SIMULATIONS OF CASCADE DAMAGE IN SILICON

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Summary

In an effort to better understand radiation damage to electronic materials, we use the binary-collision simulation code MARLOWE to model displacement cascades in silicon. We examine the average number of displacements produced by knock-on atoms as a function of their energy. The resulting vacancy-interstitial pairs are classified according to separation radius. We also examine a few particular cases of 100 keV cascades in silicon in order to highlight the importance that channeling has on the shape of displacement cascades.

Introduction

Displacement damage in silicon is investigated with a computer simulation that calculates the structure of the individual cascades of displacement damage that follow upon the initial collision of an impinging particle with a lattice atom. In order to simulate such damage cascades in electronic materials, we have used the binary-collision cascade simulation code MARLOWE, developed by Robinson and Torrens.1-3 Our main concern in this paper is with the displacement cascades themselves, and not the relation between such cascades and the damage to an electronic component, although some single electrical models are developed at the end.

There are three portions to this study. After outlining how the MARLOWE code works, we use it to estimate the number of displacements produced by external radiations that transfer an energy E to a lattice atom. These results are obtained as a function of the energy E and the resulting vacancy-interstitial pairs are grouped according to their separations. The second portion is a specific examination of several 100 keV cascades, from which we learn that there is more variety in such cascades than the usual tree structure attributed to them. Finally an attempt is made to relate the calculated distributions of vacancies and interstitials to experimental carrier removal rates from neutrons.

Calculations

Binary-Collision Simulation Code MARLOWE

In the mode in which we use it, a MARLOWE calculation is started by giving an energy E to an atom in a lattice site. This primary knock-on atom (PKA) lies in an infinite silicon crystal, which we model in its diamond lattice, at zero temperature, with the silicon lattice constant of 0.543 nm. Inclusion of temperature effects will reduce the channeling but it is unknown at what temperature this will become important. The direction of the atom's momentum is chosen randomly with respect to the crystal directions. MARLOWE operates by following the collision of this PKA with the atom (or several atoms) that lie immediately in its path. The code assesses the momenta of both particles and, if the lattice atom receives an energy greater than the displacement energy, here taken as 15 eV, both ions are then followed as they traverse the lattice. The code successively observes the next collision of the fastest moving ion, until all of the ions have energies less than some cutoff energy, usually taken of the order of the displacement energy. A local Molière potential represents the elastic scattering between atoms. The electronic energy loss is the impact parameter dependent option of the MARLOWE code.

After the above calculation is complete, a new PKA is started (in virgin crystal) and the process repeated until sufficiently good statistics are obtained. The program's output yields a large amount of information, including the ranges of the PKA's, the number of displacements created, the length of replacement sequences, the fraction of the initial energy E that goes into electronic losses, the location of the interstitials and vacancies produced, and so forth. The MARLOWE code can, of course, yield other relevant geometric and interaction parameters since it calculates the actual interactions and the location of all particles. Some such outputs are used in the electrical calculations of the last section.

Number of Displacements versus Energy

Our first effort was to determine the average number of displacements produced by a PKA of energy E. After producing a cascade, MARLOWE determines the separations of the resulting vacancies and interstitials and orders them according to the distance between an interstitial and the nearest unpaired vacancy. If the lattice site nearest an interstitial is vacant, then the vacancy and interstitial are said to form a close pair. If we assume that all close pairs recombine, we can label all of the remaining pairs as distant (a somewhat different terminology than that used by Robinson and Torrens). Further, we can assume that all pairs separated by less than n lattice constants have recombined and just count those that are further separated.

Figure (1) shows the results for the number of displacements versus PKA energy for a number of separations radii. Specifically, we show all pairs, all but close pairs, and all pairs separated by more than n=1, 2, 3, 5 and 7 lattice constants. The calculation was done in two parts. We used a cutoff energy of the same value as the displacement energy 15 eV (no displacements are produced for E less than twice the cutoff energy). MARLOWE was used to calculate the number of pairs separated produced by PKA's of energy E, where E ranged between 15 eV and 10 keV. We then fit these seven curves with a simple form, good to about 10%, for this range of energies.

