EM397 Thin Film Mechanics, Fall 2006 Term Paper Jun Zhou

Dislocations in epitaxial thin films

Abstract

Dislocations are common in epitaxial systems. For a thin film epitaxially grown on a substrate with coherent interface, it may have *spontaneously-formed* dislocations when its thickness is larger than certain value, i.e. critical thickness. The presence of dislocations can have an adverse effect on electrical performance of semiconductor materials, providing easy diffusion paths for dopants to lead to short circuits, or recombination centers to reduce carrier density. And, formation of dislocations is one of the most observed mechanisms of relaxation of mismatch strain. However, in optoelectric applications, strain alters the electronic bandgap and band edge alignment, and should be maintained. So, controlling formation of dislocations is very important in the manufacture of microelectronic and optoelectronic devices.

This term paper will review some basic concepts and try to produce some understanding about the control of dislocation formation.

1 Introduction

Semiconductor and optoelectic materials are used most effectively if they exist in the form of a single-crystal thin film. Many these materials with electronic or optoelectric properties suitable for device applications are alloys and the crystalline quality of the materials is of central importance. Films are usually grown on substrates by one of the physical or chemical vapor deposition techniques. The substrate and film materials are selected on the basis of their electronic characteristics, and it is rare to find suitable material combinations which have the same lattice parameter. More commonly, there is a mismatch in lattice parameter between them. Due to this mismatch strain, the film is strained and the strain energy stored in the film increases as the thickness of the film grows. The film tries to relax itself. Formation of dislocations is one of the most observed relaxation mechanisms. Figure 1 gives an example.

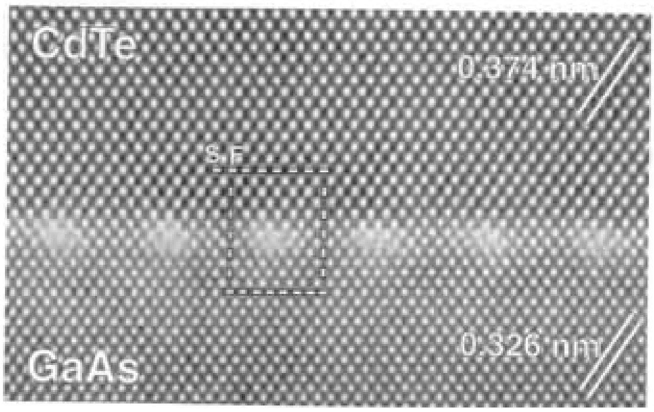

Fig.1 Atomic resolution transimission electron micrograph of an interface between CdTe and GaAs where the strain is relaxed by the introduction of edge dislocations. Schwatzman and Sinclair (1991). Reproduced from Reference [2].

Generally, dislocations in the thin films which form the electronically or optoelectrically active regions within a device are undesirable. The presence of dislocations has adverse effects on electrical performance of semiconductor materials, providing easy diffusion paths for dopants to lead to short circuits, or recombination centers to reduce carrier density. And, in optoelectric applications, strain-relieving dislocations are harmful because strain alters the electronic bandgap and band edge alignment, and should be maintained. So, controlling formation of dislocations is very important in the manufacture of microelectronic and optoelectronic devices.

In this paper, some basic concepts are reviewed first, and a simple case of expitaxial system with buffer layer is studied to get some understanding about dislocation controlling.

2 Basic concepts

Our discussion is based on the continuum theory of elasticity dislocations. For an elastic body with appropriate traction and displacement boundaries, we are interested in the energy change of the system with respect to the configuration or position of dislocation. The negative gradient of the energy may conveniently be called a force. Here it comes to a concept of *configurational force*. This force is introduced to give a description of energy changes and is not the same as ordinary surface tractions and body forces.

The formation and advance of dislocations can change background strain field and reduce the strain energy stored in the body. On the other hand, work must be done to form a dislocation. In an isolated system, where there is no energy exchange between the solid and its surroundings, the reduced strain energy must be bigger than the work required to form a dislocation to allow dislocations formed *spontaneously*.

