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Dose-rate and temperature dependent statistical damage accumulation model for ion implantation into silicon

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Abstract

Currently there are extensive atomistic studies that model some characteristics of the damage buildup due to ion irradiation (e.g. L. Pelaz et al., Appl. Phys. Lett. 82 (2003) 2038–2040). Our interest is to develop a novel statistical damage buildup model for our BCA ion implant simulator (IIS) code in order to extend its ranges of applicability. The model takes into account the abrupt regime of the crystal-amorphous transition. It works with different temperatures and dose-rates and also models the transition temperature. We have tested it with some projectiles (Ge, P) implanted into silicon. In this work we describe the new statistical damage accumulation model based on the modified Kinchin–Pease model. The results obtained have been compared with existing experimental results.
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1. Introduction

When ions strike a silicon substrate they create zones of disorder that exhibit different configurations, ranging from isolated point defects or point defect clusters surrounded by crystalline silicon, to continuous amorphous layers. Our ion implant simulator [2] does not consider a deterministic view of the defects but it takes into account a statistical approach that lets us calculate the doping and damage profiles, even in 3D [3]. Our goal is to extend the range of applicability in order to take into account the temperature and the dose-rate within our damage model.

2. Model

Our statistical approach of the damage buildup is based on a modified Kinchin–Pease model [2]. We consider the defect density as the defects at

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each box in which we have divided the target. The projectile generates damage along its trajectory. The number of point defects generated will be $n = kE/(2E_d)$, where E is the energy transferred by the projectile to the target atoms in nuclear scattering, $k = 0.8$ is a constant, and E_d is the displacement threshold energy (e.g. 15 eV for silicon) of the lattice atoms.

The net increase of point defects Δn is given by $\Delta n = nf_{\text{surv}}(1 - N/N_\alpha)$, where N is the previous local defect density, and N_α, the local defect density above which the crystal is considered to be amorphized (e.g. $N_\alpha = 20\%$ of the atomic density of silicon) and f_{surv} is the defect survival ratio that depends on the ion target combination, temperature and dose-rate as main dependencies. The increase in the number of defects is greater when the crystal is not amorphized than when the crystal is partially amorphized. Finally, the new defect density at each box will be $N = N + \Delta n/V$, V being the box volume.

Our main goal is to find an average survival factor, f_{surv}, to be used in our accumulation model that takes into account the dose-rate and the implantation temperature. The decay equation of surviving defects can be written as $n = n_0 \exp(-t/t_{\text{rec}})$, where n_0 is an average number of defects generated per cascade. According to recent works [4] the average lifetime of the IV pair can be expressed for a temperature T as $t_{\text{rec}} = t_0 \exp(\frac{E_A}{k_B T})$, where t_0 is an effective jumping period that has a value of 1.62×10^{-13} seconds and E_A is an activation energy (0.43 eV for isolated IV pairs).

The time between cascades, t_{BC}, at a given dose-rate, $\dot{D}$, can be solved as $t_{BC} = \frac{1}{\dot{D}\sigma_{\text{eff}}}$, where σ_{eff} is an effective cross-section that depends strongly on ion-target combination (increases with ion mass) and takes into account the overlapping between successive cascades.

In order to obtain an average surviving factor, we integrate the expression

$$n_0 f_{\text{surv}} t_{BC} = \sum_{i=0}^{\infty} \int_{(i)t_{BC}}^{(i+1)t_{BC}} n_0 \exp(-t/t_{\text{rec}})\, dt,$$

and get

$$f_{\text{surv}} = \frac{t_{\text{rec}}}{t_{BC}} = \dot{D}\sigma_{\text{eff}} t_0 \exp\left(\frac{E_A}{k_B T}\right).$$

However, the activation energy E_A, that covers the thermal dependence of the model, for a specific defect is dependent on the surrounding defects [1,4]. As we do not have information about particular defects we have tested the relationship between the number of IV pairs surrounding a given IV pair and the defect density, and we found it to be linear. Therefore, as a first approximation we can write $E_A = E_A^0 + \delta \frac{N}{N_\alpha}$, where the parameter δ will take into account the superlinear behavior of the amorphization versus dose.

