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A new approach to calculating the energy of systems of misfit dislocations in strained epitaxial layers

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Abstract. A new method for calculating the stored elastic energy of epitaxial strained layers containing misfit interfacial dislocations is presented. The method differs from previous approaches in that it explicitly takes into account all dislocation–dislocation interactions and interactions between dislocations and the mismatch stress. The method is unique in that it can be used to calculate the energy of finite and/or irregularly spaced systems of dislocations. Examples are given comparing the energy per unit area of finite and non-uniform systems of dislocations calculated using the present approach with that calculated for the infinite uniform case.

Thin film structures involving epitaxially strained layers (figure 1) are increasing in both scientific and technological importance, e.g. $Si_{1-x}Ge_x$ alloy films on Si substrates for microelectronic devices. In many cases of interest the film has the same crystal structure as the substrate but has a different lattice parameter which defines a mismatch strain, $f_m = (a_{layer} - a_{substrate})/a_{substrate}$. For film thickness, h, below a critical thickness, h_c, the mismatch is accommodated by a homogeneous straining of the film (pseudomorphic film) with an induced biaxial stress

$$\sigma_0 = -2\mu[(1+\nu)/(1-\nu)]f_m \tag{1}$$

and stored elastic energy

$$W_0 = LL'2\mu[(1+\nu)/(1-\nu)]f_m^2 h. \tag{2}$$

In these expressions μ is the shear modulus and ν is the Poisson ratio of the film. For $h > h_c$ the mismatch is increasingly accommodated by misfit dislocations at the interface between substrate and film as the introduction of dislocations relieves some of the mismatch strain and reduces the stored elastic energy. It is necessary to be able to calculate the stored energy for any potential configuration of misfit dislocations in order to (a) predict the minimum energy configuration which would correspond to the thermodynamic equilibrium state and (b) estimate the excess energy of an observed configuration which will provide the driving force for subsequent relaxation towards the equilibrium configuration.

This problem has been considered many times previously, e.g. [1–4], but early attempts [2, 3] did not take interactions between dislocations into account properly [5]. An attempt has been made recently to consider explicitly the interaction between dislocations [6]. However, in that treatment the interaction was limited to nearest neighbours and the total energy was not synthesized correctly in that the interactions considered do not correspond to the total

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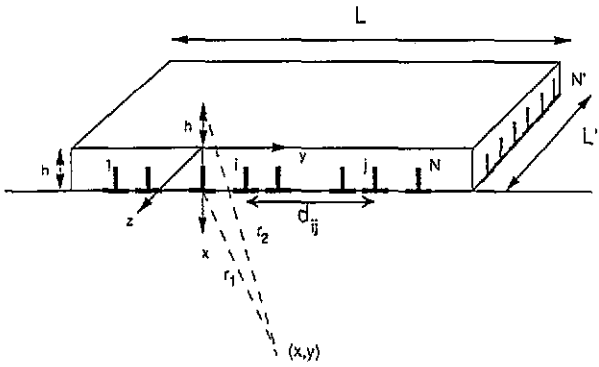

Figure 1. The geometry and coordinates of orthogonal misfit dislocations at the interface between a bulk substrate and a strained epitaxial layer.

stress distribution. Great care must be taken in synthesizing energies from the component parts of the system. In linear elasticity, as usually assumed, the stresses from various sources in the system are additive, but the energies are not because the energy density is proportional to the square of the local stress. The concept of 'interaction energy' allows the energies to be additive provided that all interactions are included and that the sources of interactions synthesize the total stress distribution. This is not the case in [6] because the interaction between each dislocation and the initial misfit stress is not included fully by considering only the energy associated with the average stress in the layer. A recent theory [4] has included these interactions rigorously, but is only valid for infinite arrays of uniformly spaced dislocations. (It has been shown using this theory that the interactions reduce the total energy with respect to that erroneously obtained by adding the dislocation self-energies to the mean strain energy [5]. Adding nearest neighbour interactions, as in [6] only serves to increase the error.)