*Work partially supported by the Defense Nuclear Agency and the Defense Advanced Research Projects Agency.
For PKA energies between 10 keV and 1 MeV we used a cutoff of 10 keV. We wrote an auxiliary program that read the MARLOWE output, particularly the remaining energy of the interstitials, and calculated the total number of displacements produced using the fits mentioned above. This procedure saved much of the considerable computer time that would have been required to follow all of the high energy cascades down to a 15 eV cutoff energy. There are statistical spreads associated with the points on Fig. (1), but they are of the order of 1% or less.

It is well known that many of the initially formed pairs recombine. Surely the close pairs will recombine-they consist of an interstitial with less than 15 eV and its nearest lattice site, which is empty. Beyond that it is hard to estimate what an effective recombination radius is. It would be interesting to reverse this process, using experimental results to estimate the final number of displacements and then determining an effective recombination radius from the MARLOWE results. Such an attempt is made in the last section.

**Single 100 keV Cascades**

In order to picture the effects of large, single cascades, we had MARLOWE follow in detail the cascades produced by PKA's with energies of 100 keV. For these runs we used an energy cutoff of 10 keV. The program prints out a table of interstitials with their remaining energies. Because the average range of a 10 keV ion is 15 nm, the damage produced by less than 10 keV ions is fairly localized at their production sites on Figs. (2) through (4). We show in the following drawings only the vacancies whose associated separations are greater than five lattice constants; we assume that all closer pairs have recombined in line with the conclusions of the following section. All the final interstitials shown on Figs. (2) through (4) have a box associated with them. The size of the box represents the residual energy of that atom when the MARLOWE code quit following that atom. More specifically, the volume of this box is proportional to the number of vacancies which an atom of that energy can be expected to create as calculated above. The recombination radius of the full calculation is used. For each of the three displayed cascades the largest box represents 13 displacements. The vacancy versus energy calculation of Fig. (1) shows that the 13 vacancies at a recombination radius of 5 are created by a 9 keV ion. In all the cascade displays we have taken a viewing angle which best portray the cascade. The length of each axis is the minimum required to contain all the points on the display. The axes are parallel to the cubic axes of the silicon crystal.

The first lesson learned from examining these 20 cascades is the considerable variety they display. There is no typical cascade. The two represented in Figs. (2) and (3) are those with the longest and shortest PKA ranges, 720 nm and 10.3 nm. The long-ranged one is shown in Fig. (2). The randomly chosen direction in which the PKA started from the origin was nearly parallel to the large channel in the (110) direction. The PKA produced a number of displacements but was gradually focused into the channel. It produced no displacements from about 510 nm to 720 nm, at which point its energy dropped below 10 keV.

Figure (3) shows the opposite extreme—a PKA that suffers a nearly head-on collision shortly after it leaves its lattice site. The final location of the PKA is shown by the heavy circle. There is a large difference of scale between the figures. Figure (2) shows a cascade which is 444 nm in extent while Figure (3) shows a cascade extending a maximum of 80 nm from the origin. Figure (4) shows another tree-like cascade but with the main fork farther from the origin. We see in Figs. (3) and (4) the tree structure, more traditionally associated with cascades, but even in Fig. (3) one of the two principal branches is focused into a channel. Further, because of channeling and because we have

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**Fig. (1):** The number of vacancies created per eV of initial energy for a silicon projectile in silicon as calculated by the MARLOWE code. The various curves represent different vacancy-interstitial recombination lengths in units of cubic lattice constants.

**Fig. (2):** Cascade of Displacements in silicon resulting from one-100 keV PKA. The path is primarily along the (110) direction and follows a channeling path. The cascade is the longest of the calculated 100 keV cascades. The x-, y-, and z-axes are 8.4, 316, and 311 nm long respectively.

**Fig. (3):** Cascade of Displacements in silicon resulting from one-100 keV PKA. The path is primarily along the (110) direction and follows a channeling path. The cascade is the longest of the calculated 100 keV cascades. The x-, y-, and z-axes are 8.4, 316, and 311 nm long respectively.

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**Fig. (4):** Cascade of Displacements in silicon resulting from one-100 keV PKA. The path is primarily along the (110) direction and follows a channeling path. The cascade is the longest of the calculated 100 keV cascades. The x-, y-, and z-axes are 8.4, 316, and 311 nm long respectively.
100 keV Silicon
Recomb. rad. = 5

Fig. (3): Cascade of displacements in silicon resulting from a 100 keV silicon originating at the origin. The PKA suffered a strong initial interaction and stopped at the first box. This cascade is one of the most dense and most tree-like of the calculated cascade. The positive x-, y-, and z-axes are 57, 44, and 47.5 nm long respectively.

