Modeling and Simulation for Epitaxial Growth with Strain

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ABSTRACT

Strain has significance for both the growth characteristics and material properties of thin epitaxial films. In this work, the method of lattice statics is applied to an epitaxial system with cubic symmetry, using linear elasticity. The energy density and force balance equations are written using a finite difference formalism that clearly shows their consistency with continuum elasticity. For simplicity, the atomic interactions are assumed to be maximally localized. For a layered material system with a material/vacuum interface and with surface steps, force balance equations are derived, and intrinsic surface stress at the material/vacuum interface is included by treating the atoms at the surface as belonging to a different material. By defining the strain relative to an appropriately chosen nonequilibrium lattice, as in the method of eigenstrains, analytic formulas in terms of microscopic parameters are found for the macroscopic monopole and dipole forces due to a step.

Keywords: modeling and simulation, epitaxial growth, strain

1 INTRODUCTION

Due to heteroepitaxial growth, thermal expansion, and alloy segregation, mechanical strain occurs in nearly all technologically interesting films. In heteroepitaxial growth of thin films (i.e. oriented growth of one material onto a substrate of a different material), strain is induced by mismatch between the lattice constants in the substrate and those in the epilayer; e.g., for silicon on germanium the lattice mismatch is -4%. Similarly, alloy segregation during growth or through annealing induces strain due to lattice mismatch between the segregated regions. Cooling after growth or thermal cycling during use in a multi-component system with different coefficients of thermal expansion leads to strain between the components.

Without strain, the competition between interfacial (i.e. attachment) and surface energy determines whether a system grows in layer-by-layer (Frank-van der Merwe) or islanding (Volmer-Weber) mode. Strain has a significant influence on the morphology and device properties of thin films. For example, the thermodynamic competition between elastic energy and interfacial energy can lead to the Stranski-Krastanov growth mode in which islanding starts after formation of a wetting layer. Strain often leads to three-dimensional structures (rather than flat films) during heteroepitaxial growth. The resulting "quantum dots" exhibit novel and desirable optoelectronic properties. On the other hand, strain drives (usually) unwanted material inhomogeneities in alloy films [1].

We consider a lattice static model [2], [3] where the energy is

$$E = \alpha \sum_{p=\pm,k=1,2} (S^p_{kk})^2 + \sum_{p=\pm,q=\pm} \{2\beta (S^{pq}_{12})^2 + \gamma S^p_{11} S^q_{22}\}. \tag{1}$$

In this expression, $S^{pq}_{k\ell}$ is a discrete version of the strain tensor and α, β and γ are microscopic elastic parameters. Intrinsic surface stress at material interfaces is included by variation of the elastic parameters and the lattice constant at the interface. The complete range of elastic parameters is included by use of nearest-neighbor springs, diagonal springs and bond bending terms (neglected in many previous models) on a simple cubic lattice.

In the bulk, minimization of the elastic energy leads to the force balance equations

$$4\alpha D^+_k D^-_k u_k + 4\beta \sum_{\ell \neq k} D^+_\ell D^-_\ell u_k + (4\gamma + 4\beta) \sum_{\ell \neq k} D^0_k D^0_\ell u_\ell = 0 \tag{2}$$

where u_k are the components of the displacement vector and D^p_k are finite difference operators. This form of the force balance equations is convenient because it is a finite difference version of the continuum elastic equations. The force balance equations at interfaces and step edges are a variant of (2), which do not have a continuum analogue in some cases.

For problems in which the underlying lattice has cubic symmetry but the material geometry includes interfaces, we generalize the energy in (1) by only keeping bond interactions that are consistent with cubic symmetry but not imposing a symmetry constraint on the strength of the interactions.

As an example, consider a system for which the film has the same elastic parameters as the substrate but a

Figure 1: Pinning of two double steps in the middle of two substrate terraces in a metastable state on a 3 monolayer epilayer. The lower, middle and upper regions are the substrate, epilayer and vacuum, respectively, and the results are shown at 4 successive times.

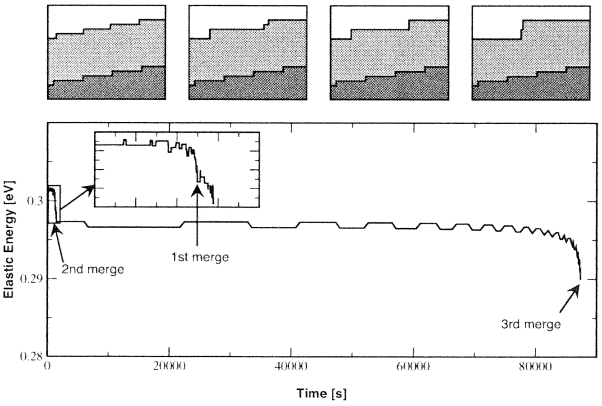

Figure 2: Example of a simulation with 4 steps on a 10 ML epilayer. The total system energy monotonically decreases, indicating the approach of the system to the thermal equilibrium. The four pictures are at 4 successive times.

lattice mismatch of ϵ_1. Model intrinsic surface stress by letting bonds on the surface of the film have a different lattice mismatch ϵ_2. For a bond (cell) in which one of the vertices is in the vacuum, set $\alpha = \beta = \gamma = 0$.

It follows from these choices [3] that the monopole force due to a step is

$$\mathbf{M} = \left(4(\alpha^2 + \gamma\sigma_3 - \gamma^2)\alpha^{-1}\epsilon_1, \quad 0\right). \tag{3}$$

The torque component of the dipole term, computed around the concave corner point of the step is

$$\mathbf{D}_T = 4\alpha\epsilon_2 - (\gamma^2/2\alpha)(5\epsilon_1 + \epsilon_2). \tag{4}$$

In addition, the strain model is coupled to an island dynamics model for epitaxial growth for which the lateral structure of the film is described as a continuum. Computational results from this combined method in 2D are shown in Figure 1, in which steps on the film surface are pinned by buried steps at the interface between substrate and film.

2 ACKNOWLEDGMENTS

Research supported in part by a Focused Research Group grant # DMS0074152 from the NSF.

REFERENCES

[1] B.J. Spencer, P.W. Voorhees and J. Tersoff, "Enhanced instability of strained alloy films due to compositional stresses" Phys. Rev. Lett., 84 (2000) 2449-52.

[2] A.C. Schindler, M. F. Gyure, D. D. Vvedensky, R. E. Caflisch, C. Connell and G. D. Simms. "Theory of Strain Relaxation in Heteroepitaxial Systems" Phys. Rev. B (2003) to appear.

[3] C. Connell, R.E. Caflisch, E. Luo and G. Simms. "A Discrete Elastic Model for Epitaxial Systems and the Force Field at a Step". in preparation.