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Position dependant critical thickness in finite epitaxial systems

Arun Kumar, Anandh Subramaniam*

Materials Science and Engineering, Indian Institute of Technology, Kanpur 208016, India

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ABSTRACT

During the growth of an epitaxial overlayer, interfacial misfit dislocations become energetically favourable on exceeding the critical thickness. In the case of finite systems (i.e. either the substrate or the epitaxial overlayer is finite), different positions along the interface are not equivalent and the critical thickness will be position dependent. Minimum of these thickness values can be visualized as the global critical thickness. The current work aims at simulating the stress state of a growing epitaxial overlayer on a finite substrate using finite element method and further use the numerical model to calculate the position dependent critical thickness along the interface. Eigenstrains will be imposed in selected regions in the domain towards this end. The variation of shear stress along the interface will be computed from the model to understand the issues related to the mechanism of formation of misfit dislocations. This includes the important question: "why interfacial dislocations cannot 'punch-in' directly from the free lateral surface?" The simulation methodology and associated concepts can readily be extended to other finite epitaxial systems like stripes and islands.

1. Introduction

In Van der Merwe growth mode (layer by layer growth), the epitaxial overlayer is coherent with the substrate, in the initial stages of growth (if the misfit between the overlayer and the substrate is small) [1]. On growth beyond a critical thickness (designated as h_c), misfit dislocations can partially relieve the coherency strains [2]. Four kinds of epitaxial overlayers can be distinguished [3]: (i) thin film on a thick substrate (which is wide in the lateral dimensions), (ii) finite substrate (in lateral dimensions) with an overlayer having full coverage, (iii) stripes (which have partial coverage on the substrate along one dimension), (iv) Islands (which have small lateral extent and have a tapering geometry). In case (i), the film can be considered to be under uniform strain and the effect of free lateral surfaces is usually ignored. The classification based on an alternate view point found in standard literature is [4]: layer by layer growth (Frank-Van der Merwe growth mode), Island growth (Vollmer–Weber growth mode) and layer growth followed by island formation (Stransky–Krastanov growth mode).

In configurations (ii–iv) as above, effects due to one or more finite dimensions play a role in determining the stress state of the system. Additionally, a system can be envisaged where the substrate is thin (i.e. has comparable dimensions to the overlayer) [5].

Van der Merwe has determined the critical thickness for an epitaxial system consisting of a thin film on thick substrate with large lateral dimensions [6]:

$$h_c = \frac{b}{8\pi(1+\nu)f_m}\left[1+\ln\left(\frac{2h_c}{q}\right)\right] \tag{1}$$

where 'b' is the modulus of Burgers vector, 'ν' is Poisson's ratio of the thin film, 'f_m' is misfit parameter, 'q' is inner cut-off radius given as $\left(q = \frac{\pi b}{2\sqrt{2}(1-\nu)}\right)$ and 'h_c' is the critical thickness of the epitaxial film.

In the analyses by Van der Merwe [7,8] and other investigators [9,10], the substrate is assumed to be rigid with all the strain and associated energy being in the film (i.e. free lateral surface effects are ignored in the model considered).

The critical thickness has been determined by force balance between coherency stresses and dislocation line stresses by Matthews and Blakeslee [11]:

$$h_c = \frac{b}{2\pi f_m}\frac{(1-\nu\cos^2\alpha)}{(1-\nu)\cos\lambda}\left[1+\ln\left(\frac{h_c}{b}\right)\right] \tag{2}$$

where 'α' is the angle between the dislocation line and its Burgers vector, 'λ' is the angle between the slip direction and that direction in the film plane which is perpendicular to the line of intersection of the slip plane and the interface.

The criterion for h_c put forth by Van der Merwe seems to work well for metallic films. People and Bean [12] considered semiconductor films to be in a metastable state (i.e. misfit dislocations do

* Corresponding author. Tel.: +91 512 259 7215; fax: +91 512 259 7505.
E-mail address: anandh@iitk.ac.in (A. Subramaniam).

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not form, even after h_c has been exceeded) and deduced a criterion based on energy balance (for the $Ge_{0.5}Si_{0.5}/Si$ system):

$$h'_c(\text{nm}) = \frac{1.9\times10^{-3}}{f_m^2}\ln\left[2.5h'_c(\text{nm})\right] \tag{3}$$

where, h'_c is the critical thickness of metastable films.

In systems which have at least one finite dimension (lateral extent of the substrate or the overlayer), the critical thickness is expected to a function of the position along the interface. This is due to the fact that the energy of the dislocation will vary as a function of its position along the interface and hence its ability to provide strain relief [5]. In these finite epitaxial systems the substrate cannot be considered rigid and the energy stored per unit area of the interface will vary a function of the position along the interface. Suhir [13] has studied stresses in finite coherent systems (single and multi-layer epitaxial systems). He has modelled the stresses as thermal induced stresses and has computed the shear stress variation along the interface as:

$$\tau(x) = \tau_{max}e^{-k(l-x)} \tag{4}$$

where $\tau_{max} = -\frac{kE_f h_f \Delta\alpha\Delta t}{(1-\nu_f)}$, $k=\sqrt{\frac{\lambda}{\kappa}}$, $\lambda \cong \lambda_f = \frac{(1-\nu_f)}{E_f h_f}$ and $\kappa = \frac{2}{3}\left(\frac{(1+\nu_f)h_f}{E_f} + \frac{(1+\nu_s)h_s}{E_s}\right)$.

