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The use of extended-defect dissolution as a probe for stress-induced interstitial diffusion anisotropy

P. Castrillo [a,*], R. Pinacho [a], M. Jaraiz [a], J.E. Rubio [a], J. Singer [b]

[a] Department of Electronics, University of Valladolid, ETSIT, Campus Miguel Delibes, 47011 Valladolid, Spain
[b] NXP Semiconductors, 850 rue Jean Monnet, 38926 Crolles, France

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ABSTRACT

In this paper, the influence of biaxial strain-induced diffusion anisotropy on the evolution of extended defects in silicon has been analyzed. Point-defect diffusion anisotropy has been modeled and implemented within an atomistic kinetic Monte Carlo framework. The anneal of {3 1 1}-defects has been simulated for self-interstitial diffusion anisotropies varying within the plausible ranges. From these simulations, it is observed that diffusion anisotropy has a significant effect on the competition between defect ripening and dissolution. In particular, it is shown that the plot of {3 1 1} density versus {3 1 1} mean size could be used to check for the existence of self-interstitial diffusion anisotropy.

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1. Introduction

Strained silicon is essential for the 45-nm node and beyond in order to improve device performance [1,2]. The strain could modify point-defect and dopant diffusion during device processing [3,4]. These modifications can be due to variations of the formation and migration energies of mobile species. Moreover, for biaxial strain, diffusion anisotropy may be induced due to inequivalence of in-plane and out-of-plane directions. At present, there is a controversy in theoretical studies about the magnitude (and even the existence) of diffusion anisotropy for point-defects and common dopants in the standard {1 0 0} orientation [5–7]. Available experimental information on diffusion anisotropy is indirect and only concerning dopants [8]. Besides, the available theoretical studies about the effect of strain on extended-defect dissolution do not consider the possible effect of anisotropic diffusion [9] and experimental data are not conclusive [10–12].

In this paper we analyze the effect of point-defect diffusion anisotropy on extended-defect dissolution. In particular, we focus on the case of {3 1 1}-oriented self-interstitial defects [13–15]. As a result, we propose {3 1 1}-defects as a probe of self-interstitial diffusion anisotropy.

2. Physical model

We consider biaxially strained {1 0 0} silicon layers, that can be obtained by epitaxial growth on a SiGe relaxed substrate [16]. Below the critical thickness for misfit dislocation nucleation, the in-plane lattice parameter of the epitaxy is imposed by the substrate ($a_{\text{in-plane}} = a_{\text{subs}}$). Thus, the biaxial strain of the silicon layer is $\varepsilon_{\text{biax}} = (a_{\text{subs}} - a_{\text{Si}})/a_{\text{subs}}$, where a_{Si} is the unstrained silicon lattice parameter. Knowing $\varepsilon_{\text{biax}}$, the stress σ_{biax} can be easily calculated according to $\sigma_{\text{biax}} = Y \cdot \varepsilon_{\text{biax}}$, where Y is the biaxial modulus.

Biaxial stress modifies the formation energy of intrinsic defects (self-interstitials, I, or vacancies, V) both when they are free point-defects and when they are bound to an extended defect. The binding energy (E_b) of an extended defect is given by the difference of the formation energy of the free and the bound I or V (i.e.: $E_b(\sigma_{\text{biax}}) = E_f^{\text{free}}(\sigma_{\text{biax}}) - E_f^{\text{bound}}(\sigma_{\text{biax}})$). For the case of {3 1 1}-defects, Guo et al. [9] calculated that E_b increases (decreases) for tensile (compressive) strain about 0.07 eV/%. This relatively small modification reflects that, for {3 1 1}-defects, E_f^{bound} has a strain-dependence rather similar to E_f^{free}.

The transport capacity of point-defects is governed by the product of diffusivity and concentration (DC). This product is the relevant magnitude for diffusion processes and it is very difficult to split it experimentally into the individual contributions of D and C [17]. The activation energy of DC is $\Delta E_f + E_m$, where ΔE_f is the energy required to get a free point defect and E_m is its migration energy. In equilibrium conditions, ΔE_f is just the formation

* Corresponding author. Tel.: +34 645 689990; fax: +34 983423675.
E-mail address: Pedro.Castrillo@tel.uva.es (P. Castrillo).

