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LLNL-PROC-406296

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August 14, 2008

ICASC-23
Phalaborwa, South Africa
August 17, 2008 through August 22, 2008

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Prepared for proceedings of ICACS 2008.

Effects of the density of collision cascades: Separating contributions from dynamic annealing and energy spikes

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(Dated: August 13, 2008)

We present a quantitative model for the efficiency of the molecular effect in damage buildup in semiconductors. Our model takes into account only one mechanism of the cascade density dependence: nonlinear energy spikes. In our three-dimensional analysis, the volume of each individual collision cascade is divided into small cubic cells, and the number of cells that have an average density of displacements above some threshold value is calculated. We assume that such cells experience a catastrophic crystalline-to-amorphous phase transition, while defects in the cells with lower displacement densities have perfect annihilation. For the two limiting cases of heavy (500 keV/atom ^{209}Bi) and light (40 keV/atom ^{14}N) ion bombardment of Si, theory predictions are in good agreement with experimental data for a threshold displacement density of 4.5 at.%. For intermediate density cascades produced by small 2.1 keV/amu PF_n clusters, we show that dynamic annealing processes entirely dominate cascade density effects for PF_2 ions, while energy spikes begin contributing in the case of PF_4 cluster bombardment.

INTRODUCTION

Bombardment of semiconductors with cluster ions often results in an enhanced buildup of stable lattice defects near the sample surface, where collision cascades generated by the atomic components of a cluster ion spatially overlap. This phenomenon, referred to as the *molecular effect* (ME) in damage accumulation, has been studied for several decades (see, for example, [1–3] and references therein). The ME efficiency γ can be defined as the ratio of the concentrations of stable lattice defects produced by cluster and atomic ions when the following bombardment parameters are kept constant: ion energy normalized to amu, ion fluence normalized to the number of displacements per atom (DPA), and ion beam flux normalized to DPA s^{-1} [4].

The ME is related to an enhanced damage formation efficiency for denser collision cascades. Two fundamentally different mechanisms could contribute to the dependence of the damage production efficiency on the cascade density: *dynamic annealing* [5] and *energy spikes* [1–3, 6]. Nonlinearity of dynamic annealing processes (i.e., processes of migration and interaction of radiation-generated point defects during bombardment) results in a more efficient formation of stable defects for denser cascades. This mechanism has recently been discussed in detail in [7]. The formation of energy spikes involves collective processes during the thermalization of collision cascades (i.e., for times $\lesssim 10$ ps [1, 2]) for cascade densities above some critical value. The following criteria for energy spike formation are currently well accepted in the literature: [1–3, 6, 8] (i) the collisions in the cascade are so dense that they can no longer be considered as pair collisions, leading to a decrease in an effective displacement energy of lattice atoms; (ii) the average fraction of displaced atoms in a collision cascade exceeds the critical fraction of displacements necessary for the disordered crystalline lattice to experience a catastrophic transformation into an amorphous state; and (iii) the average energy (per lattice atom) within the volume of a collision cascade exceeds the critical energy (per lattice atom) required for substrate melting.

Both energy spike and dynamic annealing processes could operate simultaneously. In some cases, one process could dominate. For example, we have recently shown that, for Si bombarded at room temperature with 40 keV/atom N_1 and N_2 ions, the ME is due to dynamic annealing [7], while for GaN bombarded with keV heavy ions, energy spikes appear to dominate the cascade density dependence of the damage production efficiency [9].

Any quantitative analysis of the ME requires calculations of the density of collision cascades. However, the three-dimensional shape of collision cascades is complex, and even the definition of such a density is not straightforward [2, 4, 10]. In this paper, we present a new algorithm for calculations of the efficiency of the ME in damage buildup in semiconductors. In this algorithm, we assume that the ME is due to only one mechanism: the formation of nonlinear displacement spikes. A comparison of such theoretical predictions with experimental data allows us to separate contributions from energy spikes and dynamic annealing. Our results point to an increasing role of energy spikes in ion-beam defect processes in Si with increasing mass of PF_n cluster ions.

TABLE I: Parameters used in calculations, where $N_{atom}^{cascade}$ is the number on individual atomic cascades analyzed, $N_{cluster}^{cascade}$ is the number of molecular cascades analyzed, and R_{pd} is the position of the maximum of the nuclear energy loss profile.

