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Continuum modeling of post-implantation damage and the effective plus factor in crystalline silicon at room temperature

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Abstract

The role of computer simulation in predicting intrinsic diffusion effects is amplified with the shrinkage of MOS devices. In this work, post-implant damage distributions are obtained from atomistic Monte Carlo (MC) simulations. Based on diffusion-limiting kinetics, the evolution of the damage at room temperature with time is studied. It is shown that evolution of the point defects follow the Ostwald ripening process, where larger defect clusters grow at the expense of smaller ones. A qualitative study of the effective plus factor is also conducted, taking into account various clustering and recombination processes. Clustering is found to significantly affect the remaining amount of damage, which in turn affects subsequent diffusion processes.

Keywords: Diffusion-limited kinetics; Ostwald ripening; Transient enhanced diffusion

1. Introduction

Progress of the semiconductor industry follows Moore's law, which simply states that the size of a transistor on a silicon chip must be reduced by a factor of two every 18 months. Accurate implant and diffusion models are thus desirable for optimization of the shrinking transistor with ultra-shallow source and drain junctions.

The diffusion constant, D in Fick's law [1] describes only the macroscopic diffusion in thermal equilibrium while the diffusion that limits scaling of transistors today takes place in a microscopic scale far from equilibrium. As much as diffusion is undesired especially when enhanced, annealing is nevertheless needed to fulfill sheet resistance demands. Transient enhanced diffusion (TED) [2] in silicon remains one of the greatest challenges in device scaling. TED is known to be associated with elevated levels of Si self-interstitials from implant which agglomerate to form "rod-like defects" known as {311} defects. This anomalous diffusion is further complicated by the presence of small interstitial clusters (SIC) which contribute significantly to the creation of larger clusters by a process called Ostwald ripening [3]. In this work, we conduct a qualitative simulation study of the clustering phenomena of a hypothetically uniform point defect distribution with and without recombination effects. The results are compared against a theoretical diffusion model and the evolution of the point defect clusters with time is also investigated. In the final section, spatially variant damage distributions obtained from atomistic full-cascade Monte Carlo simulations are employed for clustering and recombination studies.

2. Diffusion-limited reaction model and simulation method

The high concentration of point defects generated by the implantation process and their significant diffusivities result in mutual annihilation even at room temperature (RT). Further complicating the process, they form complexes by clustering with similar defect species, eventually morphing into {311} defects and dislocation loops. In this section, we present a simplified reaction model on the mutual annihilation, clustering and cluster recombination of the point defects. In the equations to follow, I represents mono-interstitials, V represents mono-

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Table 1
Forward and backward reaction rates in current model

Process	Reaction	Forward rate	Backward rate
Bulk recombination	$I+V \Leftrightarrow \varnothing$	$4\pi r (D_I+D_V)$	Equal to forward rate
Point defect clustering	$I+I_N \Leftrightarrow I_{N+1}$	$4\pi r\, N^{1/3} (D_I+D_{IN})$	$D_I \exp(-E_N^I/kT)/a^2$
	$V+V_N \Leftrightarrow V_{N+1}$	$4\pi r\, N^{1/3} (D_V+D_{VN})$	$D_V \exp(-E_N^V/kT)/a^2$
Cluster recombination	$I_N+V \Leftrightarrow I_{N-1}$	$4\pi r\, N^{1/3} (D_V+D_{IN})$	See Eq. (3)
	$V_N+I \Leftrightarrow V_{N-1}$	$4\pi r\, N^{1/3} (D_I+D_{VN})$	See Eq. (6)

Constants r and a represent the capture radius ($r=0.235$ nm) and average interatomic spacing ($a=0.271$ nm), respectively. Point defect clusters assumed immobile ($D_{IN}=D_{VN}=0$ except when $N=1$).

vacancies, I_N and V_N represent interstitial and vacancy clusters of size N, while D denotes the diffusivities of a certain species indicated by the subscript and asterisks denote equilibrium quantities.

The governing rate equations in this work are given in Table 1, with the rate constants [4] using a constant capture radius ($r=0.235$ nm) to avoid a large number of unknown parameters. The forward clustering and recombination reactions are based on the assumption of a diffusion-limited process, and hence depend only on the diffusivities, cluster size and capture radii. Assuming only I and V to be mobile, the diffusivities of I_N and V_N are taken to be zero. The diffusivities of I and V are given by $D_I=0.01\ \exp(-0.9/kT)$ and $D_V=0.001\ \exp(-0.43/kT)$, respectively [5]. The backward rates of the clustering reactions depend on the reverse energy barrier and the binding energies of the small clusters ($N<5$) are taken from molecular dynamics calculations [6], while the binding energies for the larger clusters ($N>5$) are taken from Pelaz's work [7]. The backward reaction rate constants for cluster recombination are derived from detailed equilibrium as shown in Eqs. (1)–(6).

