Understanding the role of strain in Si-Ge devices

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Abstract

The effect of strain on the structural morphology of thin films of Si-Ge alloys and SiO_2 is investigated through the use of empirical potential models.

1   Introduction

The influence of strain in Si-Ge and strained Si technologies is of considerable current interest since it affects process integration for Heterostructure Bipolar Transistors (HBTs), Modulation Doped Field Effect Transistors (MODFETs), and SiGe-on-insulator devices. As a step towards investigating the role of strain on dopant diffusion for thin films, we have correlated the change in morphology of silicon based substrates under tension and compression to the change in the potential energy surface (PES) for both a Stillinger-Weber-modeled silicon and a MEAM-modeled [1] SiO_2 surface using a virtual AFM-like "probe". The importance of strain on the segregation of Ge and consequent roughening of the thin films of SiGe is also shown.

2   Simulation Details and Results

Experimentally, a thin film of SiGe is observed to be smoother under tension than under compressive conditions [2]. To explore the origin of this result computationally, we measure the interaction between the Si (100) surface under varying strain conditions and a silicon "probe" and determine the minimum energy configuration (Fig. 1). We observe a reduction in the extent of the regions of attraction for the silicon surface under tensile strain as compared to an unstrained surface. In contrast, there is a marked increase in extent of the regions showing attraction for the film under compression. This can be linked qualitatively to the change in morphology observed experimentally. Since compressed films are seen to be more attractive to a silicon probe, this implies that, during thin film growth, depositing atoms will have a choice of adsorption regions, leading to a roughening of the film. In comparison, atoms will have to overcome a large barrier to diffuse in films under tensile stress and will be tend to adsorb on lattice sites, leading to smoother films. We also find that SiGe thin films overlaying a Si(100) surface give rise to a PES similar to that for pure Si(100) under compressive stress due to the underlying strain imposed by the Si layers.

Similar simulations were carried out for a MEAM-modeled oxide surface [1]. An α-quartz crystal (100) surface was relaxed for a period of 40ps under conditions of

compressive and tensile stress and the potential energy surface of the relaxed surface was mapped out using a silicon probe and compared to an unstrained substrate. We observe a quantitative behavior similar to the Si(100) study (Fig. 2) with the compressed surface being more attractive to the probe as compared to a substrate under tensile strain. Films of varying thickness are being probed to see the effects of system size.

The effect of strain on the morphology in $Si_{1-x}Ge_x$ alloys was investigated by varying the concentration of Ge and observing the extent of segregation in thin films on a Si(100) surface. Using a Monte Carlo technique, starting from random initial configuration of Si-Ge atoms, swaps were made between atoms of the two species until an equilibrium energy configuration was obtained. The bottommost silicon layers were kept fixed at their equilibrium lattice positions to impose a compressive strain on the SiGe film. An additional dynamic buffer layer of Si was kept between the fixed silicon layers and the region where swaps between Si and Ge were allowed. This allows the SiGe layers to feel the effect of the underlying strain without introducing any artifacts of the simulation conditions. Absence of a dynamic Si layer leads to an artificial bimodal distribution. As shown in Fig. 3, there is a marked segregation of the Ge atoms to the surface of the film with the top few layers being dominated by Ge. This aggregation alleviates the compressive strain imposed by the underlying Si(100) layers, accompanied by an expansion of the top few layers, as seen by the change in average height of the layers shown in Fig. 4. The next few layers reach an equilibrium concentration which is higher than the average bulk Ge concentration. A crossover to a Si rich region occurs in the lower layers, in which an equilibrium concentration of Ge much lower than the average bulk concentration is achieved. For low concentrations of Ge (x=0.1), this crossover regime is difficult to observe given the statistical noise in the data. This study confirms experimental evidence for segregation in strained SiGe alloys [3,4] and is similar in spirit to a recent computational study of segregation of Ge at a dislocation boundary [5].

We considered the role of strain in step formation on the (100) surface and its relation to the roughness of the film. Using the semi-empirical Stillinger-Weber potential, the change in step energy of a pure Si (100) film under strain confirmed previous computational results [2] (Fig. 5). We compared these results to the change in step energy of a ultra-thin Ge layer deposited on top of a relaxed Si(100) surface. The segregation effects seen in Monte Carlo simulations suggest that such an arrangement mimics equilibrium SiGe/Si(100) systems adequately. We find a reduction in the value of the step energy formation for the SiGe/Si(100) system identical to those seen in compressed Si which shows that SiGe films have a large density of steps and are consequently rougher than thin films made from unstrained silicon, again confirming experimental data [2].