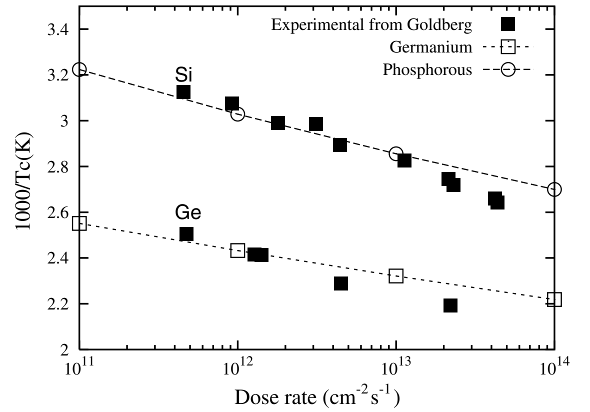

Fig. 1. Transition temperature as a function of ion dose-rate for 80 keV Si and Ge implants to a dose of 10^{15} cm^{-2} [5]. We compare phosphorous simulated points with silicon experimental points.

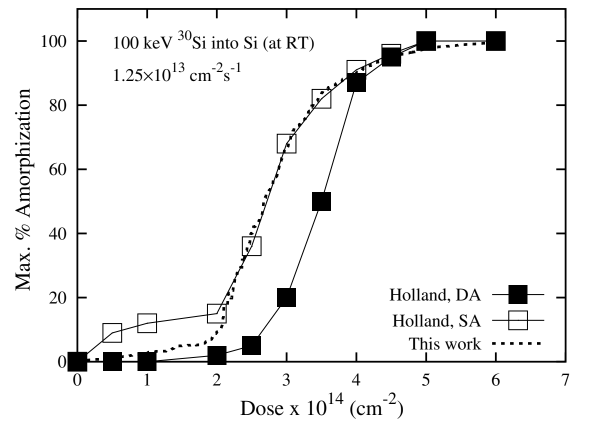

Fig. 2. Superlinear behavior of the model. Experimental points from single (SA) and double (DA) alignment RBS are from Holland [6]. The parameters used are $E_A^0 = 1.1$ eV, $\delta = 0.7$ eV and $\sigma_{\text{eff}} = 4.6\, 10^{-21}$ cm^2.

There exist a strong correlation between these fitting parameters (mainly between $\sigma_{\rm eff}$ and $E_{\rm A}^{0}$) and several sets of them can match the experiment. We show a unique set that covers as much of the experimental profiles we have and we show the goodness of the model. With this model we have fitted the parameters $E_{\rm A}^{0}$, $\sigma_{\rm eff}$ and δ in order to reproduce the experimental SIMS results and to have nearly the same transition temperature when the dose-rate changes reported in the literature [5] (see Fig. 1). The transition temperature is defined for a given dose and dose-rate as the temperature at which the damage is about 50%. Note we do not have experimental results for phosphorous, but these are expected to be near the silicon ones. In Fig. 2 we illustrate the superlinear behavior of the model and compare with results from Holland [6].

3. Results

In order to validate the model we have simulated several implantations with different projectiles using different temperatures and dose-rates:

(i) Germanium with 70 keV implanted into silicon{1 0 0}. In Fig. 3 (top) we can see the comparison of simulated doping profiles with experimental SIMS [7,8] with a dose-rate of $10^{18}\,{\rm cm}^{-2}\,{\rm s}^{-1}$ and a temperature of 250 °C and several doses. We note the excellent agreement between simulated and experimental data. With a lower dose-rate ($10^{11}\,{\rm cm}^{-2}\,{\rm s}^{-1}$) we also obtain good results (see Fig. 3 (bottom)). At room temperature and a high dose-rate ($10^{18}\,{\rm cm}^{-2}\,{\rm s}^{-1}$) as observed in Fig. 4 the model also works well. The fitted param-

