

# Nucleation behaviors and interactions of SiGe/Si (001) islands:

## modeling and experiments

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Self-organisation of SiGe islands with homogeneous size and high density remains a challenging issue for both fundamental interests and nano- and opto-electronic applications. Up to now it was concluded that the elastic field between SiGe islands is repulsive. In recent work, we observed a nice alignment of islands that nucleate adjacently with both their sides and their corners almost in contact. This observation contradicts the theoretical conclusions and deserves a joined theoretical/experimental study to understand the mechanism.

The combination of first-principle and continuum calculation paved the way towards quantitatively understanding the surface energy variation as a function of deposited layers (wetting effect) and the influence of strain on surface energy both for facet (105) and (001) has been calculated by Shklyaev[1] and Lu[2]. Based on these results, the 2D-3D transition and the formation of (105)-facet-bounded huts turns to be quantitatively understandable. In this study, we developed a continuum model on the basis of first-principle results about wetting effect and strain dependence of surface energy[1][3], in order to describe the nucleation behaviors and the island-island interactions. Our results are found to be in good agreement with experimental observations; especially we found that, from calculations and experiments, the coherent islands are attractive rather than repulsive as ones usually concluded.

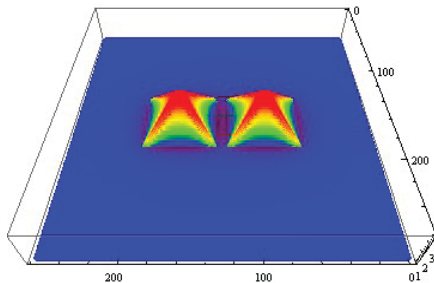


Fig. 1: Strain-dependent surface energy influences island-island interaction

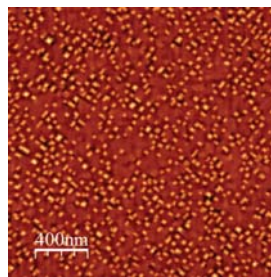


Fig 2: AFM image of SiGe/Si(001) hut islands

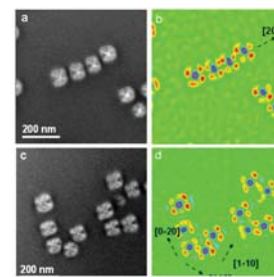


Fig. 3: TEM plan-view images (left) and strain phase image (right) of Ge/Si(001)

[1] Shklyaev OE, MJ Beck, M Asta, MJ Miksis, and PW Voorhees. Role of strain-dependent surface energies in ge/si (100) island formation. Physical review letters, 94(17):176102, 2005.

[2] Guang-Hong Lu and Feng Liu. Towards quantitative understanding of formation and stability of ge hut islands on si (001). Physical review letters, 94(17):176103, 2005.

[3] Guang-Hong Lu, Martin Cuma, and Feng Liu. First-principles study of strain stabilization of ge (105) facet on si (001). Physical Review B, 72(12):125415, 2005.