I-cluster recombination: $I_N+V \Leftrightarrow I_{N-1}$ (Forward rate=k_{FI1}, Backward rate=k_{RI1}). At equilibrium,

$$R_{ICR} = k_{FI1}[I_N][V^*] - k_{RI1}[I_{N-1}] \approx 0 \quad (1)$$

I-clustering: $I_{N-1}+I \Leftrightarrow I_N$ (Forward rate=k_{FI2}, Backward rate=k_{RI2}). At equilibrium,

$$R_{IC} = k_{FI2}[I_{N-1}][I^*] - k_{RI2}[I_N] \approx 0 \quad (2)$$

Subst. (2) into (1),

$$k_{RI1} = k_{FI1}\left[\frac{k_{FI2}}{k_{RI2}}\right][I^*][V^*] \quad (3)$$

V-cluster recombination: $V_N+I \Leftrightarrow V_{N-1}$ (Forward rate=k_{FV1}, Backward rate=k_{RV1}). At equilibrium,

$$R_{VCR} = k_{FVI}[V_N][I^*] - k_{RV1}[V_{N-1}] \approx 0 \quad (4)$$

V-clustering: $V_{N-1}+V \Leftrightarrow V_N$ (Forward rate=k_{FV2}, Backward rate=k_{RV2}). At equilibrium,

$$R_{VC} = k_{FV2}[V_{N-1}][V^*] - k_{RV2}[V_N] \approx 0 \quad (5)$$

Subst. (5) into (4),

$$k_{RV1} = k_{FV1}\left[\frac{k_{FV2}}{k_{RV2}}\right][I^*][V^*] \quad (6)$$

The equilibrium concentrations of interstitials (I*) and vacancies (V*) have been taken from tight-binding calculations of Tang and Colombo [8]. Using this model, user-defined rate equations are set up in the continuum process simulator DIOS [9]. Results are presented at RT, since complex interactions of the defects are known to occur immediately after implantation and may be dominant even at low temperatures [10].

3. Results and discussion

3.1. Spatially uniform point defect distribution

The clustering kinetics of point defects is first examined by employing hypothetically uniform distributions of I and V at 10^{20} cm^{-3}. This section of work concentrates only on the clustering of point defects without diffusion and recombination (both bulk and cluster) effects, and hence a uniform defect concentration is deemed sufficient for this qualitative study. Following the reaction rates for clustering given in Table 1, and assuming a maximum cluster size of $N=10$, the evolution of the point defect clusters with time is given in Fig. 1(a) and (b) for I and V, respectively. Starting with V at 10^{20} cm^{-3}, V_N start to form quickly. By 10^{-4} s, V_2 start to pre-dominate, followed by smaller clusters. V_2 remain metastable for about 10^5 s (28 h) before dissolving, and we see a slight increase in the concentration of larger clusters. Throughout this period of time, V concentration has dropped several orders of magnitude from the initial 10^{20} cm^{-3}, reaching a meta-stable state at about 6×10^{10} cm^{-3} after 10^{-3} s, and finally reducing to negligible amounts in one day. The remaining species consists of mainly V_3 and larger sized clusters. The formation of I_N, on the other hand, takes place at a much slower rate. I_2 become predominant only after 1000 s, and do not dissolve within the time frame simulated, unlike V_2. I concentration remains constant at 10^{20} cm^{-3} for a much longer period before finally depleting. V_N form more quickly and readily than I_N because of the larger diffusivity of V at RT, leading to a higher forward clustering rate. This finding is consistent with Deep Level Transient Spectroscopy (DLTS) measurements which see V_2 as the only stable defect species at RT [10].

Expanding the system size to $N=50$, the same rate equations are solved for clustering at the typical annealing temperature of 850 °C. The results are shown in Fig. 2(a) and (b) for I and V, respectively after time periods of 1 and 10 s. From Fig. 1(a) and (b), we know that clustering begins as early as 10^{-4} s for V while significant amounts of I_N are seen only after 1000 s at RT. At 850 °C, I_N are already seen after 1 s, although I still dominate and only small cluster sizes ($N\leq20$) are present. After 10 s, the formation of larger I_N is seen. A particularly low concentration of I_2 clusters is observed; interstitials are mainly trapped in I_3 clusters (and as I). This