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energy of the point defect from surface ($\Delta E_f = E_f^{free}$). In contrast, during transient enhanced diffusion (TED) conditions, ΔE_f for self-interstitials is given by the binding energy required to get a free I from an extended {3 1 1}-defect ($\Delta E_f = E_b^{\{311\}}$) [13].

Under biaxial stress, the transport in the perpendicular direction, $DC_{33}(\sigma_{biax})$, is modified according to [8]:

$$\frac{DC_{33}(\sigma_{biax})}{DC(0)} = \exp\left(\frac{\sigma_{biax}V_{33}}{kT}\right) \quad (1a)$$

and in the in-plane direction, $DC_{11}(\sigma_{biax})$, is modified as:

$$\frac{DC_{11}(\sigma_{biax})}{DC(0)} = \exp\left(\frac{\sigma_{biax}V_{11}}{kT}\right), \quad (1b)$$

being $DC(0)$ the transport capacity for unstrained material, k the Boltzmann constant, T the temperature, and V_{33} and V_{11} the so-called apparent activation volumes in the perpendicular and in-plane directions, respectively. These activation volumes are the combination of the stress dependences of ΔE_f and of the migration energy in the corresponding direction (E_{m33} or E_{m11}):

$$V_{33} = \frac{-d(\Delta E_f + E_{m33})}{d\sigma_{biax}} \quad (2a)$$

$$V_{11} = \frac{-d(\Delta E_f + E_{m11})}{d\sigma_{biax}} \quad (2b)$$

As a consequence, under TED conditions, DC_{33} and DC_{11} would be affected in the same amount by the stress dependence of $E_b^{\{311\}}$.

If we focus the attention on the anisotropy, the ratio between the in-plane and perpendicular transport capacities can be written as:

$$\frac{DC_{11}}{DC_{33}} = \exp\left(\frac{A\varepsilon_{biax}Y\Omega}{kT}\right) \quad (3)$$

where Ω is one atomic volume and A is an adimensional anisotropy coefficient defined as $A = (V_{11} - V_{33})/\Omega$ [8]. As one can see in Eq. (3), the product $A\varepsilon_{biax}$ determines the diffusion anisotropy. If $A\varepsilon_{biax}$ is positive, in-plane diffusion is higher than the perpendicular one, being the opposite if $A\varepsilon_{biax}$ is negative. Moreover, one can notice from Eq. (2) that A does not involve ΔE_f and, therefore, would be the same in equilibrium and in TED conditions.

As far as we know, there are no experimental values of A for self-interstitials. A calculated value of +0.2 can be inferred from Ref. [7]. Anisotropy data for interstitial diffusers, that might be similar to that of Is, are very scattered. In the case of boron, experimental values of A for the standard {1 0 0}-orientation ranging from +1.2 to −1.1 have been inferred from the comparison of the perpendicular diffusivity under biaxial strain and the diffusivity under hydrostatic pressure [8,18,19]. In addition, the calculated values of A derived from ab-initio calculations are from 0 to +0.5 (with an upper limit of +0.8) for boron [5–8] and −1.4 for carbon [20]. To help elucidate this puzzle, we have found that the plot {3 1 1}-defect size versus {3 1 1}-defect density is selectively sensitive to the presence of I diffusion anisotropy. It might even provide a means for a quantitative estimate of the anisotropy coefficient A.

3. Model implementation

Our study has been carried out within the framework of atomistic non-lattice Kinetic Monte Carlo (KMC). The model described in the previous section has been included in the process simulator DADOS [21]. Ion-implant generated Is and Vs are calculated within the Binary Collision Approximation and loaded into DADOS. This simulation scheme has been proven to reproduce very well the phenomenology of extended-defect evolution for the relaxed material [15,21]. A description of our extended-defect implementation, focused on {3 1 1}-defects, is given in Ref. [15]. In particular, we assume that the length of a {3 1 1}-defect ($L_{\{311\}}$) depends on the number of Is (n_I) as $L_{\{311\}} \approx 0.43\, n_I^{2/3}$ nm.