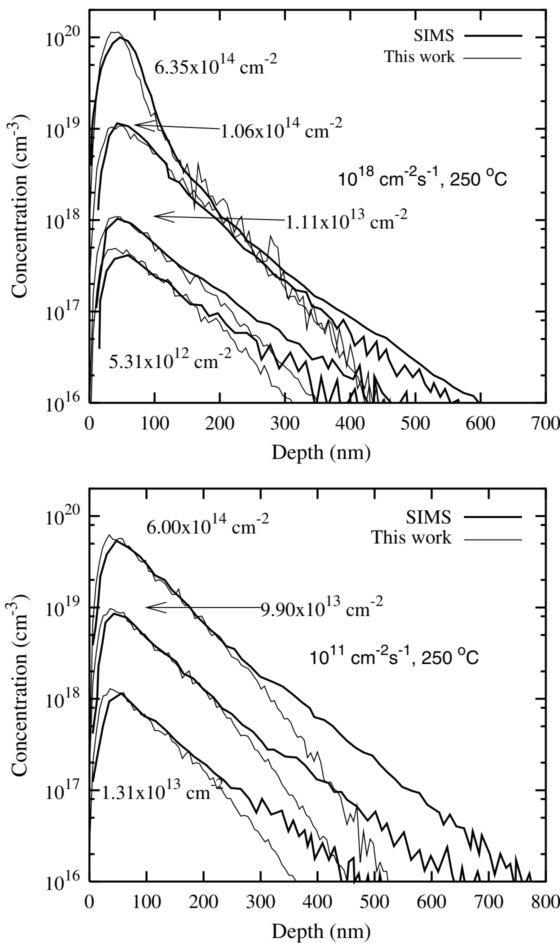

Fig. 3. Germanium with 70 keV into silicon{1 0 0} at 250 °C. We compare the SIMS experimental results [7] with our simulation results. (Top) Dose-rate = $10^{18}\,{\rm cm}^{-2}\,{\rm s}^{-1}$. The amorphous layer in the experiment is about 67.5 nm (for the higher dose). The simulation yields a 65 nm amorphous layer. (Bottom) Dose-rate = $10^{11}\,{\rm cm}^{-2}\,{\rm s}^{-1}$.

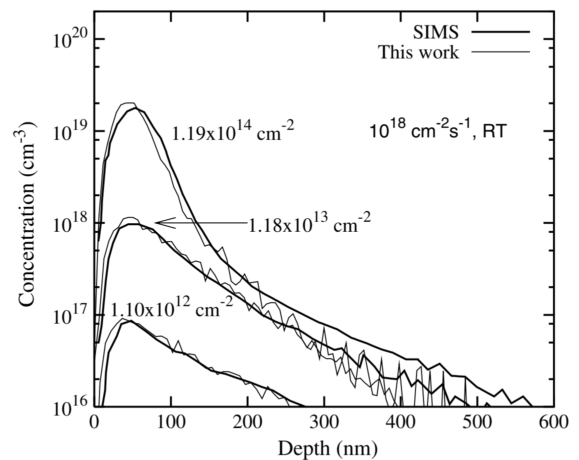

Fig. 4. Germanium implanted with 70 keV into silicon{1 0 0}, at room temperature. Dose-rate = $10^{18}\,{\rm cm}^{-2}\,{\rm s}^{-1}$. We compare the SIMS experimental results [7] with our simulation results. The measured amorphous layer was about 75 nm for the higher dose. The simulation yields a 50 nm amorphous layer.

