Modeling of the effects of dose, dose rate, and implant temperature on transient enhanced diffusion

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Atomistic simulations are used to study the effects of implant parameters on transient enhanced diffusion (TED). We analyze 10 keV Si implants in a wide range of doses from 10^8 to 10^{14} ions/cm^2, dose rates from 10^{10} to 10^{14} ions/cm^2 s, and implant temperature from room temperature to 1000 °C. Different regimes with different dependence of TED on these parameters are observed. For high doses, high dose rates, and low implant temperatures, the Frenkel pairs are accumulated during ion implantation, and the resulting damage is very dense. During the postimplant annealing, the recombination of Frenkel pairs is efficient, and the extra interstitials generated by the implanted ions provide the main contribution to the enhanced diffusivity. For low doses, low dose rates, and high implant temperatures, there is little interaction between neighboring cascades during annealing. The recombination of Frenkel pairs is not complete, and many interstitials and vacancies from each cascade survive recombination and contribute significantly to TED. © *1999 American Institute of Physics.* [S0003-6951(99)02214-7]

Ion implantation provides a controlled way of introducing dopants in Si for the fabrication of integrated circuits. The depth and concentration of the doping profile can be determined by the energy and dose of the implant. However, transient enhanced diffusion (TED) of the dopants occurs during the postimplant anneal necessary to cure the damage generated during ion implantation. In spite of the inherent complexity of the process associated with the annealing of the damage, the ''+1'' model has been able to predict TED with considerable success.[1] This model implies that the Frenkel pairs rapidly recombine without contributing significantly to TED, and only the excess interstitial generated as the implanted ion becomes substitutional controls TED. Several experiments[2–4] and calculations[5] confirm the validity of this model for usual implantation conditions: light implanted ions (B, P, or Si), high doses (10^{13}–10^{14} ions/cm^2), high dose rates ($>10^{12}$ ions/cm^2 s), and low implant temperature (around room temperature). According to the +1 model, the enhanced diffusivity is independent of the implanted ion, since all the ions generate only one excess interstitial. It increases linearly with dose, since the number of excess interstitials equals the number of implanted ions. And TED is independent of dose rate and implant temperature, since these factors only change the accumulated damage but not the number of excess interstitials.

There are some deviations from the +1 model when the implantation parameters differ significantly from the above conditions. We have found that the enhanced diffusivity increases with the mass of the implanted ion due to more silicon recoils producing a larger separation between interstitial and vacancy profiles.[6] Packan *et al.*[7] have observed that the enhanced diffusivity increases sublinearly with the dose. Jones *et al.*[4] reported that variations in the implant temperature, between 5 and 40 °C, and beam current between 0.035 and 0.35 mA/cm^2, do not influence the final amount of B diffusion after the postimplant anneal. However, Masters *et al.*[8] have shown that both the dose rate between 10^{11} and 10^{13} protons/cm^2 s and implant temperature from 600 to 900 °C, do influence B enhanced diffusion during implantation. Also, Venezia *et al.*[9] have observed the effects of implant temperature between room temperature (RT) and 400 °C on B and Sb diffusion.

In this letter we study by atomistic simulation the influence of dose, dose rate, and implant temperature on the enhanced diffusivity of dopants in Si. We provide a comprehensive understanding of the different regimes for doses between 10^8 and 10^{14} ions/cm^2, dose rates between 10^{10} and 10^{14} ions/cm^2 s, and implant temperatures between RT and 1000 °C.

The implantation cascades are simulated with MARLOWE,[10] and the coordinates of Si self-interstitials and vacancies are transferred to the Monte Carlo diffusion code DADOS.[11] They are given random hops according to their respective diffusion hop rates at the implant temperature. Clusters of point defects are formed when the mobile point defects jump within the capture radius of other point defects or pre-existing clusters. The dissolution of the clusters occurs by the emission of a point defect at a rate determined by their binding energy. The simulation parameters are the same as in Ref. 12. New implantation cascades are added at intervals of time determined by the dose rate until the specified dose is reached. Then, additional annealing at the same or different temperature can be carried out for a specified amount of time. The surface is considered as a perfect sink for point defects.[13] To implement the +1 model in our atomistic simu-

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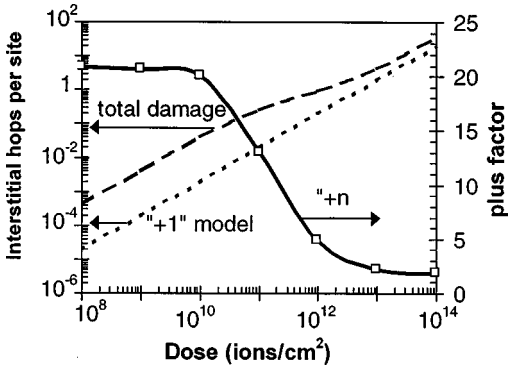

FIG. 1. Total number of interstitial hops per lattice site vs implantation dose using the total damage and the plus one model for a 10 keV Si room temperature implant, 10^{12} ions/cm^2 s, annealed at 800 °C for 1000 s. The plus factor ($+n$) is the ratio between the total number of hops using the two models.

