1. Publication Nº
INPE-4254-PRE/1127

2. Version

3. Date
Jul., 1987

5. Distribution
☐ Internal ☒ External
☐ Restricted

4. Origin
LAS

Program
MATER/MATHET

6. Key words - selected by the author(s)
STRAINED EPITAXIAL LAYERS
SUPERLATTICES
COMMENSURATE-INCOMMENSURATE TRANSITIONS
PHASE TRANSITIONS

7. U.D.C.: *539.2*

8. Title *INPE-4254-PRE/1127*

EQUILIBRIUM STABILITY OF STRAINED EPITAXIAL LAYERS ON A RIGID SUBSTRATE

10. Nº of pages: *07*

11. Last page: *06*

12. Revised by

Ram Kishore

13. Authorized by

Marco Antônio Raupp
General Director

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14. Abstract/Notes

A simple theory of the equilibrium stability of an strained epitaxial layer on a rigid substrate is presented. We generalize the Frank-van der Merwe model of a single layer and consider N layers of adsorbate on a substrate. Continuum elasticity theory is used to describe each layer, but the coupling between layers is treated in a discrete fashion. Our method interpolates between a few layers and the thick film limit of standard dislocation theory, and in this limit the standard results are obtained. In addition, we develop a variational approach which agrees well with our exact calculations. The advantage of our method over previous ones is that it allows to perform stability analyses of arbitrary superlattice configurations.

15. Remarks *Submitted for publication in the "Proceedings of the 3rd. Escola Brasileira de Física de Semicondutores", Campinas, SP, 1987.*

EQUILIBRIUM STABILITY OF STRAINED EPITAXIAL LAYERS ON A RIGID SUBSTRATE*

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ABSTRACT - A simple theory of the equilibrium stability of an strained epitaxial layer on a rigid substrate is presented. We generalize the Frank-van der Merwe model of a single layer and consider N layers of adsorbate on a substrate. Continuum elasticity theory is used to describe each layer, but the coupling between layers is treated in a discrete fashion. Our method interpolates between a few layers and the thick film limit of standard dislocation theory, and in this limit the standard results are obtained. In addition, we develop a variational approach which agrees well with our exact calculations. The advantage of our method over previous ones is that it allows to perform stability analyses of arbitrary superlattice configurations.

1. INTRODUCTION

With the advent of the Molecular Bean Epitaxy, a great deal of work has been devoted to the study of coherently strained layered structures. The importance of these structures for applications as electronic devices is by now well established.[1] However, there still remain some fundamental questions regarding the stability of these structures as the thickness increases.

In this work we present a simple theory of equilibrium stability of a strained epitaxial layer on a rigid

* *Supported in part by an ONR contract (S.C.Y.), the MRL program at Brown University (J.M.K. and S.C.Y.) and an NSF-CNPq contract of cooperation between Brown University and INPE.*

substrate.[2] We generalize the Frank-van der Merwe[3] model of a single layer and consider N layers of adsorbate on a substrate. Continuum elasticity theory is used to describe each layer, but the coupling between layers is treated in a discrete fashion. The analyses is performed at zero temperature but certainly the statistical mechanics treatment of this model for finite temperatures will be a challenging problem. Even for the case of two layers of adsorbate in the absence of a substrate some interesting results are obtained.[4] The critical thickness for a given misfit is obtained by computing the energy of a single misfit dislocation as a function of thickness. When this energy vanishes, the equilibrium critical thickness is reached. Our method interpolates between a few layers and the thick film limit of standard dislocation theory. We also develop a variational approach which agrees well with the exact calculations and gives the standard result in the thick film limit. The advantage of our approach over previous ones is that it allows to perform the stability analyses of arbitrary superlattice configurations. Here, we present and discuss the main results. A detailed account of this work will be published elsewhere.[2,4]

