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G. Subramanian, K.S. Jones, M.E. Law, M.J. Caturla, S. Theiss, T. Diaz de la Rubia

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G.Subramanian*, K.S. Jones*, M.E.Law**, M.J.Caturla***, S.Theiss***, T.Diaz de la Rubia***
*Department of Materials Science & Engineering, 525 Engineering Bldg.
**Department of Electrical and Computer Engineering, 525 Engineering Bldg.
SWAMP Center, University of Florida, P.O.Box 116400, Gainesville, FL 32611
***Lawrence Livermore National Laboratory, Livermore, CA 94550

ABSTRACT

{311) defects and dislocation loops are formed after ion-implantation and annealing of a silicon wafer. Recent Transmission Electron Microscopy studies by Li and Jones have shown that sub-threshold dislocation loops nucleate from {311} defects. In our study, the conjugate gradient method with the Stillinger Weber potential is used to relax different configurations such as {311} defects with a maximum of five chains and perfect dislocation loops. From the formation energies thus obtained we find that there is an optimal width for each length of the {311} defects. Moreover the relative stability of {311}s and loops is studied as a function of defect size. We observe that at very small sizes the perfect loops are more stable than the {311}s. This may provide an explanation for the experimental observation by Robertson *et al* that, in an annealing study of end of range damage of amorphized samples, 45% of the loops had nucleated in the first 10 minutes of anneal. We propose that homogeneous nucleation, as against unfaulting of the {311}s, could be the source of these loops.

INTRODUCTION

Shallow junctions , produced by ion-implantation, are a necessity if microelectronic devices of smaller dimensions are to be realized. It is well known that {311} defects and dislocation loops are formed upon annealing subsequent to ion-implantation. It is also known that {311} defects, as a source of interstitials , contribute significantly to the phenomenon of transient enhanced diffusion (TED) of dopants such as boron in ion implanted silicon during post-implant annealing [1]. Transient enhanced diffusion has a deleterious effect on the formation of shallow junctions The formation and evolution of these {311} defects is of great interest to researchers. On the other hand, the source of dislocation loops has been a subject of conjecture for a number of years. It has been observed by transmission electron microscopy (TEM) that concomitant with the dissolution of {311} defects, some small loops grow in size [2]. Similar connection between the

dissolution of {311} defects and the growth of loops has been observed by other groups [3].

Recently, Li and Jones have shown through TEM studies that sub-threshold dislocation loops nucleate from {311} defects by unfaulting of the latter [4]. Robertson *et al* have reported that in the case of end-of-range damage of ion implanted silicon 45% of the dislocation loops were formed in the first 10 minutes of anneal [5]. In this work, we report, for the first time , through simulations, the stability of the {311} defects depending on the length and width of the interstitial chains that constitute this defect. We also analyze, through simulations, the relative stability of the {311} defects and perfect dislocation loops. The methodology of the simulations has been the conjugate gradient technique using the Stillinger –Weber (SW) [6] interatomic potential.

COMPUTATIONAL DETAILS

The Stillinger-Weber potential used in this work is the most widely used interatomic potential for silicon. In our simulations, we used a 27000 atom computational cell. This large cell size ensures that the lattice displacement field created by the relaxed extended defects is contained within the cell. For {311} defects the interstitial configuration used here is similar to that used by Kim *et al* [7]. The interstitial chains constituting the {311} defect are extended along the <011> direction and they lie on the {311} plane. Laterally, the interstitital chains are added along the <233> direction. The adjacent interstitial chains are separated from each other by a distance of $\frac{a\sqrt{11}}{2\sqrt{2}}$ where a is the lattice parameter. This configuration is then relaxed using the conjugate gradient method with the SW interatomic potential. As a consequence of this relaxation we obtain the formation energy of the {311} defects as a function of the number of interstitials in the defect. Calculations are done for different number of chains up to a configuration five chains wide. Similarly, the circular configuration of the perfect dislocation loop is created with Burgers vector a/2 <110>. Subsequently, the loop configuration is relaxed using the conjugate gradient method to yield formation energies for varying loop size.