100 keV Silicon
Recomb. rod. = 5

Fig. (4): A tree-like cascade of displacements in silicon resulting from a 100 keV silicon ion. The positive x-, y-, and z-axes are 77, 50, and 35 nm long respectively.

allowed the closer pairs to recombine, there are large gaps in the structure of the trees. Prior calculations of cascade structure were based on amorphous models which were incapable of depicting the more discrete character evident from a full lattice calculation.

While average quantities calculated from the results of these 20 cascades are well determined by MARLOME, the standard deviations associated with most of these quantities are significant compared with the mean values. One should be cautious in using average cascades to represent all cascades.

Relation to Carrier Removal Rates

Simple vacancies in silicon are believed to be mobile at room temperature. Three possible mechanisms will trap the vacancy: 1) combination with an oxygen impurity to form a stable complex, 2) combination with an interstitial which effectively annihilates both defects or 3) combination with another vacancy to form the stable divacancy. These last two competing mechanisms can be quantified in a simple model by the use of the MARLOME code. If we use the PKA spectrum resulting from a 1 MeV neutron on silicon as given by van Lint, and integrate over the energy, the total energy cross section is about 10 keV-cm⁻². The normally observed carrier removal rate in silicon is experimentally found to be near 6 cm⁻¹. Therefore the PKA energy that goes into removing a carrier is about 1.6 keV. Figure (1) gives the number of vacancies created in silicon by a silicon PKA with the vacancy-interstitial recombination length as a parameter. If the carrier removal is associated with the divacancy, the required two unrecombined vacancies forming the divacancy and resulting from 1.6 keV of PKA energy require a vacancy to energy ratio of 1.3 x 10⁻⁴ vacancies/keV.

The curves in Fig. (1) are fairly flat in the main range of interest, the energies of most of the PKA's, a few tens of keV. In this range, to obtain the above experimentally derived vacancy to energy ratio, a vacancy-interstitial recombination length of 5 to 7 lattice constants is required, i.e., 2.7 to 3.8 nm. With such long recombination lengths, approximately 95% of the vacancies have annealed by recombination with an interstitial. This recombination ratio agrees with Leadon's model for short term annealing.

Fig. (4): The radial distribution function of vacancy pairs for a 300 eV silicon recoil in silicon averaged over 400 projectiles. Various vacancy-interstitial recombination lengths are used as a parameter. All lengths are in units of L = 0.543 nm, the cubic lattice constant.
Damage volumes caused by neutrons and their intermediary PKAs are difficult to define unambiguously. As shown previously, displacement damage is a statistical process and varies from one damage volume to another. Even if some average is taken, specification of a dimension or a density cannot describe accurately a spatially varying defect density. One method of presenting spatial information is the use of the radial distribution function (RDF) between vacancies, i.e., the number of vacancy pairs which are separated by a given distance. Such information is available from MARLOWE and is presented in Fig. (5). The code was run for 400 PKA's of energy 300 eV and all ions were followed down to below the displacement energy. The distribution was then averaged. All lengths are given in units of L = 0.543 nm, the lattice constant. The ordinate of the RDF gives the number of pairs per cubic lattice spacing expected on the average. The abscissa is the length parameter but here is presented as the cube of the number of lattice spacings in order to maintain the density meaning of varying width histograms. A 300 eV silicon has an average range of 2.1 L but the RDF shows a significant tail beyond the average range. The RDF is given as a parameter of the vacancy-interstitial recombination length. Because of the small range here, the recombination significantly reduces the vacancy density. The statistics even with 400 particles become poor at large recombination lengths. If our previously estimated recombination length of 5 to 7 L is valid, the annealing factors derive from the 300 eV RDF are too large to explain the annealing data. Thus higher energy PKAs are needed to simulate the terminal cluster damage. This is consistent with Holme's calculation based on electrical measurements of a 6 nm (11 L) diameter electrically active damage volume.

Conclusion

In summary, we see that the nature of the collision cascade is changed dramatically when the effects of channeling and focusing are included in the simulation. In addition, this work has shown that displacement damage in silicon is diffuse for dimensions greater than 10 nm and that channeling along the (110) direction is an important effect. Damage cascades resulting from 100 keV silicon vary wildly in size. Fewer than 30% of the cascade interstitials are more than a cubic lattice constant from a matching vacancy.

References