

## Quantitative Analysis of Shape Transition of Ge Islands on Si(100) with nc-AFM

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Ge on Si(001) has been widely considered as a model system for understanding strained heteroepitaxy. Due to the 4.2% lattice mismatch, compressively strained Ge layer evolves and self-organizes into coherent (dislocation-free) 3D islands. In equilibrium, small islands are elongated or square pyramids, while larger islands develop a more complex multi-faceted dome shape through a first-order shape transition. In-situ measurements of shapes for Ge islands grown in UHV are illustrated in the non-contact AFM(nc-AFM) figs. (a),(d),(f),(h) below as the island sizes increase. The shape change arises from strain relaxation; dome shape is preferred after a critical island size. While the physical nature of the pyramid-to-dome transition is known, there were only few attempts to understand this transition in a more quantitative way. Specifically, the magnitudes of nucleation barriers in this first-order shape transition have not been discussed. Here we use nc-AFM to examine the evolution of Ge island facets and compare it with a simple yet realistic strain relaxation model [1]. It is found that the barrier for nucleating a Ge island from the wetting layer is  $\sim 2-3$  meV/atom, and the barrier of pyramid-to-dome shape transition at the critical island size is  $\sim 1-2$  meV/atom. These barriers are derived from a thermodynamic total energy inclusive of surface energy and strain energy. Therefore, detailed atomic processes controlling the kinetics of shape changes are not yet addressed in this study.

[1] I. Daruka, J. Tersoff, A.-L. Barabasi, Phys. Rev. Lett. **82**, 2753 (1999).

