CORRELATION BETWEEN DISLOCATION DISTRIBUTION DENSITY AND INTERFACE RELAXATION STRESS IN EPITAXIAL THIN LAYER ON A FLEXIBLE SUBSTRATE

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Foundations

In development and fabrication of optical electronic devices the growth of thin semiconductor layers on a bulk substrate is one of the most important and demanding parts of the process. If the matching between the substrate and the layer is almost perfect, the growth of the film is two-dimensional. At initial stage, a thin layer forms which undergoes plastic relaxation once it exceeds some critical thickness. If on the other hand, the lattice mismatch between the film and the substrate is large, the film grows by nucleation mechanism where three-dimensional islands emerge, grow and eventually coalesce. It has been observed experimentally that particular growth mode depends on a balance between the interfacial energies of the substrate and epitaxial layer and the lattice mismatch between the layers. The stress associated with misfit strain between the thin sheet and a substrate is the main source and the driving force for formation of structural defects. Thin films contain a large number of lattice defects, which in turn tend to degrade the performance of the devices. The natural response of the system under such circumstances is formation of strain relaxing mechanisms that can have adverse effects on electronic performance of semiconductor materials. In the unstrained or relaxed epitaxial film, the substrate and the film retain their bulk lattice constants and the film is not commensurate with the substrate. In this case, the mismatch is accommodated locally by the misfit dislocations where the average spacing between misfit dislocations depends on the misfit constant. In this work we consider the problem of relaxation of coherency stresses by lattice misfit dislocations, which can be represented as edge dislocations distributed along the interface, and can be associated with the concept of dislocation density according to the mathematical theory of continuous distributions of dislocations.

Methodology

Consider a planar thin film deposited on a substrate with a thickness, h_f which is much smaller than the lateral dimensions of a thin plate–like structure. Remote edges of the layer in lateral directions are far enough so that the mechanical fields in these areas can be ignored. The bottom and the top surface of the layer with the total height h are free of applied traction. Under such conditions the layer is invariant under translation in either of the lateral directions. As a result, all fields are independent of in–plane coordinates of the layer. We also assume that deformations, curvature and dislocation density tensor do not depend on in–plane coordinates and are functions of normal coordinate only. Moreover, the material of epitaxial system is assumed isotropic and heterogeneous with different elastic modulus in the film and the substrate. The structural deformations of the system in the form of deflection due to plastic curving are assumed small so that geometrically nonlinear effects are not considered in the derivation. It is shown that the curvature of the system which stems from the plastic part of the distortion tensor, depends on the dislocation densities in the film and the substrate and not only on a misfit dislocation density in the interface between both phases. The curvature of the epitaxial system also depends on elastic heterogeneity of the system and is influenced by the mismatch in elastic constants of the film and the substrate. The self–equilibrated feature of stress distribution across the width of the system can be directly verified by integration across the whole thickness. The relaxation stress at the interface between the film and the substrate can be calculated as a stress difference between both fields at the top and the bottom of the interface. The difference gives a jump in relaxation stress which depends on the plastic curvature of the system, difference between elastic modulus of the film and the substrate, dislocation distribution densities in the film and the substrate and a misfit dislocation distribution density as well. The stress jump in relaxation normalized by elastic modulus of the substrate can be written as

$$\frac{[\![\sigma]\!]}{E_s} = \mathrm{g}_0(\xi,\eta)(\alpha_f - \alpha_s)h + \mathrm{g}_1(\xi,\eta)\widehat{\alpha}_m$$

where functions g_0 and g_1 depend on dimensionless parameter ξ describing geometry of the system whereas η describes the strength of elastic mismatch between the film and the substrate. Here $\widehat{\alpha}_m$ represents the misfit dislocation density, α_f and α_s are the corresponding dislocation densities in the film and the substrate. Interfacial stress jump dependence on both geometric parameters defined on the domain $\xi = E_f/E_s \in [0,1] \times \eta = h_f/h \in [0,1]$ for the case where dislocation densities in the film and the substrate are both zero, i.e., for $\alpha_s = \alpha_f = 0$ can be graphically represented as