'E_f' and 'E_s' are the Young moduli, 'ν_f' and 'ν_s' are Poisson ratios and 'h_f' and 'h_s' are heights of the thin film and substrate respectively, '$\Delta\alpha$' is the difference in thermal expansion coefficients of the thin film and substrate, 'Δt'; is the temperature differential.

Two important mechanisms have been extensively discussed in literature with regard to the mechanism of generation of misfit dislocations [1]. These are formation of a misfit segment in: (i) a threading dislocation, (ii) a dislocation half-loop extending from the free-surface of the film. Dislocations loops may have to nucleate before extending to the interface to form misfit segments. The thickness of the film at which a half-loop of radius R_c can nucleate is given by [14]:

$$h_c^{\text{half-loop}} = R_c\cos\phi \tag{5}$$

where, R_c is determined by solving the following equation: $R_c = \frac{b}{16\pi\varepsilon}\frac{(2-\nu)}{(1+\nu)\cos\phi\cos\lambda}\left[\left\{1+\ln\left(\frac{8R_c}{e^2 b}\right)\right\}+\frac{e^2 b}{8}\right]$. The value of $e^2 = 1$ for a circular loop.

In finite epitaxial systems, one more possibility can be envisaged for the formation of a misfit dislocation: the 'punching-in' of an interfacial dislocation from the free lateral surface (due to interfacial shear stresses). Even for the case of nucleation of a dislocation in a homogenous material, multiple criteria have been considered in literature. These include: shear stress based criterion [15], shear stress gradient based criterion [16], criterion based on non-local effects [17], etc. It is generally accepted that a shear stress in the range of G/30–G/10 is required for the nucleation of an edge dislocation ($\tau_{critical}^{nucleation}$) in a homogenous material [18]. The criterion for the nucleation of interfacial dislocations is not fully understood as yet and hence in the current work the range for a homogenous crystal is used for comparisons.

The reader may refer to the works of de Hosson et al. [19,20] for correlation between linear elastic and atomistic models to understand the effect of bond strength, misfit and interaction parameter on the atomic structure of the interfacial misfit dislocation. Using atomistic model, they have given a better explanation of the interface structure in case of large misfit where dislocations core start interacting. At smaller misfits (where interfacial misfit dislocations are separated by large distance and can be considered as isolated), atomistic and linear elastic models give nearly same approximate solutions.

The current investigation aims at the following tasks: (i) simulate a epitaxial film on a substrate with finite lateral extent using finite element method, (ii) determine the stress state and energy of the system as a function of the thickness of the film, (iii) compute the variation of the interfacial shear stress, (iv) determine the critical thickness as a function of the position of the dislocation along the interface using the numerical model. Additionally, attempt will be made to answer the following important question: "why interfacial dislocations cannot punch-in directly from the free lateral surface?" $Ge_{0.5}Si_{0.5}/Si$ system will be used as a model system [21–23] to illustrate the methodology and comprehend the important issues with regard to the mechanism of formation of misfit dislocations.

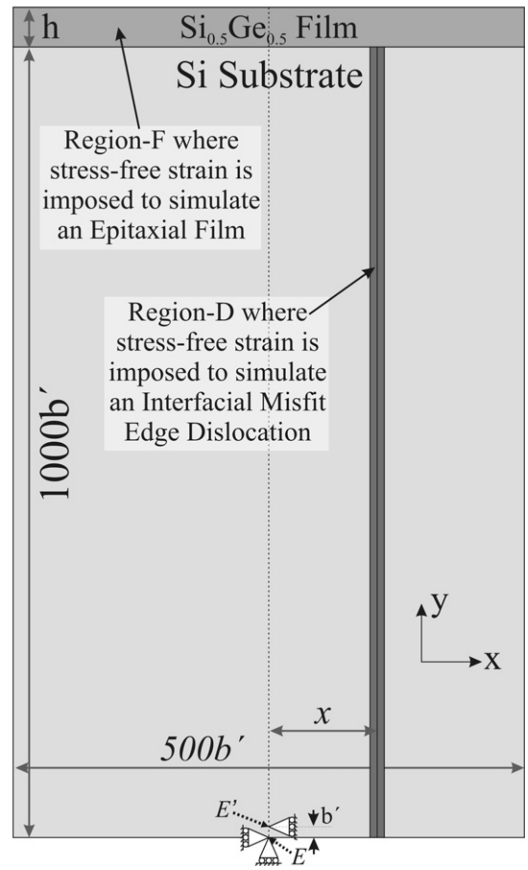

Fig. 1. Schematic of the finite element model used for the simulation of an epitaxial thin film ($Si_{0.5}Ge_{0.5}$) on a thick substrate (Si), which is finite in the lateral dimension (*x*-direction). The regions where eigen-strains are imposed are shown, along with the boundary conditions used.

2. Finite element methodology

To simulate the stress state of an epitaxial system and a misfit dislocation, the finite element model as shown in Fig. 1 is considered. It is to be noted that the substrate is thick and finite in the lateral dimension. The figure (Fig. 1) shows the schematic of the model with a $Si_{0.5}Ge_{0.5}$ film on a Si substrate; along with the boundary conditions imposed.

The stress state of the epitaxial thin film ($Si_{0.5}Ge_{0.5}$) is modelled by imposing stress-free strains (eigen-strains) in region-F (as marked in Fig. 1). This strain corresponds to the lattice mismatch between the film and the Si substrate and is imposed as the *x*-component of the eigen-strain tensor (i.e. ε_{xx}). The value of this strain is: $(a_f - a_s)/a_f = 0.02$.

The stress state of the interfacial misfit edge dislocation is simulated by imposing eigen-strains in region-D as marked in Fig. 1. This corresponds to the insertion of a plane of atoms in the substrate