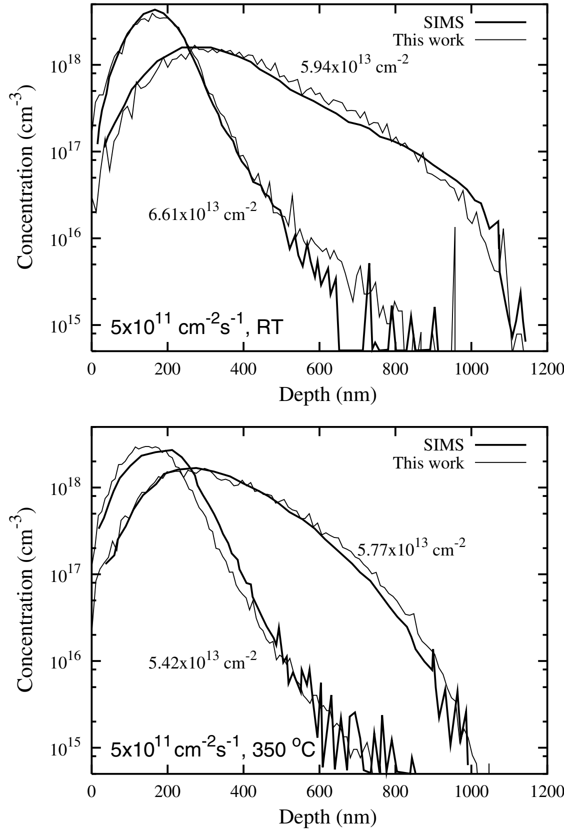

Fig. 5. (Top) Phosphorous doping profiles obtained by 140 keV implantation into {1 0 0} Si with different angles ((0°, 0°) left curves and (7°, 22.5°) right curves) and doses at room temperature. (Bottom) P implanted at 350 °C. The dose-rate is in both plots $5\times10^{11}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$. The SIMS data are from [9].

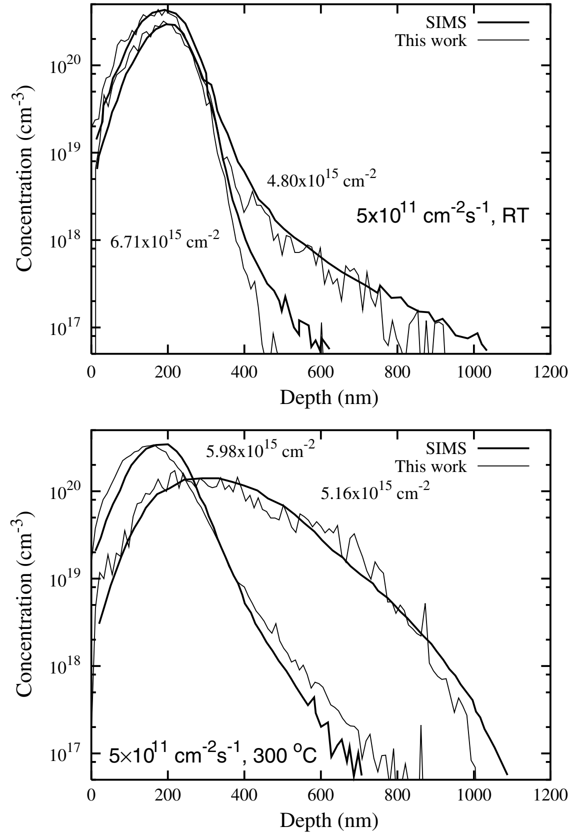

Fig. 6. (Top) Phosphorous doping profiles obtained by 140 keV implantation into {1 0 0} Si with different angles ((0°, 0°) left curves and (7°, 22.5°) right curves) and high doses at room temperature. The thickness of the amorphous layer determined by RBS/C is 280 nm, The simulations yielded a thickness of 270 nm. (Bottom) P implanted at 300 °C. The dose-rate in both plots is $5\times10^{11}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$. The SIMS data are from [9].

eters used are $E_A^0 = 2.0\,\mathrm{eV}$, $\delta = 0.7\,\mathrm{eV}$ and $\sigma_{\mathrm{eff}} = 10^{-26}\,\mathrm{cm}^2$.

(ii) Phosphorous with 140 keV implanted into silicon{1 0 0} at different doses and temperatures. The dose-rate is $5\times10^{11}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$. In Fig. 5 we compare implantations with simulations at different angles and doses at (top) room temperature and (bottom) at 350 °C. The agreement is very good in both cases. Fig. 6(top) at room temperature and (bottom) at 300 °C shows the comparison between simulated results and SIMS profiles [9] with higher doses. Again, we note the excellent agreement between them. The fitted parameters used are $E_A^0 = 1.1\,\mathrm{eV}$, $\delta = 0.7\,\mathrm{eV}$ and $\sigma_{\mathrm{eff}} = 10^{-18}\,\mathrm{cm}^2$.

4. Conclusions

We show a novel statistical damage accumulation model that takes into account the abrupt regime of the crystal–amorphous transition. It provides good results for different temperatures and dose-rates and reproduces accurately the transition temperature. In order to more widely validate the model we will need more experimental data.

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