3 Conclusions

We find a qualitative similarity between the computationally efficient PES calculations and the far more computationally intensive step energy calculations, which suggest that PES calculations are an economical alternative to determine regimes of attraction and repulsion. The similarity of the response of surfaces

composed of Si(100), SiGe and oxide show that strain affects different substrates in analogous ways. We confirmed experimental observations of surface segregation and quantified the Ge equilibrium composition profile under strain which will be crucial in understanding dopant transport in ultra-thin "SGOI" devices.
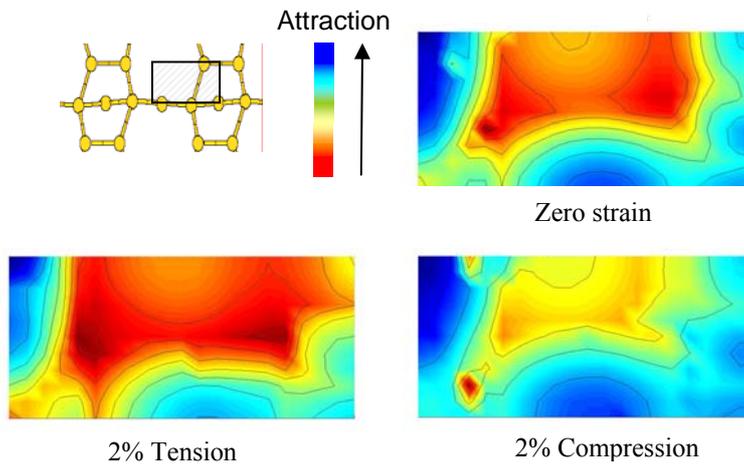

Figure 1. Potential Energy Surface of strained Si(100). The schematic diagram shows the region where the Si(100) surface was probed by a silicon atom.
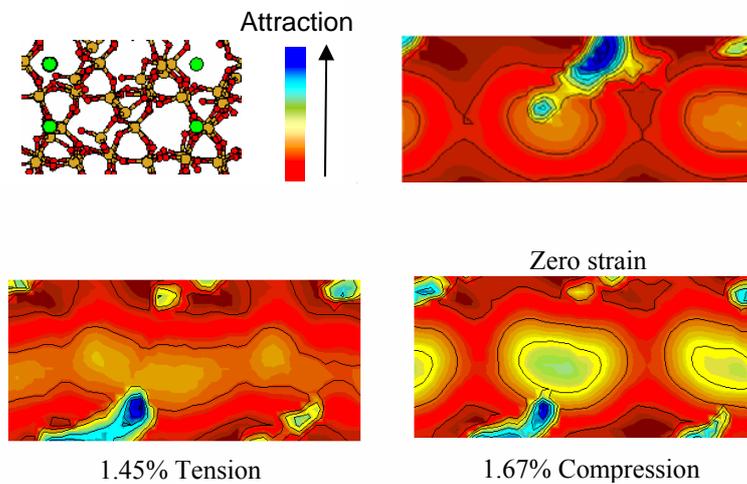

Figure 2. Potential Energy Surface of strained α-quartz(100). The strain values represent the stability limits of the MEAM-modeled crystal line α-quartz. The atomic inset shows the amorphization of the top few layers of the quartz crystal with the green dots delineating the outer limits of the Si probe.
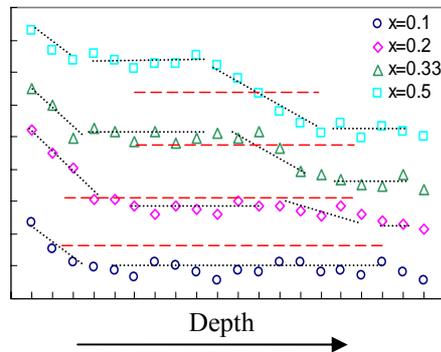
Fig. 3: Concentration profile of Ge atoms as a function of the depth of simulation cell. The red dashed lines denote the average concentration and the dotted lines are guides in visualising the various regimes. x is bulk concentration of Ge in film. x-axis spacing is 0.2. y-axis spacing is 1 atomic layer.
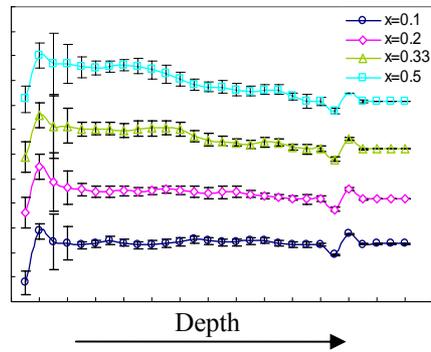
Fig. 4: Difference in height between successive layers as a function of the depth of the simulation cell. Error bars correspond to the deviations from the average height. Anomalous behavior of the first layer is due to the presence of a surface. x-axis spacing is 0.05 Å. y-axis spacing is 2 atomic layers.
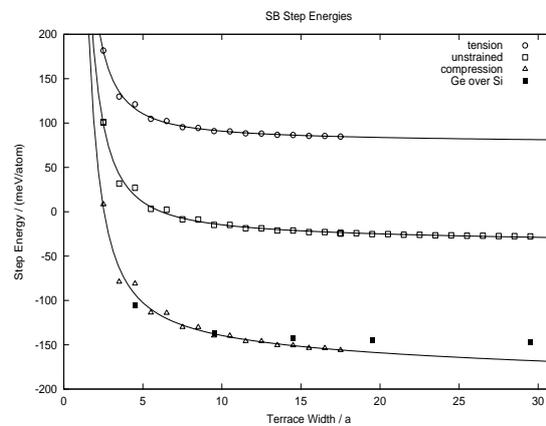

Fig. 5: Step energy calculations as a function of strain. Results for a film of Ge over Si mirror those for pure Si under compressive strain.

References

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