RESULTS AND DISCUSSION

The total formation energies obtained using the conjugate gradient method are plotted in fig(1) as a function of number of interstitials. It is evident from this figure that as the defect size increases, the least energy configuration has progressively increasing widths. This trend is for the first four chains only. The

five-chain wide defect has a higher formation energy compared to the four- chain wide defect for the defect sizes accessible from this simulation. A closer inspection of the data suggests that the five-chain defect will become more stable than the four-chain defect at a larger defect size.

Fig(2) shows the formation energy per interstitial of the {311} defect as a

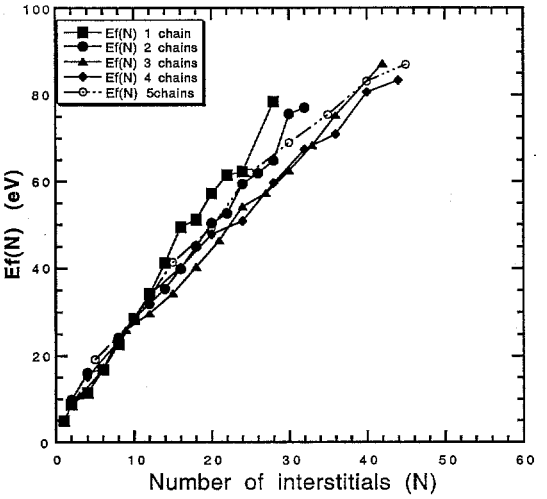

Fig 1: Formation energy versus defect size of {311} defect for different number of chains

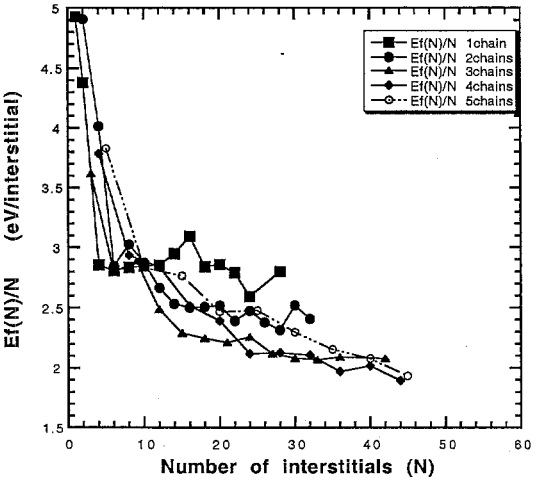

Fig 2: Formation energy per interstitial versus defect size of {311} defect for different number of chains

function of the defect size for different number of chains that constitute the defect. This figure demonstrates that the formation energy of the defect decreases as the defect size increases. Moreover, as in fig(1), the trend seems to be that the most stable defect width (number of chains) increases as the defect size increases. The formation energy per interstitial curves (fig(3)) for the perfect loop and {311}s show a decreasing energy trend with increasing defect size. Moreover, the formation energy per interstitial curve for the perfect loop follows closely the most stable {311} energy curves for defect sizes greater than 20 interstitials. Fig(4) (after Robertson *et al* [5]) shows the percentage of loop nucleation as a function of anneal time. It is evident from this plot that 45% of loops were nucleated during the first 10 min of anneal. We propose that homogeneous nucleation as opposed to {311} unfaulting may be the dominant mechanism of loop nucleation during this time interval. Unfaulting of the {311}s occurs after a further anneal at 750^{0}C, thereby suggesting that there is an energy barrier for the unfaulting process.

