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On the Two to Three Dimensional Growth Transition in Strained Silicon Germanium Thin Films

B. G. Demczyk*, A. H. King**, R. J. Gambino***

*Air Force Research Laboratory, SHNX, Hanscom AFB, MA 01731
**School of Materials Engineering, Purdue University, West Lafayette, IN 47907
***Department of Materials Science & Engineering, SUNY, Stony Brook, NY 11794

The transition from two dimensional (Frank-Van der Merwe) [1] growth to a layer-by-layer plus island mode (Stranski-Krastanov) [2] has generally been approached theoretically through examination of kinetic instabilities [3-5]. Although many surfaces do indeed develop nearly sinusoidal morphology profiles, in other cases, growth takes place as discrete, faceted islands. Metastable equilibrium models have been developed for the nucleation of discrete islands [6,7], but not specifically the two to three dimensional growth transition. Utilizing a model adapted from classical nucleation theory [8], we calculate a "critical thickness" for island formation, taking into account the surface energies of the deposit and the substrate and the elastic modulus of the deposit, using the following relation:

$$h = h_c = (2\,\gamma_i - \gamma_f)/\,M\varepsilon^2 \qquad [1]$$

where γ_i and γ_f, are the surface energies of the island and film, respectively, M, the biaxial modulus and ε, the lattice strain (misfit). Elastic constants were taken from reference [9]. In Table I, values of critical thickness for the two-to-three dimensional growth transition (equation 1) are listed, along with an approximate value of the critical thickness for dislocation formation, h_{cd} as per the Mathews equilibrium theory [10]. For $Si_{0.3}Ge_{0.7}$ alloys, linear extrapolation of both elastic moduli and surface energies were made. Even though critical thickness values for the maximum strain cases are similar, the Ge/Si (001) film showed a clear tendency toward island formation (Figure 1a), while the Si/Ge (001) film remains largely planar, though heavily faulted (Figure 1b). It is energetically favorable to relax the misfit strain through creation of islands only when the surface energy of the deposit (Ge) is lower than the that of the Si substrate. The alloy on Si (001) forms faceted islands that extend all the way to the substrate (Figure 1c), similar to the Ge/Si (001) case. In the alloy on Ge (001), however, the island height is only about one half of the total film thickness (Figure 1d) and the underlying film contains a high density of dislocations, which serve to largely relieve the misfit strain. Subsequent film growth, unencumbered by strain, is driven by surface energy minimization-i.e. formation of faceted islands with major facets near {111}. Alloys on (111) were found to relieve strain by island formation under conditions of both compression and tension. In these cases, defects do form, but are constrained to glide on such inefficient slip planes (either in the interface or at high angles to it) that the strain cannot be completely relieved and island formation is required.

In general, islands form to affect a reduction of the surface energy of the deposit-substrate system. Absent of strain, islands are expected to form where the surface energy of the deposit is lower than that of the substrate. Even if it is slightly higher, islands may

still lower the total energy by incorporating low energy facets into their structure. In addition, even though the "critical thickness" for island formation is generally higher than that for dislocations, islands can still serve to relieve the misfit strain if dislocation motion is frustrated, such as on (111) substrates. In the case of films growing on thin underlayers, however, the “substrate” itself may deform. This can lead to such results as, for example, Ge on an alloy being resistant to island formation despite being in a state of compression. Thus some novel heterostructures may be synthesized.

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References

[1] F. C. Frank and J. H. van der Merwe, Proc. Roy. Soc. Lon. A **198**, 205 (1949).
[2] I. N. Stranski and V. L. Krastanow, Akad. Wiss. Lit. Mainz. Math-Natur. K1 IIb **146**, 797 (1939).
[3] D. J. Srolovitz, Acta metall. **37**, 621 (1989).
[4] B. J. Spencer, P. W. Voorhees and S. H. Davis, Phys Rev. Lett. **67**, 3696 (1991).
[5] B. G. Orr, D. Kessler, C. W. Snyder and L. Sander, Europhys. Lett. **19**, 33 (1992).
[6] N. Grandjean, J. Massies and F. Raymond, Jpn. Jl. Appl. Phys **33**, L1427 (1994).
[7] J. Tersoff and F. K. LeGoues, Phys Rev. Lett. **72**, 3570 (1994).
[8] B. G. Demczyk, A. H. King and R. J. Gambino, in preparation.
[9] X. Wang, G. L. Zhou, T. C. Zhou, C. Sheng and M. R. Yu, in *Silicon Molecular Beam Epitaxy*, Mater. Res. Soc. Symposium Proc., V. 220, J. C. Bean, S. S. Iyer and K. L. Wang, eds, Materials Research Society, Pittsburgh, PA (1991), p. 241.
[10] J. W. Mathews and A. E. Blakeslee, J. Cryst. Gwth **27**, 118 (1974): **29**, 27 (1975).

TABLE 1. Critical Thickness (nm) for Island Formation

System	(001)	h_{cd}	(111)	
Ge/Si	2.0	2.0	1.5	
Si/Ge	2.2	2.0	1.7	
SiGe/Si	4.5	3.3	3.8	
SiGe/Ge	27.1	11.0	21.2	

h_{cd} = Mathew's equilibrium theory

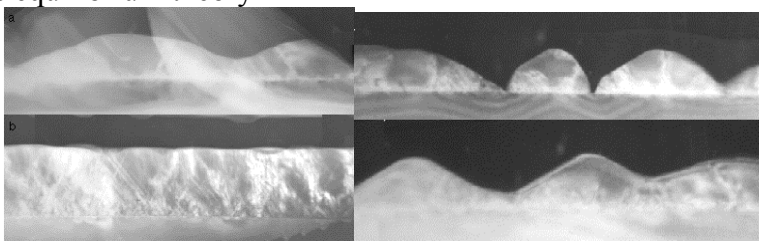

Fig. 1: Cross sectional transmission electron micrograph of a) Ge/Si (001), b) Si/Ge (001), c) SiGe alloy on Si (001), d) SiGe alloy on Ge (001). Note: beam direction is along <110> of the substrate.