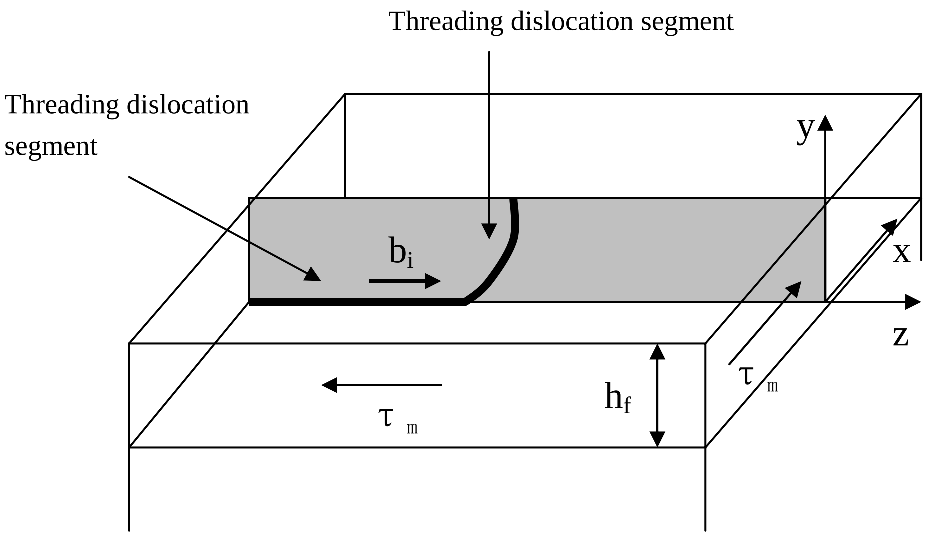

Fig.2 Schematic illustration of a model system with screw dislocation

For convenience and simplification, only screw dislocations are considered in this paper. Considering a strained film deposited on a substrate, the mismatch strain is

$$\varepsilon_{xz} = \frac{1}{2}\gamma_m ,$$

then the corresponding stress due to mismatch is

$$\sigma_{xz} = \tau_m = \mu_f \gamma_m ,$$

and all other stress components are zero in background mismatch field. The interface misfit segment of the strain-relieving dislocation lies in the interface y = 0 along the negative z-aixs. Its Burgers vector is in the z-direction and is denoted by $b = b_z$.

The work per unit length required to create the interface misfit dislocation (far behind the threading segment) is

$$W_d(h) = \frac{\mu_f b^2}{4\pi} \ln \frac{2h_f}{r_0},$$

and the work per unit length done by the background stress field (far behind the threading segment) in forming this dislocation is

$$W_m(h) = -\tau_m b h_f = -\mu_f b \gamma_m h_f .$$

Then the critical thickness is determined by

$$W_d(h_c) + W_m(h_c) = 0 \text{, i.e., } \frac{\mu_f b^2}{4\pi} \ln \frac{2h_c}{r_0} - \mu_f b \gamma_m h_c = 0 .$$

