Stress effects on point defect supersaturation and defect evolution

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In state-of-the-art nano-scale ultra large scale integration (ULSI), stress engineering is essential to improve device performance. We studied stress effects on interstitial supersaturation and defect cluster size distribution and evolution by analyzing B marker transient enhanced diffusion (TED) data in a carefully designed strain containing structure. Samples were prepared by Ge pre-amorphisation and regrowth, leaving an end-of-range (EOR) defect band inside the strained layer (Fig.1). Interstitial supersaturations were inferred from the ratio of B diffusivities in pre-amorphized and unimplanted samples. Defect cluster evolution and energetics were then extracted from the supersaturation data by inverse modeling. The method was also applied to unstrained control samples. The inset to Figure 2 shows how stress affects the mean formation energy per interstitial as a function of the cluster size.

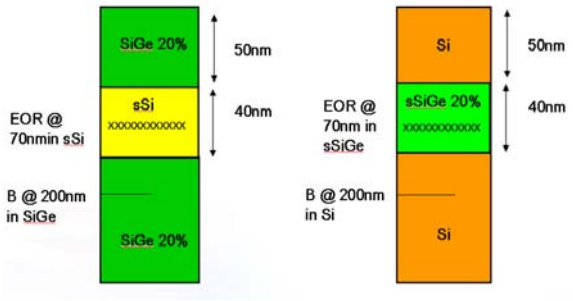

Figure 1: Schematic illustration of strained-Si and strained-SiGe structures used in experiments

Density function theory (DFT) calculations have been done to compare with the cluster formation energies derived from inverse modeling. Results for small interstitial clusters and <311> defects, together with previous DFT results [1,2], are shown in Fig. 2. Full tensor elements of induced strain were calculated for various <311> defects and dislocation loops. The results show that, under tensile stress,
a) TED lasts longer because stress stabilizes interstitial clusters more effectively than isolated interstitials,
b) small <311> defects are more effectively stabilized than larger ones
c) <311> defects are strongly oriented with respect to the strain field, consistent with TEM observations and recent DFT results for small interstitial clusters [2].

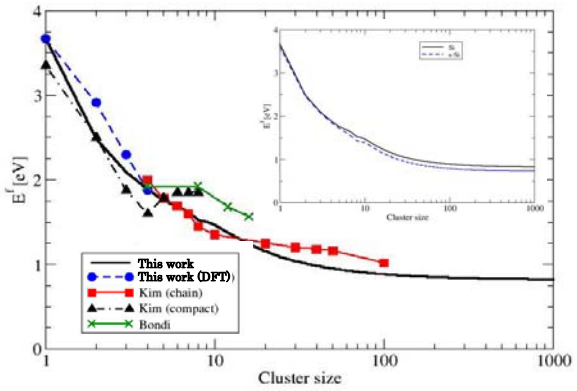

Figure 3: Formation energy per interstitial as a function of cluster size, for unstrained Si and for strained Si (the broken line in inset).

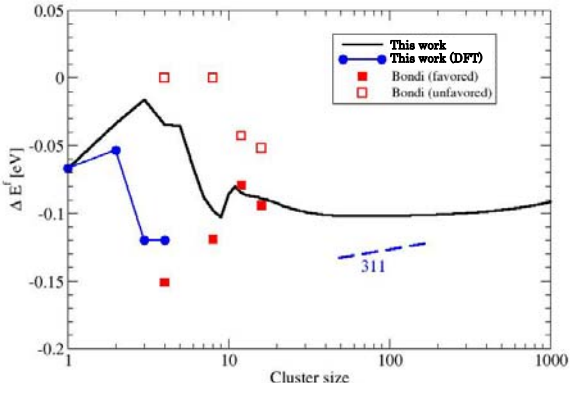

Figure 2: The strain-induced change in cluster formation energy for strained Si on 20%Ge, expressed as average energy per interstitial

References

[1] J. Kim, F. Kirchhoff et al., Phys. Rev. Lett. **84**, 503 (2000); J. Kim et al., Proc. Int. Conf. on Computational Nanoscience (ICCN2001).
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