In general, however, experimental observations show that the dislocations are not uniformly-spaced and are finite in number, e.g. [7]. Thus the existing exact theory [5] does not strictly apply to most situations of practical interest. In the present work a new approach to calculating the stored elastic energy of strained layers containing misfit dislocations is presented that can be applied to finite systems and/or irregularly spaced dislocations.

The method of calculation employed here is based on the following principles:

(a) starting from the pseudomorphic configuration the incremental energies are summed as each dislocation is introduced sequentially;

(b) linear elasticity is assumed so that the stresses and strains from different sources can be superposed;

(c) the energy increment for introducing any given dislocation is equal to the work done by displacing the surfaces of an imaginary 'cut' in the material by a Burgers vector, b (defined as the vector from start to finish after a right-handed circuit of lattice sites in the defective crystal), against the internal stresses acting on the surfaces of the cut, i.e. [8]

$$\Delta W = -\int \sigma_{\text{initial}} \cdot b \, \mathrm{d}S - \frac{1}{2}\int \Delta\sigma \cdot b \, \mathrm{d}S \tag{3}$$

The stress distribution on the faces of the cut is σ_{initial} before the deformation takes place and $\sigma_{\text{initial}} + \Delta\sigma$ when deformation is complete. Thus $\Delta\sigma$ is the self-stress field of the dislocation being introduced. The cut can be along any surface starting at the dislocation core and ending either at a free surface or infinity. In this method the core is regarded as a hollow cylinder of radius q (approximately equal to b), and thus the calculated energy

is that stored in the region outside the core. For convenience we select the cut surface as starting at the dislocation core on the plane $x = h - q$ (figure 1) and extending in the x direction to the surface of the epitaxial layer.

For a single set of N dislocations spaced on the y-axis and aligned parallel with the z direction (figure 1) this leads to the following expression for the total energy

$$W_N = W_0 - N\sigma_0 b_y h L' + N E_D L' + \frac{L'}{2}\sum_{i\neq j}^{N} E_I(d_{ij}) \tag{4}$$

in which E_D is the self-energy of a dislocation and $E_I(d_{ij})$ is the energy of interaction between a pair of dislocations separated by distance d_{ij}. The second term in (4) is the work done against the misfit stress, the third is the self-energy of non-interacting dislocations and the fourth term is the summation of all the interactions between pairs of dislocations in the system (the factor of two arises because the summation as written counts the energy of a given pair of dislocations twice; as d_{ij} and d_{ji}). The energy given by (4) does not depend on assuming any periodicity or average spacing of the dislocations.

In general the crystallographic constraints will lead to more than one set of dislocations being present. Here we consider systems in which there are two sets of dislocations of the same type with orthogonal dislocation lines and f_m the same in each direction (this will apply to epitaxial layers grown on the {100} face of cubic crystals, but the analysis can be extended to any geometry). For each dislocation in the second set there will be present an additional stress due to the overall strain caused by the first set. In the coordinate system of the first set the overall strains due to the first set are

$$\langle\epsilon_{yy}\rangle = Nb_y/L \qquad \langle\epsilon_{zy}\rangle = Nb_z/2L' \tag{5}$$

and the corresponding stresses relevant to the Burgers displacement of the second set are

$$\langle\sigma_{zz}\rangle = [2\mu\nu/(1-\nu)]\langle\epsilon_{yy}\rangle \qquad \langle\sigma_{zy}\rangle = 2\mu\langle\epsilon_{zy}\rangle. \tag{6}$$

These are converted into stresses for the second set by the transformation $(x, y, z) = (x', z' - y')$. The inclusion of these stresses leads to the following expression for the energy of a strained epilayer containing a two-dimensional network of N by N' dislocations:

$$W_{N,N'} = W_0 - \sigma_0 b_y h(NL' + N'L) + NN'\mu h\{b_y^2[2\nu/(1-\nu)] - b_z^2\} + (NL' + N'L)E_D + \frac{L'}{2}\sum_{i\neq j}^{N} E_I(d_{ij}) + \frac{L}{2}\sum_{i'\neq j'}^{N'} E_I(d_{i'j'}). \tag{7}$$

In this derivation the energy associated with the intersections of the two orthogonal sets of dislocations is neglected.