Set $r_0 = b/2$ and $\gamma_m = 0.01$, we have

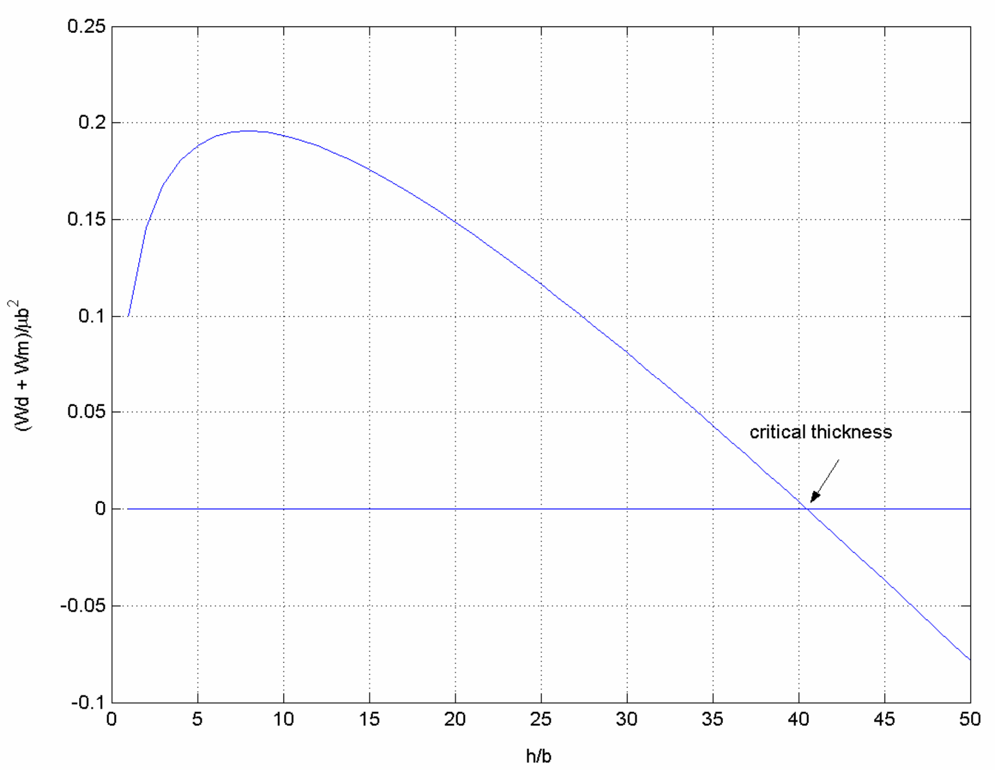

Fig.3

The critical thickness is $h_c \approx 40b$.

3 A simple case – Epitaxial system with buffer layer

It is desirable to relax all mismatch strain in film which carries functional characteristics. In Ge/Si epitaxial film structure, people use buffer layer to get a low-mismatch layer of Ge:

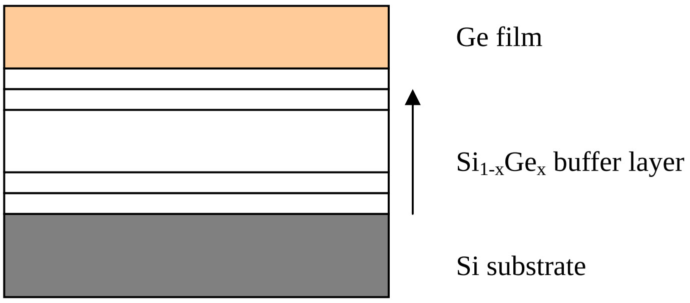

Fig.4 Schematic illustration of Ge/Si system with buffer layer

In the buffer layer, the composition of SiGe alloy is graded from Si substrate to Ge film. The thickness of the buffer layer is about 1 μm , which is not nice for industry where "reducing the dimensions" is highly desired.

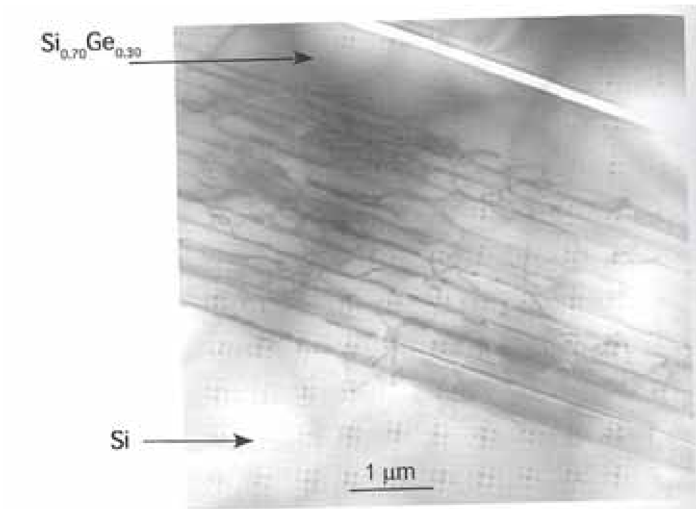

Fig.5 Cross-sectional TEM image showing a dislocation-free SiGe cap layer which is grown on a graded SiGe buffer layer. Fitzgerald(1995). Reproduced from Reference [2].

Is it necessary to alter the composition smoothly? How about big steps to give sharp changes in composition, for example, Si – $Si_{0.75}Ge_{0.25}$ – $Si_{0.5}Ge_{0.5}$ – $Si_{0.25}Ge_{0.75}$ – Ge structure? Let's study a little bit about this kind of structures.

The Ge film acts like an unstrained capping layer on the $Si_{0.25}Ge_{0.75}$ layer. First, considering the effect of capping layer on the dislocation formation in $Si_{0.25}Ge_{0.75}$ layer:

The formation of dislocation at the $Si_{0.5}Ge_{0.5}$/$Si_{0.25}Ge_{0.75}$ interface requires distortion of both $Si_{0.25}Ge_{0.75}$ and Ge layers. On the other hand, only the stress field in $Si_{0.25}Ge_{0.75}$ does work as the dislocation is formed. Thus, the critical condition

$$W_d(h_c) + W_m(h_c) = 0 \text{, i.e., } \frac{\mu_b b^2}{4\pi} \ln \frac{2(h_{bc} + h_f)}{r_0} - \mu_b b \gamma_m h_{bc} = 0,$$

where the modulus difference is ignored.