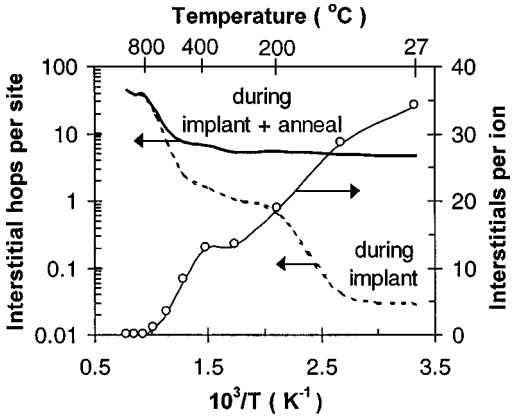

FIG. 2. Total number of interstitial hops per lattice site vs the inverse of the implant temperature for a 10 keV 10^{13} ions/cm^2 Si, 10^{12} ions/cm^2 s implant, as implanted and after 800 °C, 1000 s anneal. The residual damage (interstitial remaining per implanted ion) after implantation is plotted by the line with circles.

lation we follow the same scheme as described above but instead of including all the Frenkel pairs generated in each cascade, we only consider the implanted ion. We discuss TED in terms of interstitial hops at a depth 10 times the projected range of the implanted ions. The total number of interstitial hops per lattice site is proportional to the time averaged diffusivity of interstitial diffusing dopants, such as B.[6] The ratio between the number of hops using the total damage to that using the $+1$ model we define as the effective plus number ''$+n$.''[6]

First, we study the dose dependence. Figure 1 is a plot of the total number of interstitial hops per lattice site versus the implantation dose for 10 keV Si implants at RT with a dose rate of 10^{12} ions/cm^2 s, and annealed at 800 °C for 10 min. Three different regimes are observed. For high doses (above 10^{13} ions/cm^2), the number of interstitials hops increases linearly with dose and it is close to the number using the $+1$ model. For low doses (below 10^{10} ions/cm^2), the number of hops also increases linearly with dose but it is approximately 20 times the number obtained using the $+1$ model. For intermediate doses (between 10^{10} and 10^{13} ions/cm^2) the number of interstitial hops increases sublinearly with dose, as reported by Packan *et al.*[7]

This result can be understood as follows. The damage generated in one single cascade is dense; some recombination takes place very rapidly and the surviving Si interstitials and vacancies form clusters. According to MARLOWE calculations, the average number of Frenkel pairs generated by a 10 keV Si cascade is 155. A significant fraction of them are recombined at RT, leaving approximately 50 Frenkel pairs per implanted ion after RT implantation. For high doses, the residual damage from different cascades overlap and it is not possible to distinguish individual cascades. The average distance between Si interstitials and vacancies is very small. During the postimplant anneal, the recombination is efficient, and only the extra interstitials generated by the implanted ions moving onto lattice sites, contribute significantly to TED, giving validity to the $+1$ model.

For extremely low doses, the implantation cascades do not overlap and the average distance between cascades is larger than the distance to the surface. The interstitials and vacancies that escape from the original cascade diffuse until they are annihilated at the surface. Since all the cascades behave independently, the number of hops is proportional to the number of cascades. The factor of 20 for ''$+n$'' indicates that, for a 10 keV Si implant, some interstitials of the Frenkel pairs are diffusing significant distances and contribute about 20 times more hops than the interstitial kicked out by the implanted ion. For intermediate doses the distance between cascades is comparable to the distance to the surface. The interstitials that escape from one cascade diffuse until they are recombined with defects of other cascades or are annihilated at the surface. The value of $+n$ decreases with increasing dose because the implantation cascades are closer to each other and the number of hops that the interstitials give before recombination decreases.

We have investigated the influence of the substrate temperature by simulating the implantation of 10 keV Si ions, to a dose of 10^{13} ions/cm^2 and a dose rate of 10^{12} ions/cm^2 s, into Si between RT and 1000 °C. The implantation cascade is not changed with the substrate temperature and only the annealing of the damage during implantation at elevated temperature is taken into account. In Fig. 2 we plot the total number of interstitial hops as a function of the reciprocal of the implant temperature, after implantation and after a postimplant anneal at 800 °C for 10 min. At low implant temperature (below 400 °C) a significant number of Frenkel pairs of each cascade survive in the form of interstitial or vacancy clusters. The number of interstitial hops during implantation increases with temperature, due to the release of some free interstitials during the Ostwald ripening of the interstitial clusters.[9] However, in this temperature range, the number of interstitial hops during implantation is negligible compared to the total number of hops during the anneal. After the postimplant anneal the measured B diffusivity (proportional to the total number of hops) is approximately the same for all implant temperatures in this range, in agreement with Jones *et al.*[4]