2. THE MODEL

We consider N layers of adsorbate on a substrate. For simplicity, each overlayer is assumed to become incommensurate with the substrate in one direction only. We further assume that each layer can be described by continuum elasticity theory, but the coupling between them is treated in a discrete manner. This allows for abrupt changes in the system in the direction normal to the substrate. A general Hamiltonian for this system can be written in terms of the density of each layer, described by the function

$$\rho_n(x) = \rho_0 \, \mathrm{Re} \, e^{iG_n x} \, e^{i\theta_n(x)} , \qquad (1)$$

where the reciprocal lattice vector $G_n = \frac{2\pi}{a_n}$ is the natural periodicity of the n^{th} layer.[2] Displacements are allowed only in the x-direction. For the case of a rigid substrate and N identical layers, the Hamiltonian describing the system can be written as

$$H = \int \left[\frac{K}{2} \sum_{n=1}^{N} \left(\frac{d}{dx} \theta_n(x) - \delta\right)^2 + v \sum_{n=1}^{N-1} \left(1 - \cos(\theta_n - \theta_{n+1}\right) + h(1 - \cos \theta_1) \right] dx . \qquad (2)$$

The first term in (2) describes the elastic energy required to strain each layer, the second term describes the coupling between layers and the final term is the effect of the rigid substrate potential which acts only on the first layer. δ is proportional to the mismatch between the overlayer and the substrate.

3. RESULTS AND DISCUSSION

To proceed with the calculation we have to minimize the energy with respect to the $\theta_n(x)$, but this will lead to a system of coupled sine - Gordon equations which are somewhat intractable even when N=2. To simplify the calculation without changing significantly the physics involved, we replace the cosine interaction by a periodic parabolic interaction $V(\theta)$ defined by

$$V(\theta) = \frac{1}{2}\theta^2 \quad , \qquad -\pi \leqq \theta \leqq \pi \ ,$$

$$V(\theta+2\pi) = V(\theta) \ . \tag{3}$$

Although the calculations were performed using this approximation, we do not expect the behavior will depend on the particular choice of potential. Performing now the minimisation leads to a set of linear equations of motion for $0 \leqq \theta_n \leqq \pi$. The general solution of the system of differential equations has the form $\theta_i(x) = \sum_{j=1}^{N} a_{ij} e^{k_j x} + b_{ij} e^{-k_j x}$. Two possibilities arise: either there is a soliton in $\theta_i(x)$ which corresponds to the removal or addition of a column of atoms to the i^{th} layer or there is not. The former corresponds to the boundary condition $\theta_i(-L/2)=0$, $\theta_i(L/2)=2\pi$ for a system of length L, and the latter to $\theta_i(-L/2)=\theta_i(L/2) = 0$.

We have investigated the energy of the soliton configurations from the registred state analyticaly for N= 1, 2, 3 and 4 and numericaly for N > 4. We find that the configurations with lowest critical misfit always fall into two classes. For sufficiently small h/v the onset of stability is determined by a configuration with a soliton in every layer corresponding to a conventional misfit dislocation at the interface. For h/v > 1.2, we find that the first layer remain essentially connensurate with the substrate, except for an elastic distortion in form of a twist, where $\theta_1(-L/2) = \theta_1(0) = \theta\ (L/2) = 0$ and $\theta_1(x) = -\theta_1(-x)$. Each of the remaining N-1 layers has a soliton which corresponds to a misfit dislocation between the first and second layers. The soliton width increases with distance from the substrate.