The critical thickness increases due to the capping layer as the figure below shows. So capping layer tends to stabilize the configuration against dislocation formation.

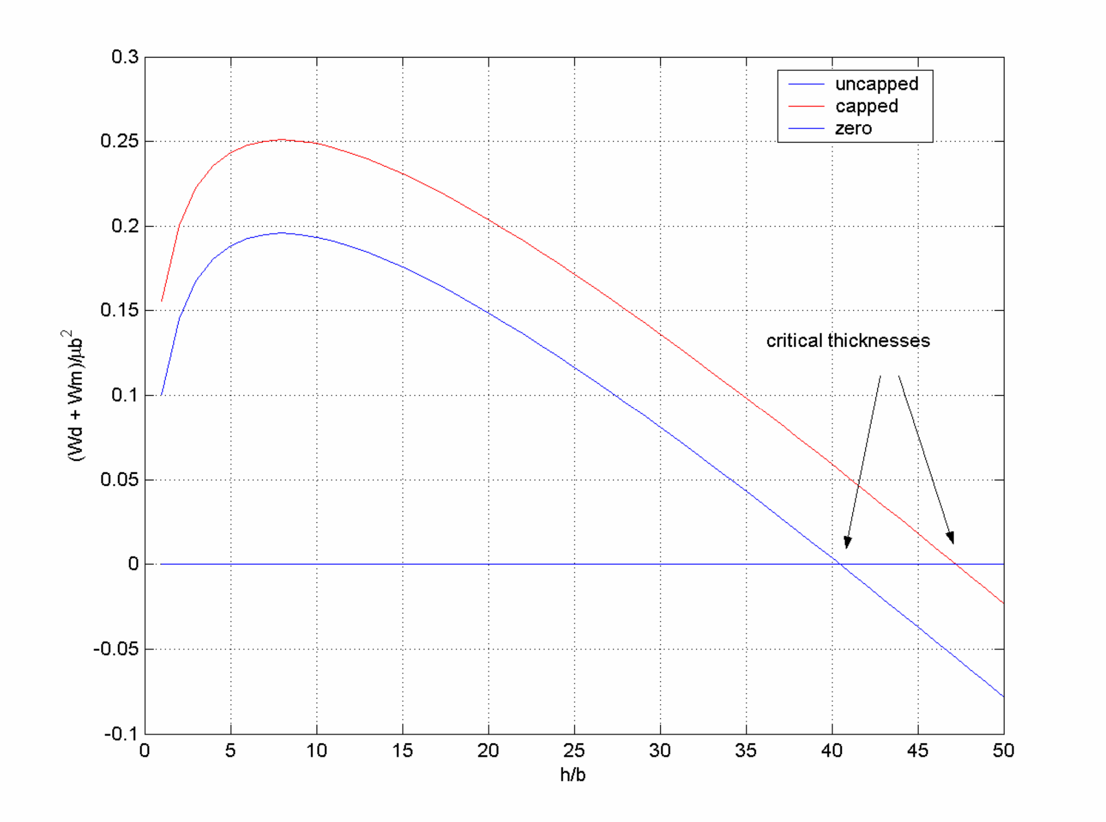

Fig.6

Then, we include the influence of modulus difference. Due to this difference, there is one more configurational force acting on the dislocations near the interface. For a screw dislocation, the force exerted by the interface is attractive if the dislocation is in the more stiff material with the larger shear modulus, and vice versa. The configurational force takes the following form:

$$F_{\text{int}} = -\frac{\mu_f b k_\mu}{4\pi |y|},$$

where, $k_\mu = \dfrac{\mu_f - \mu_s}{\mu_f + \mu_s}$ represents the difference of moduli (Hirth and Lothe 1982, see Ref. [2]).

The force acts in the positive y-direction if $\mu_s > \mu_f$, and vice versa. If $\mu_s > \mu_f$, there is a stable equilibrium position for the dislocation within the film at the distance

$$y_{eq} = -\frac{\mu_f b k_\mu}{4\pi\tau_m}$$

from the interface. If $\mu_s < \mu_f$, there is no stable equilibrium position for the dislocation in the film. For a layer sandwiched between two layers, for example, the $Si_{0.5}Ge_{0.5}$ sub-layer (sub-layer 2) between $Si_{0.75}Ge_{0.25}$ (sub-layer 1)and $Si_{0.25}Ge_{0.75}$ (sub-layer 3), it feels two configurational forces from two interfaces (1/2 and 2/3 interfaces).