In our simulations, the surface is assumed to be a perfect sink for Is (i.e. the recombination occurs with no barrier) [22] whereas lateral and bottom boundaries are assumed to act as perfect mirrors (i.e. the jump is rejected) [23]. This assumption for the bottom boundary is valid for the realistic cases of both silicon on silicon (with low trap density and back surface far away) and silicon on SiGe (assuming that DC_{33} for Is in the SiGe substrate is lower than in a tensile Si layer grown on it). No misfit dislocations are assumed.

Concerning the splitting of the strain dependence of the DC product, we assume that strain modifies ΔE_f whereas the migration rate is unaffected. Strain-induced diffusion anisotropy is implemented assigning different jump probability for Is in the in-plane and perpendicular directions, according to Eq. (3). Following Ref. [9], the strain dependence of binding energies of {3 1 1}-defects has been assumed to be independent of size, with a value of 0.07 eV/% [9].

4. Simulation results

As a representative case, we have simulated a 5×10^{13} cm^{-2} 40 keV Si^+ implant followed by an 815 °C anneal. This process is non-amorphizing, does not involve dopants, and gives rise to {3 1 1}-defects detectable by Transmission Electron Microscopy (TEM) [13,14]. We have used a simulation cell with an implant-area of 200 nm × 200 nm and a depth of 500 nm that is large enough to contain the whole implant cascade damage, which is within a depth of 400 nm. We have verified that larger depths do not lead to relevant differences in the simulation results.

First, following Ref. [9], we have performed simulations assuming no anisotropy ($A = 0$) for both tensile (+1%) and compressed (−1%) material, and we have compared them to the unstrained one [24]. In Fig. 1(a) and (b), we have represented the anneal time evolution of {3 1 1}-defect areal density ($d_{\{311\}}$) and mean length ($\langle L_{\{311\}}\rangle$), respectively. Only {3 1 1}-defects longer than 5 nm ($n_I > 40$) are taken into account in order to emulate the TEM threshold sensitivity. As it can be seen in the figure, and in agreement with Ref. [9], tensile stress retards and compressive stress accelerates defect evolution. This is due to the strain-induced modification of E_b and, consequently, of I-emission rate of {3 1 1}'s. In Fig. 1(c), $\langle L_{\{311\}}\rangle$ has been plotted versus $d_{\{311\}}$ and the time variable has been omitted. As a reference, lines corresponding to different values of the total self-interstitial areal density (ρ_I) are indicated in the figure. As it is apparent in Fig. 1(c), the three cases follow the same evolution path, although with a different time scale.

Fig. 1(c) is useful to visualize the three stages of {3 1 1} evolution during the annealing: (1) *Nucleation stage*: Is and Vs recombine and excess Is are trapped by clusters. As a result many small {3 1 1}-defects start to grow, entering into the TEM-detectable size range. This is reflected in the figure, where $d_{\{311\}}$ and ρ_I increase and $\langle L_{\{311\}}\rangle$ is maintained near the minimum detectable size. The maximum of ρ_I (~2.5×10^{13} cm^{-2}) is only half of the +1 model prediction because Is in small clusters are not taken into account. (2) *Ripening stage*: After nucleation, defect dynamics is driven by the emission of Is from {3 1 1}'s. Emitted Is can be trapped by other {3 1 1}'s or (to a lower extent) are annihilated at the surface. As a consequence, large {3 1 1}'s (more stable) grow, small {3 1 1}'s disappear, and the total amount of Is scarcely decreases (quasi-conservative ripening) [13–15]. Thus, $\langle L_{\{311\}}\rangle$ increases, $d_{\{311\}}$ decreases, and ρ_I slightly diminishes. (3) *Dissolution stage*: When the mean distance between {3 1 1}'s becomes larger than the distance to the surface,

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