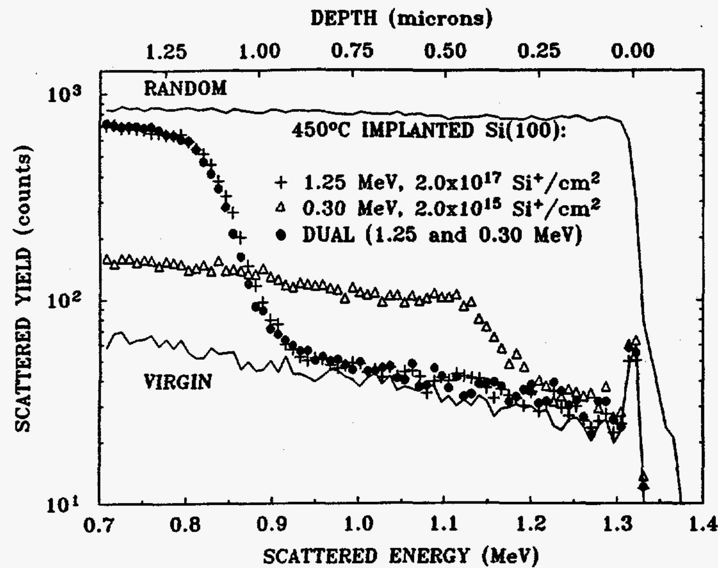

Fig. 4. Spectra comparing the [100] aligned yield from samples with and without a probe beam implantation at 450°C. The probe consisted of a 2×10^{15} cm^{-2} fluence of 300 keV self-ions. The spectra show the effects of the probe in a virgin Si(100) crystal, and one predamaged at 1.25 MeV with self-ions to a fluence of 2×10^{17} cm^{-2}. A random yield is also shown.

The probe results clearly show that the damage growth near the eor is affected by the state of the lattice, i.e., damage forms (under the conditions studied) within a virgin lattice but not in one with a high-vacancy concentration. The absence of damage near the probe's eor within the predamaged lattice suggests that cascade phenomena such as displacement spikes do not contribute to the damage process at elevated temperatures. A spike, first proposed by Brinkman[16,17] to account for eor damage, is a violently disturbed region formed by the high density of atomic displacements produced by an ion as it slows down. Since the spike mechanism for forming damage involves the collective motion of a large number of atoms, a relative small density of pre-existing defects within the vicinity of a spike is not expected to significantly impact either its size or density. Therefore, the absence of eor damage within the predamaged lattice leaves one to conclude that displacement spikes are of no consequence at elevated temperatures and must be completely relaxed through defect recombination. Rather, it appears that eor damage forms in the virgin lattice as a result of the inability of the lattice to accommodate the atomic excess produced by implantation. Since a virgin lattice contains insufficient vacant sites to accommodate the implanted atoms, it is reasonable to assume that interstitial type defects will be formed. This is consistent with reports of interstitial-type defects near the eor such as the loops, rods, and intermediate defect configurations[18].

CONCLUSIONS

New effects related to ion-induced damage accumulation at high-temperature in Si(100) were demonstrated. The use of self-ions in this study showed the effects to be independent of the ion-solid chemistry. Mechanisms were elucidated, including one based on kinematic separation of Frenkel pairs to account for the vacancy excess within the superficial layer which gives rise to negative lattice strain. A technique utilizing a self-ion beam was shown to be effective in eliminating pre-existing, vacancy-type defects. The results from studying the interaction between the self-ions and pre-existing defects demonstrated that cascade effects are of little or no importance to damage accumulation at elevated temperatures, even near the eor. Rather, damage appears to form near the eor simply because implanted atoms cannot be accommodated within the lattice without damage formation.

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