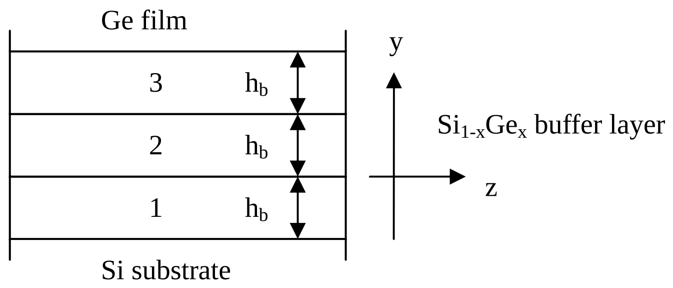

Fig. 7

For a dislocation in sub-layer 2, there are three forces acting on it: the force $F_m = -\tau_m b$ (along negative y-direction, per unit length), exerted by background mismatch field, and two forces per unit length by two interfaces:

$$F_{\text{int}1/2} = -\frac{\mu_2 b k_{\mu 1/2}}{4\pi y} = \frac{\mu_2 b\Delta}{4\pi(2\mu_2 + \Delta)}\frac{1}{y},$$

$$F_{\text{int}2/3} = \frac{\mu_2 b k_{\mu 2/3}}{4\pi(h_b - y)} = \frac{\mu_2 b\Delta}{4\pi(2\mu_2 - \Delta)}\frac{1}{h_b - y},$$

where $\mu_{Si} - \mu_1 = \mu_1 - \mu_2 = \mu_2 - \mu_3 = \mu_3 - \mu_{Ge} = \Delta$ is assumed [3]. The dislocation can have stable equilibrium position y_{eq} which is the root of equilibrium equation:

$$F_m + F_{\text{int}1/2} + F_{\text{int}2/3} = 0,$$

$$y_{eq} = \frac{1}{2}\left\{h_b - \frac{(\frac{\Delta}{\mu_2})^2}{2\pi[4-(\frac{\Delta}{\mu_2})^2]\gamma_m} \pm \sqrt{[h_b - \frac{(\frac{\Delta}{\mu_2})^2}{2\pi[4-(\frac{\Delta}{\mu_2})^2]\gamma_m}]^2 - \frac{\frac{\Delta}{\mu_2}h_b}{\pi(2+\frac{\Delta}{\mu_2})\gamma_m}}\right\}.$$

Set $\gamma_m = 0.01$, $\mu_2 = 45.6GPa$ [3], and study how the equilibrium positions vary when modulus difference Δ and sub-layer thickness h_b changes. See figures 8 and 9.