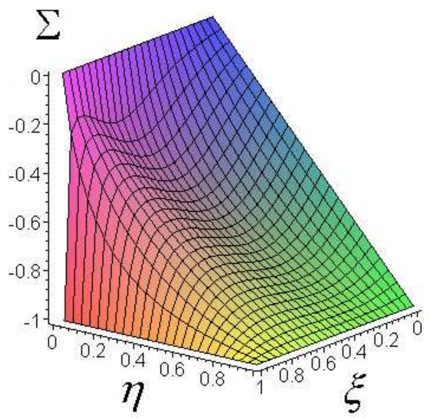

Fig. 1 Interfacial stress jump $\Sigma = [\![\sigma]\!]/(E_s\widehat{\alpha}_m)$

Derived relation shows that the jump in relaxation stress depends linearly on the misfit dislocation distribution density, as well as on the difference in dislocation distribution densities between the film and the substrate. Obtained results exhibit good correlation with experimental findings given in [1] and [8]. Linear dependence on $\widehat{\alpha}_m$ is generic property of the model. On the other hand, a linear relationship for the case when difference α_f-α_s is different from zero holds true only for systems where spatial distribution of both dislocation density fields remain uniform within each layer throughout a deformation process.

Final remarks

Distortion across an interface of a two phase epitaxial system is represented by the system of misfit dislocation and dislocations in the film and the substrate. The model is based on the distributed dislocation theory where for the purpose of modeling the system of distributed dislocation densities is used in the form of discontinuous function representing the magnitude of the dislocation density in the film, in the substrate, and at an interface. Results can be obtained in the closed form for what essentially represents a kinematically a one–dimensional problem, even under quite general conditions, where the epitaxial system is considered heterogeneous and heterogeneity extends through the thickness of the layers. Heterogeneity is postulated as a mismatch in elastic properties of the film and the substrate. Mismatch between the elastic modulus of the film and the substrate definitively has a significant impact on the magnitude of the resulting curvature of the system. This also holds true if the magnitude of dislocation density in the film and the substrate is different. Detailed analysis of particular cases, especially those with very thin thickness of the film with homogeneous elastic properties, retrieves the Stoney formula as a special case of a general solution. However, putting more emphasis on the quantitative aspect of the problem requires an extensive parametric study.

References

1. Boulle, A., Guinebretiere, R. and Dauger, A. Phenomenological analysis of heterogeneous strain field in epitaxial thin films using x–ray scattering, *J. Phys. D: Appl. Phys.*, **38** (2005) 3907–3920.
2. Cammarata, R. C. Surface and interface stress effects on interfacial and nanostructured materials, *Mat. Sci. Engng./A*, **237** (1997) 180–184.
3. Freund, L. B. The mechanics of dislocations in strained–layer semiconductor materials, *Advances in Applied Mechanics*, **30** (1994) 1-66.
4. Gutkin, M. Yu., Romanov, A. E. and Aifantis, E. C. Nonuniform misfit dislocation distributions in nanoscale thin layers, *Nanostructured Materials*, **6** (1995) 771–774.
5. Jagannadham, K. and Marcinkowski, M. J. Loss of coherency across an interface, *J. Appl. Phys.*, **48** (1977) 3788–3787.
6. Krishnamurthy, R. and Srolovitz, D. J. A general solution for two–dimensional stress distributions in thin films, *J. Appl. Mech.*, **71** (2004) 691–696.
7. Mathews, J. W. Coherent interfaces and misfit dislocations, *"Epitaxial Growth. Part B"*, Edited by Matthews J. W. Academic Press, (1975).
8. Park, T. -S., Suresh, S., Rosakis, A. J. and Ryu, J. Measurement of full–field curvature and geometrical instability of thin film–substrate systems through CGS interferometry, *J. Mech. Phys. Solids*, **51** (2003) 2191–2211. *Acta Mater.*, **46** (1998) 3063–3075.