Ion	Energy (keV)	R_{pd} (nm)	$N_{atom}^{cascade}$ (10^3)	$N_{cluster}^{cascade}$ (10^3)
Bi	500	92	4.5	10
N	40	75	30	40
P	65	60	15	–
F	40	60	30	–
PF_2	145	60	–	20
PF_4	225	60	–	20

CALCULATION OF MOLECULAR EFFECT EFFICIENCY

The output of well known TRIM code [11] simulations contains the coordinates of all the lattice displacements generated. In the TRIM calculations reported here (version SRIM 2006.02), the threshold displacement energy of Si atoms was 13 eV (based on experimental data from [12]), and replacement collisions were excluded from the analysis. In our algorithm, all vacancy coordinates, calculated with the TRIM code, are saved for a statistically large number of cascades for every ion-energy combination (see Table I). An individual cascade (i.e., a set of vacancy coordinates) of a cluster ion is constructed from a sum of randomly chosen individual cascades generated by the atoms forming the cluster ion. The overall volume of each individual collision cascade is divided into cubic cells with a size of 2.5 nm. For every cell, an average density of displacements is calculated as the ratio of the number of lattice vacancies to the total number of atoms in the cell.

Since energy spike processes are expected to have a threshold dependence of the damage production efficiency on the cascade density, we assume that a crystalline-to-amorphous phase transition occurs in a given cell when the average density of vacancies in it exceeds some threshold value n_c. For vacancy densities below n_c, we assume that no stable defects are produced. The ME efficiency γ for a given depth is calculated as the ratio of the number of cells with vacancy densities above n_c for a cluster ion and randomly chosen atomic ions forming the cluster. The result is averaged for a statistically large number of cluster and atomic ions.

RESULTS AND DISCUSSION

We first consider the case of irradiation of Si at liquid nitrogen temperature with 500 keV/atom Bi_1 and Bi_2 ions studied experimentally in [10]. For such heavy-ion, low-temperature irradiation, the formation of energy spikes should dominate cascade density effects in Si [10]. Hence, our current model, which ignores dynamic annealing altogether, should be valid. Figure 1 shows both experimental and theoretical depth profiles of γ for Bi. Theoretical profiles are shown for different values of n_c. It is seen from Fig. 1 that theoretical and experimental curves agree for $n_c = 4.5$ at.%. Below, we will use this n_c value in all calculations for the other ion-energy

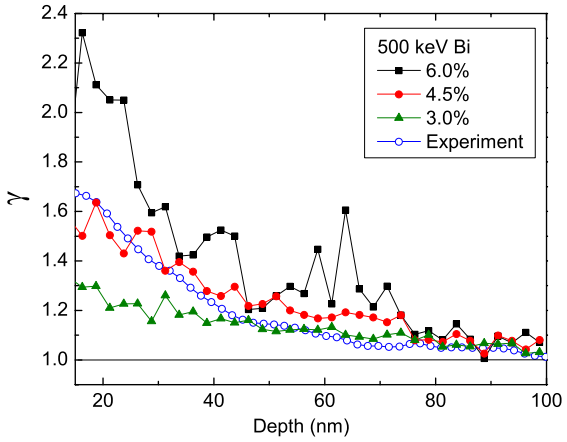

FIG. 1: Depth dependence of the molecular effect efficiency γ in Si bombarded at liquid nitrogen temperature by 500 keV/atom Bi_1 and Bi_2 ions. Threshold densities of displacements for the formation of energy spikes are given in the legend. Experimental data are taken from [10].

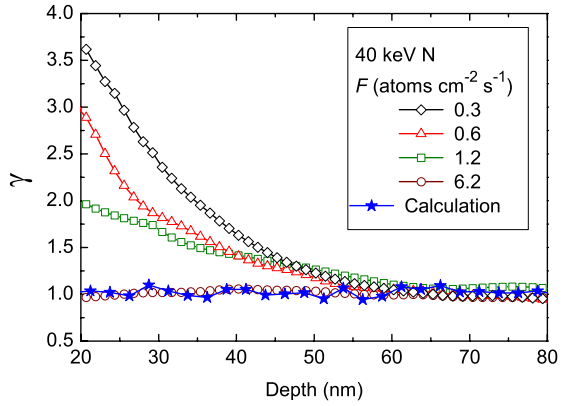

FIG. 2: Depth profiles of the efficiency of the molecular effect γ in Si bombarded at room temperature with 40 keV/atom N_1 and N_2 ions for four different values of ion beam flux, as indicated. The theoretical curve is for a threshold displacement density of 4.5 at.%. Experimental data are taken from [7].