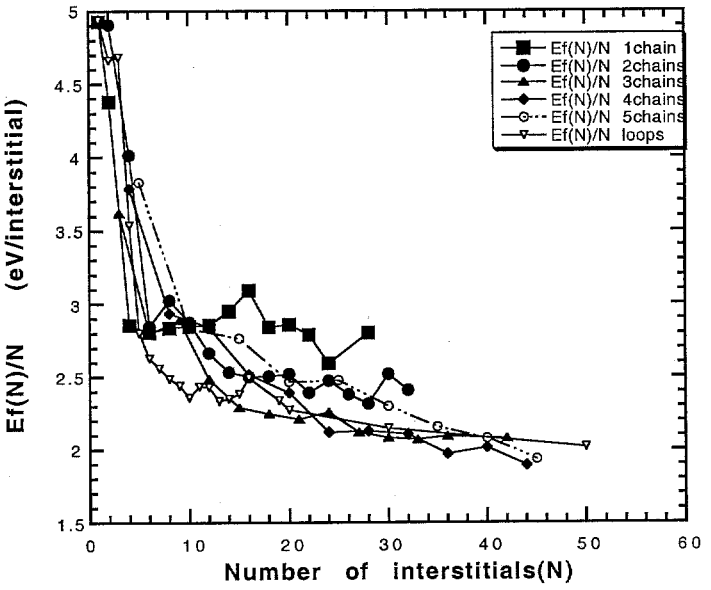

Fig.3: Formation energy per interstitial versus defect size for {311} defect with different number of chains and for perfect dislocation loop

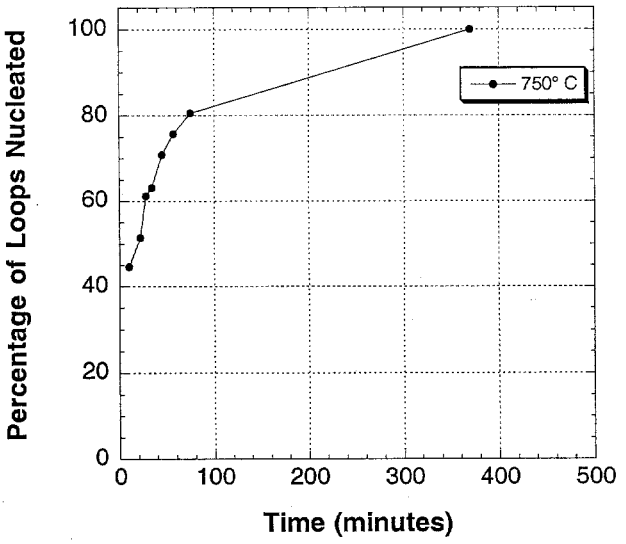

Fig.4: Percentage of dislocation loops formed as a function of annealing time. (After Robertson *et al* [5])

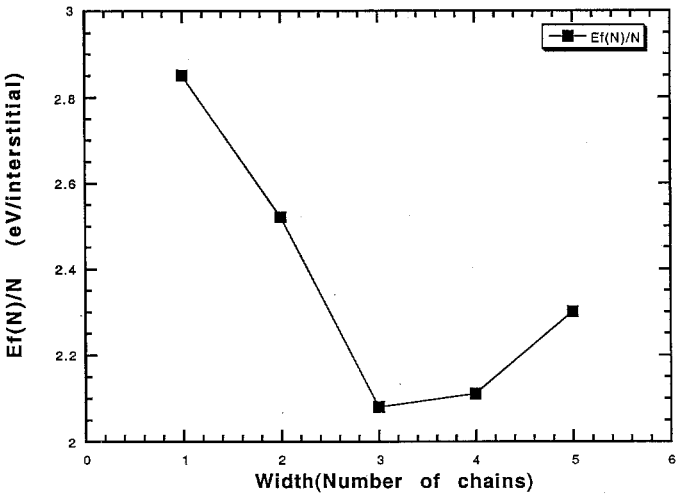

Fig.5: Formation energy per interstitial versus width (Number of chains) for {311} defect size N=30

Fig. 5 depicts the formation energy per interstital as a function of width (number of chains) for a defect size of 30 interstitials. This helps in understanding the trend of energy values vs width size indicating the relative stability of {311} defects for different number of chains.

CONCLUSIONS

We have done atomisitic simulations using the conjugate gradient method with the Stillinger-Weber potential to obtain the formation energy of {311} defects for defect widths up to 5 chains. We observe that the most stable {311} defect has progressively increasing width with increasing defect sizefor the defect sizes studied. We have also computed the formation energy of perfect dislocation loops for increasing number of interstitials in the defect. It is observed that the formation energy curve of the loops is aligned with the formation energy curve of the most stable {311} defect for defect sizes greater than 20 interstitials. We conclude that nucleation of loops, during the initial 10 minutes of anneal at 750°C may be due to homogeneous nucleation and that subsequently, there is a energy barrier for unfaulting of the {311}s to form loops. This unfaulting occurs during further anneals at 750^0C.

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