of missing low-resolution structure factors may improve the synthesis.

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Unstressed Superlattices

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Abstract

A method for calculating residual stresses in superlattices has been developed in the general form. Allowances have been made for the misfit dislocations, lattice mismatch and difference in the thermal expansion coefficients. The condition for the absence of residual stresses in superlattices has been obtained analytically in the case of both coherent growth and misfit dislocations.

Introduction

The main feature of the growth of semiconductor structures consisting of alternating layers of chemically different materials is the mismatch between the bulk lattice constants of different materials at epitaxy temperature, interfacial misfit dislocations and the difference in linear expansion coefficients.

Recently there has been strong interest in the heteroepitaxial growth of III-V compound* semiconductors on Si. However, there are serious problems concerning the growth of III-V semiconductors on Si substrates, one of which is the high density of dislocations generated and the other is residual stress in the growing films due to the large lattice mismatch and the difference in expansion coefficients of III-V films and Si substrates.

In this paper a method for calculating residual stresses in superlattices has been developed in the general form. Allowances have been made for the misfit dislocations, lattice mismatch and difference in thermal expansion coefficients of layers. The condition for the absence of residual stresses in superlattices has been obtained analytically in the case of both coherent growth and misfit dislocations.

* 3-5 compounds in IUPAC (1988) nomenclature.

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Theoretical considerations

A. Pseudomorphous growth

Consider the case of growth of a thin plate of an isotropic single crystal on a substrate. A_i is the lattice constant at epitaxy temperature, A_n is the lattice mismatch at epitaxy temperature,

$$A_n = (A_1 - A_2)/A_1, \tag{1}$$

a_i is the coefficient of thermal expansion of a layer (Fig. 1). The mismatch caused by the difference between the coefficients of thermal expansion of layers is

$$(a_1 - a_2)T \tag{2}$$

where T is the difference in temperature. The mismatch due to the misfit dislocations is $db = d_b$, where b is the Burgers vector, d is the density of misfit dislocations.

At equilibrium the stress distribution inside the composite satisfies the following equations.

(*a*) The force balance equation

$$F_1 - F_2 = 0. \tag{3}$$

(*b*) The moment balance equation

$$-F_1(t_1/2) + F_2(t_1 + t_2/2) = M_1 + M_2, \tag{4}$$

where the moments M_1 and M_2 are given by

$$M_1 = [E_1/(1-u_1)R] \int_{-h}^{t_1-h} x^2 w \, dx = [E_1 w/3(1-u_1)R][(t_1-h)^3 + h^3], \tag{5}$$

$$M_2 = [E_2/(1-u_2)R] \int_{t_1-h}^{t_1-h+t_2} x^2 w \, dx = [E_2 w/3(1-u_2)R][(t_1-h+t_2)^3 - (t_1-h)^3]. \tag{6}$$

Here R is the radius of curvature of the composite, t_i is the thickness of the plate, u_i is Poisson's ratio, w is the width of the layers and h is the shift of the neutral axis of the composite from $x = -t_1$ (see Fig. 1). The expression for h can be written as

$$\begin{aligned} h &= u + v - B/3A, \\ u &= [-q + (q^2 + p^3)^{1/2}]^{1/3}, \\ v &= [-q - (q^2 + p^3)^{1/2}]^{1/3}, \\ 2q &= 2B^3/27A^3 - BC/3A^2 + D/A, \\ 3p &= (3AC - B^2)/3A^2, \\ A &= 2E_1/(1-u_1), \\ B &= -3[E_1 t_1/(1-u_1) + E_2 t_2/(1-u_2)], \\ C &= 3\{E_1 t_1^2/(1-u_1) + [E_2/(1-u_2)] \times [(t_1+t_2)^2 - t_1^2]\}, \\ D &= -\{E_1 t_1^3/(1-u_1) + [E_2/(1-u_2)] \times [(t_1+t_2)^3 - t_1^3]\}. \end{aligned} \tag{7}$$

This expression is obtained from the balance equation of moments

$$\int_0^{t_1-h} E_1 x^2 \, dx/(1-u_1)R + \int_{t_1-h}^{t_1-h+t_2} E_2 x^2 \, dx/(1-u_2)R = \int_{-h}^{0} E_1 x^2 \, dx/(1-u_1)R. \tag{8}$$

(*c*) The boundary conditions

$$\frac{(1-u_1)F_1}{t_1 w E_1} + \frac{(1-u_2)F_2}{t_2 w E_2} + \frac{t_1 + t_2}{2R} = (a_1 - a_2)T + A_n + d_b. \tag{9}$$