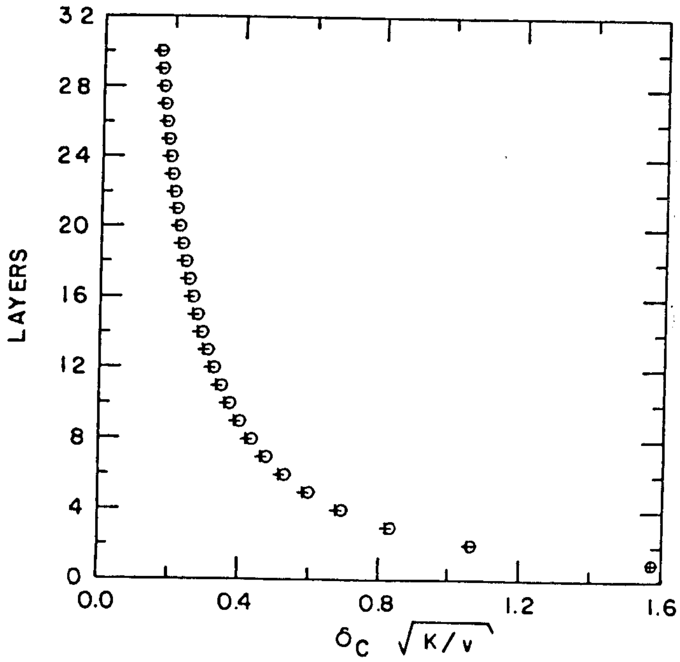

Fig.[1] - Critical misfit δ_C as a function of the number of layers, according to the exact (cross) and variational (circle) calculations.

The results of the calculation of the critical misfit are indicated in Fig.[1]. For larger N, this method becomes time consuming, so we have also performed a variational calculation. Using the information gleaned from the calculations described above, we assume a soliton in each layer centered at x=0, and in the limit $L \to \infty$ the phase $\theta_n(x)$ is assumed to have the following variational form

$$\begin{aligned} \theta_n(x) &= \pi e^{k_n x} , \quad x < 0 \\ &= 2\pi - \pi e^{-k_n x} , \quad x > 0 . \end{aligned} \tag{4}$$

In addition we make the ansatz that to minimize the energy ε_N we take $k_n = \lambda n^{-\alpha}$, with the result that the critical misfit given by $\delta_c = \varepsilon_n / 2\pi N$ takes the form $\delta_c = \frac{\pi}{2} \sqrt{v/K} \frac{\sqrt{A_N B_N}}{N}$

where $A_N = \sum_{n=1}^{N} n^{-\alpha}$, $B_N = \sum_{n=1}^{N-1} \frac{[(n+1)^\alpha - n^\alpha]^2}{(n+1)^\alpha + n^\alpha} + h/v$.

When N is large we find that the minimum value of the energy will be reached when $\alpha=1$, so that the critical misfit finally reduces to the form

$$\delta_c = \frac{\pi}{2\sqrt{2}} \sqrt{\frac{v}{K}} \frac{\mathrm{Ln}\, N}{N} . \qquad (5)$$

This is the same dependence as the more conventional theory of misfit dislocations.[5] The agreement of the variational calculation with the exact solution is quite good (see fig.[1]).

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TÍTULO

Equilibrium stability of strained epitaxial layers on a rigid substrate.

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OBSERVAÇÕES E NOTAS

Submitted for publication in the "Proceedings of the 3ª Escola Brasileira de Física de Semicondutores", Campinas, SP, 1987.

Palavras Chaves: STRAINED EPITAXIAL LAYERS, SUPERLATTICES, COMMENSURATE-INCOMMENSURATE TRANSTIONS, PHASE TRANSITIONS

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Nº DA PUBLICAÇÃO: 4254-PRE/1126 PÁG.:

CÓPIAS: Nº DISCO: LOCAL:

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AUTORIZO A PUBLICAÇÃO: ☐ SIM ☐ NÃO __/__/__

OBSERVAÇÕES E NOTAS

Palavras chaves: STRAINED EPITAXIAL LAYERS
SUPERLATTICES
COMMENSURATE - INCOMMENSURATE TRANSITIONS
PHASE TRANSITIONS

WORK SUBMITTED FOR PUBLICATIONS IN THE "Proceedings of the 3rd. Escola Brasileira de Física de Semicondutores", Campinas - SP, 1987

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