For high implant temperatures (above 700 °C), most of the damage generated in each cascade is annealed out during implantation. The residual damage is small, and there is little interaction between cascades; this is similar to the low dose regime. Many interstitials escape from each cascade and diffuse until they are annihilated at the surface. The number of

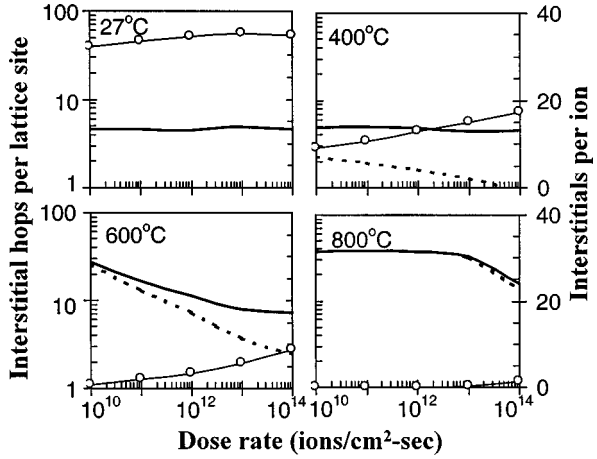

FIG. 3. Total number of interstitial hops per lattice site vs dose rate for a 10 keV 10^{13} ions/cm^2 Si implant as implanted (dashed line) and after 800 °C, 1000 s anneal (solid line), for implants at 27, 400, 600, and 800 °C. The number of hops per site as implanted at RT is constant at 0.028. The residual damage after implantation is represented by the line with circles.

interstitial hops is constant and it is 20 times the value given using the +1 model, indicating the annealing of independent cascades during implantation. Above 1000 °C equilibrium thermal diffusion dominates since the number of defects created by the implant is small compared to the intrinsic defect concentration at elevated substrate temperatures.

For intermediate implant temperatures (between 400 and 700 °C), the implantation cascades are partially annealed during ion implantation, and there is some interaction between the residual damage of each cascade, similar to the intermediate dose regime. Still there are Frenkel pairs left after implantation, which are annihilated during the postimplant anneal at higher temperatures. The number of interstitial hops during implantation is comparable to the number of hops during the postimplant anneal. The number of interstitial hops increases with implant temperature, due to the release of free interstitials from the dissociation of interstitial clusters, at the same time that the residual damage during ion implantation decreases. The reduction in the number of Frenkel pairs in neighboring cascades during implantation causes a reduction in the interaction between cascades.

In a similar fashion, we have studied the influence of the dose rate for 10 keV Si at four different implant temperatures: 27, 400, 600, and 800 °C. We vary the dose rate between 10^{10} and 10^{14} ions/cm^2 s, while keeping the dose constant at 10^{13} ions/cm^2. A postimplant anneal at 800 °C for 1000 s is carried out in all cases. The total number of interstitial hops versus the dose rate for the four implant temperatures is showed in Fig. 3. Different dose rate dependences are found depending on the implant temperature. At RT the total number of interstitial hops during implantation is very low compared with the total number after high temperature annealing. Interstitial and vacancy clusters are stable at RT, and therefore, the damage is accumulated during ion implantation. During the high temperature anneal recombination is very efficient and most of the TED occurs in the plus one regime. After the postimplant anneal the total number of hops is independent of the dose rate, in agreement with the experimental results by Jones *et al.*[4] A noticeable dependence of the number of interstitial hops during implantation on the dose rate is found at 400 °C. This is due to the release of some free interstitials from small clusters that anneal slowly at 400 °C. However, the contribution of the hops during implantation is still small compared with the total number of hops after the postimplant anneal. Therefore, the total number of hops after anneal is again independent of dose rate, similar to the implant at RT.

The effect of the dose rate becomes significant at 600 °C. At very low dose rate, the time between cascades is long enough to allow the anneal of each cascade independently. As the dose rate increases, less damage is annealed out during the implantation. The damage builds up and fewer interstitials escape recombination. At 800 °C the interstitial and vacancy clusters are not stable and each cascade has little or no interaction with neighboring cascades. Only at very high dose rates ($\sim 10^{14}$ ions/cm^2 s) there is some residual damage after implantation and some reduction in the number of hops. Dose rates below 10^{13} ions/cm^2 s produce approximately the same total number of interstitial hops. The time average diffusivity is proportional to the total number of hops and inversely proportional to the total time. The total implantation time is inversely proportional to the dose rate. Therefore, in the high temperature regime, the time average diffusivity, measured during the actual implantation only, is proportional to the dose rate, in agreement with Masters *et al.*[8]

In summary, when implantation cascades are annealed independently, many interstitials escape recombination for a long enough period to contribute significantly to TED. This situation happens at low doses, high implant temperatures, and low dose rates. At high doses, low temperatures, and high dose rates, the damage is accumulated during ion implantation. During a high-temperature postimplant anneal, recombination of Frenkel pairs is efficient and only the extra interstitial generated by the implanted ion controls TED.

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