The expression for stresses S_i in each layer should be written as

$$S_i = \pm F_i/t_i w + zE_i/2R, \tag{10}$$

where the coordinate $z = 0$ in the middle of each layer,

$$F_1 = F_2 = 4wt_1t_2E_1E_2Q[(a_1 - a_2)T + A_n + d_b] \times \{t_1t_2E_1E_2w(t_1+t_2)^2 + 4Q[t_1E_1(1-u_2) + t_2E_2(1-u_1)]\}^{-1} \tag{11}$$

and

$$-1/R = 2wt_1t_2E_1E_2(t_1+t_2)[(a_1-a_2)T + A_n + d_b] \times \{t_1t_2E_1E_2w(t_1+t_2)^2 + 4Q[t_1E_1(1-u_2) + t_2E_2(1-u_1)]\}^{-1}, \tag{12}$$

$$Q = [E_1 w/3(1-u_1)][(t_1-h)^3 + h^3] + [E_2 w/3(1-u_2)][(t_1-h+t_2)^3 - (t_1-h)^3]. \tag{13}$$

If $(a_1 - a_2)T + A_n + d_b = 0$, then $R = \infty$, $F = 0$ and $S = 0$. This is the condition for the absence of residual stresses in the heterostructure in the case of pseudomorphous growth. This condition is that the sum of three mismatches is equal to zero: the lattice mismatch at epitaxy temperature, the mismatch caused by the difference between the coefficients of thermal expansion of layers and the mismatch introduced by the misfit dislocations.

B. Coherent growth

In this case, d_b is zero. If $(a_1 - a_2)T + (A_1 - A_2)/A_1 = 0$ then $S = 0$. This condition is like that outlined by Aleksandrov (1972). The condition

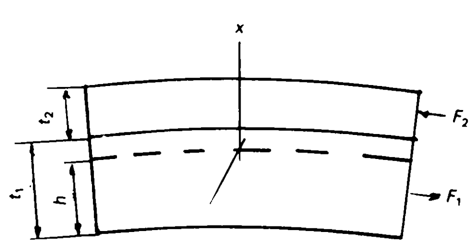

Fig. 1. Schematic diagram of the formation of a two-layer composite plate.

for the absence of residual stresses in the heterostructure in the case of coherent growth has been obtained analytically. This condition is that the sum of the following mismatches is equal to zero: the mismatch caused by the difference between the coefficients of thermal expansion of layers and the lattice mismatch at epitaxy temperature.

The growth conditions can be satisfied with such a radius of curvature of the substrate at epitaxy temperature at which, on heterostructure straightening and cooling, the stresses caused by both the difference between the coefficients of expansion of layers and the difference between the lattice constants at epitaxy temperature are eliminated. In this case, the necessary density of dislocations is introduced.

The method of calculation has been used in analyzing the residual stresses of a 14 layer InGaAsP/InP coherently developed heterolaser with a superlattice. The moments were determined relative to the neutral plane and the middle part of each layer. It is shown that in the case of moments obtained in different ways, their total values only differ in the ninth sign and the values of stresses in the layers differ in the fourth sign. The validity of the results of calculating stresses in which the moment values are determined relative to the middle part of each layer has been confirmed.

Concluding remarks

The condition for the absence of residual stresses in superlattices has been obtained analytically for the cases of both coherent growth and misfit dislocations. In the case of pseudomorphous growth, this condition is that the sum of three mismatches is equal to zero: the lattice mismatch at epitaxy temperature, the mismatch caused by the difference between the coefficients of thermal expansion of the layers and the mismatch introduced by the misfit dislocations.

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A Multisolution Method of Phase Determination by Combined Maximization of Entropy and Likelihood. III. Extension to Powder Diffraction Data

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Abstract

The mathematical techniques used in the derivation of intensity statistics and of probabilistic relations between structure factors for single-crystal data are here extended so as to encompass the phenomenon of intensity overlap, which is encountered with diffraction data collected from microcrystalline powders or from other disordered specimens. It is shown that the loss of information caused by intensity overlap in powder diagrams may be put on the same footing as the usual loss of phase for single-crystal data by a judicious use of a multiplicity-weighted metric and of the n-dimensional spherical geometry associated with that metric. Structure determination from powder diffraction data is thus cast in the form of a 'hyperphase problem' in which the dimensionality varies from one data item to another. This geometric picture enables probability distributions for overlapped intensities to be derived not only under the standard assumption of a uniform distribution of random atoms - thus extending Wilson's statistics to powder data - but also for non-uniform distributions such as those occurring in maximum-entropy phase determination [Bricogne (1984). *Acta Cryst.* **A40**, 410-445]. The corresponding conditional probability distributions and likelihood functions are then derived. The possible presence of known fragments is also considered. These new distributions and likelihood functions lead to new methods of data normalization, to new statistical tests for space-group assignment, to a generalization of the 'heavy-atom' method, to the extension to powders of a new multisolution method of structure determination [Bricogne & Gilmore (1990). *Acta Cryst.* **A46**, 284-297] recently applied to single crystals [Gilmore, Bricogne & Bannister (1990). *Acta Cryst.* **A46**, 297-308] and to a new criterion for conducting crystal structure

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