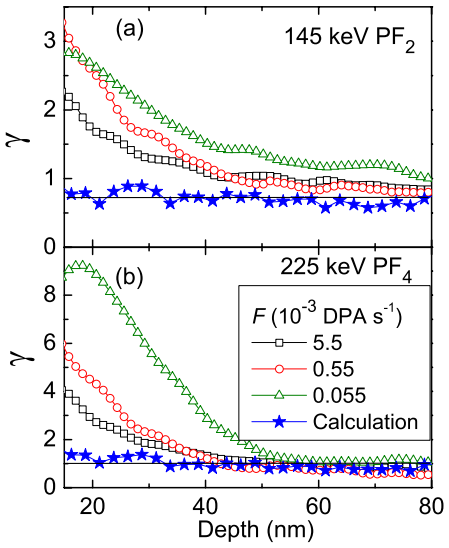

FIG. 3: Depth profiles of the efficiency of the molecular effect γ in Si bombarded at room temperature with 2.1 keV/amu PF_2 (a) and PF_4 (b) ions for three different values of ion beam flux, as indicated. The theoretical curve is for a threshold displacement density of 4.5 at.%. Experimental data (except for the curev for the ion beam flux of 5.5×10^{-5} DPA s^{-1}) are taken from [4].

combinations.

Figure 2 compares experimental (taken from [7]) and theoretical depth profiles of γ for the case of Si bombarded at room temperature with 40 keV/atom N_1 and N_2 ions for different values of ion beam flux. It is seen from Fig. 2 that our model based on energy spikes predicts the absence of the ME for all depths (i.e., $\gamma = 1$) in agreement with experiments for irradiation with large beam flux values. Indeed, as discussed in detail in [7], the strong ion flux dependence of the ME efficiency in this case is evidence that dynamic annealing rather than energy spikes is the underlying mechanism of the ME for light-ion bombardment of Si.

Finally, Fig. 3 shows results for Si bombarded at room temperature with PF_2 [Fig. 3(a)] and PF_4 [Fig. 3(b)] ions. The experimental γ depth profiles shown in Fig. 3 were obtained based on our ion channeling data reported in [4] (and based on our previously unpublished data for the lowest beam flux value) as the ratio of the concentrations of stable defects produced by a PF_n cluster and P atomic ions. A strong ME is seen in Fig. 3, particularly for PF_4 ions, for which five individual cascades of P and F atoms overlap in the near surface region, resulting in γ as large as ~ 9. Figure 3 also shows that γ decreases with increasing beam flux, indicating that dynamic annealing processes contribute to the ME [7]. However, γ reduces with increasing depth, even for the largest value of the beam flux studied (5.5×10^{-3} DPA s^{-1}), leaving the uncertainty about the possible contribution of energy spikes.

Theoretical depth profiles of γ shown in Figs. 3(a) and 3(b) help us separate the roles of dynamic annealing and energy spikes processes for PF_n ion bombardment. It is seen from Fig. 3 that our energy-spike-based model predicts a small ME (with $\gamma \approx 1.5$ near the surface) for the case of PF_4 ions and no ME for the case of PF_2 ions. Hence, dynamic annealing processes are primarily responsible for the ME for PF_2 ion bombardment, while energy spikes contribute to the ME observed for PF_4 ion bombardment of Si.

SUMMARY

In summary, we have presented an algorithm for calculations of the molecular effect in semiconductors based on nonlinear energy spikes. Our model is in agreement with experimental data for the ME in Si bombarded with 500 keV/atom $Bi_{1,2}$ and 40 keV/atom $N_{1,2}$ ions, for which the ME is due to energy spikes and dynamic annealing, respectively. Our model predicts that for PF_2 ions dynamic annealing processes are responsible for the ME observed, and energy spikes have a (minor) contribution to the ME for PF_4 ion bombardment of Si.

The authors thank T. Kuchumova for help with calculations. Work in St. Petersburg was supported by grant RFFI 08-08-00585. Work at LLNL was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

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