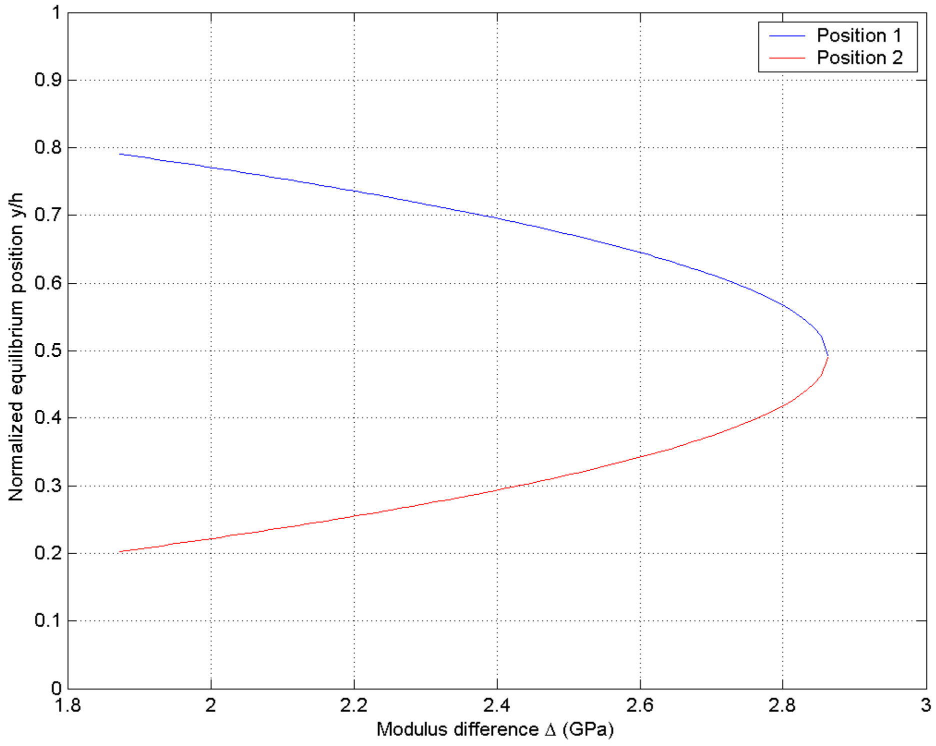

Fig. 8 Variation of equilibrium positions with respect to modulus difference. $\mu_2 = 45.6GPa$, $\gamma_m = 0.01$.

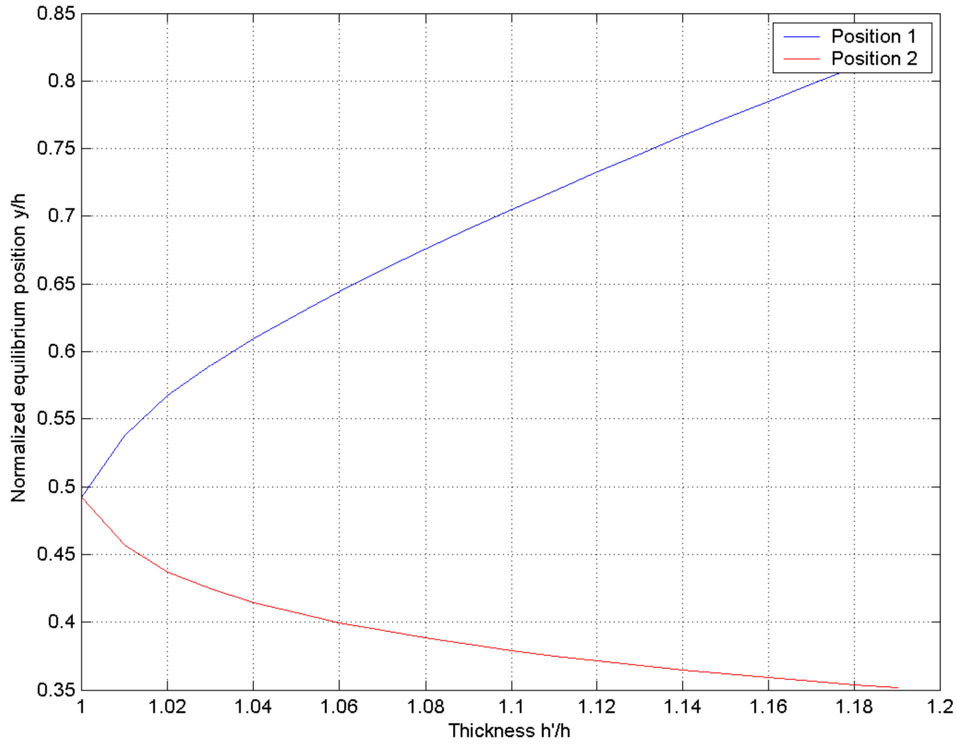

Fig. 9 Variation of equilibrium positions with respect to sub-layer thickness. $\Delta = 2.873GPa$,

$$\mu_2 = 45.6GPa\ ,\ \ \gamma_m = 0.01$$

When Δ increases, the dislocation prefers to stay near the middle of the sub-layer; in other words, the dislocation could be confined within this sub-layer for big Δ. When sub-layer thickness h_b increases, the equilibrium positions go away from the middle of the sub-layer. Δ denotes the modulus difference, that is the difference of composition ratios of two adjacent buffer sub-layers. These results suggest the confinement of dislocations could be controlled by using relatively large compositional change among buffer sub-layers and relatively thin sub-layers.

4 Summary

Some basic aspects of the continuum theory of elastic dislocation have been reviewed. A simple case of epitaxial system with buffer layer is studied and provides a little understanding about the confinement of dislocations within buffer layer. Sharp steps of the composition of buffer layer, and relatively thin buffer sub-layers can enhance the confinement of dislocations.

References:

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