Effects of curvature on the equilibrium properties of nanostructures

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There exist various strain relaxation mechanisms, that effect the properties of epitaxially grown nanostructures, such as Ge nanoislands on a Si substrate. The epitaxial strain is typically relaxed through a mechanism involving some sort of plastic deformation (such as dislocations) and the equilibrium composition profile at device temperatures is the result of the interplay between such strain relaxation mechanisms and inter-diffusion. Recently [1] there have been experimental studies illustrating the possibility of yet another mechanism through the bending of the substrate (e.g. Ge nanoislands grown on SOI), resulting in defect free structures. Atomistic simulations can be used in order to probe the effect of such a mechanism on the equilibrium properties at various temperatures and thus provide a comparison between flat and curved geometries, the former of which has been already extensively studied [2]. We simulate the effect of a curved substrate, similar to what is experimentally observed using continuous space Monte Carlo simulations and we notice a considerable alteration of the curved vs the flat composition profiles (Fig. 1).

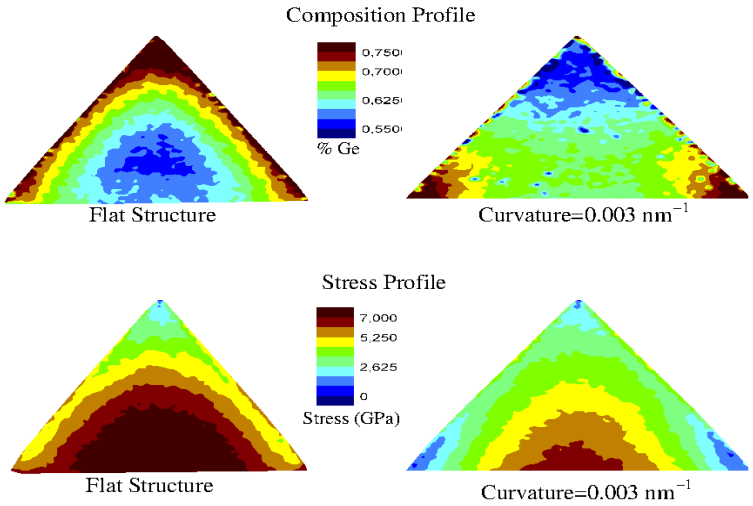

Figure 1: Top: The equilibrium composition profile after intermixing at 900K for a flat and a curved pyramid composed of 65% Ge. Bottom: The stress profile prior to intermixing.

References

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