The self-energy per unit length of a dislocation at a distance h below a free surface is given from (3) by (neglecting the non-elastic core energy)

$$E_D = -\frac{1}{2}\int_0^{h-q} (b_y\sigma_{yy}(x,0) + b_x\sigma_{xy}(x,0) + b_z\sigma_{zy}(x,0))\,dx \tag{8}$$

and the interaction energy per unit length by

$$E_I(d) = -\frac{1}{2}\int_0^{h-q} (b_y\sigma_{yy}(x,d) + b_x\sigma_{xy}(x,d) + b_z\sigma_{zy}(x,d))\,dx. \tag{9}$$

The stresses are those for a single dislocation located on the line $(h, 0, z)$ and the contributions from b_x and b_y (edge components) are calculated from the stress function χ by double differentiation [9]

$$\sigma_{xx} = \partial^2\chi/\partial y^2 \qquad \sigma_{yy} = \partial^2\chi/\partial x^2 \qquad \sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$
$$\sigma_{xy} = \partial^2\chi/\partial x\partial y \qquad \sigma_{yz} = \sigma_{zx} = 0. \tag{10}$$

The stress function, for the case in which the elastic constants of the substrate and the epitaxial layer are equal, is [9]

$$\chi = \{\mu b_x/[2\pi(1-\nu)]\}[y(\ln r_2 - \ln r_1) - 2hxy/r_2^2]$$
$$+ \{\mu b_y/[2\pi(1-\nu)]\}[-(x-h)\ln r_1 + (x-h)\ln r_2 - h + (2hx/r_2^2)(x+h)] \tag{11}$$

where r_1 and r_2 are shown in figure 1. The stresses resulting from b_z, the screw component, are [9]

$$\sigma_{yz} = -\frac{\mu b_z}{2\pi}\left(\frac{x-h}{r_1^2} - \frac{x+h}{r_2^2}\right) \qquad \sigma_{xz} = \frac{\mu b_z}{2\pi}\left(\frac{y}{r_1^2} - \frac{y}{r_2^2}\right). \tag{12}$$

These stresses completely satisfy the necessary boundary condition that all components normal to the free surface (i.e. x components) be zero at the free surface ($x = 0$). (For the screw contributions this is satisfied exactly by an image construction, equation (12), but the image construction is not sufficient for the edge contributions and equation (11) contains extra terms in addition to those resulting from the image.) The boundary condition is satisfied for each individual dislocation in the system and therefore the total energy expressions do not depend on any assumptions concerning the nature of the dislocation distribution (e.g. periodic spacing). Substitution of these stresses into equations (8) and (9) leads to the following expressions for E_D:

$$E_D = \frac{\mu}{4\pi}\left[\frac{(b_x^2 + b_y^2)}{(1-\nu)}\left(\ln\left(\frac{2h-q}{q}\right) - \frac{2h(h-q)}{(2h-q)^2}\right) + b_z^2 \ln\left(\frac{2h-q}{q}\right)\right] \tag{13}$$

and $E_I(d)$, when both h and d are much greater than q:

$$E_I(d) = \frac{\mu b_x^2}{4\pi(1-\nu)}\left(\ln(4a^2+1) - \frac{4a^2(12a^2+1)}{(4a^2+1)^2}\right)$$
$$+ \frac{\mu b_y^2}{4\pi(1-\nu)}\left(\ln(4a^2+1) + \frac{4a^2(4a^2+3)}{(4a^2+1)^2}\right) + \frac{\mu b_z^2}{4\pi}\ln(4a^2+1) \tag{14}$$

where $a = h/d$. Both E_D and E_I are logarithmically divergent in an infinite medium (i.e. as h tends to infinity). The interaction energy falls off rapidly as the interdislocation distance increases beyond h because the free surface limits the 'range' of the stress field of each dislocation and screens one dislocation from the others.

By using the above expressions (equations (13) and (14)) for E_D and E_I in equation (7) the total stored elastic energy of a finite and/or irregular two-dimensional net of orthogonal dislocations having arbitrary Burgers vector may be calculated.

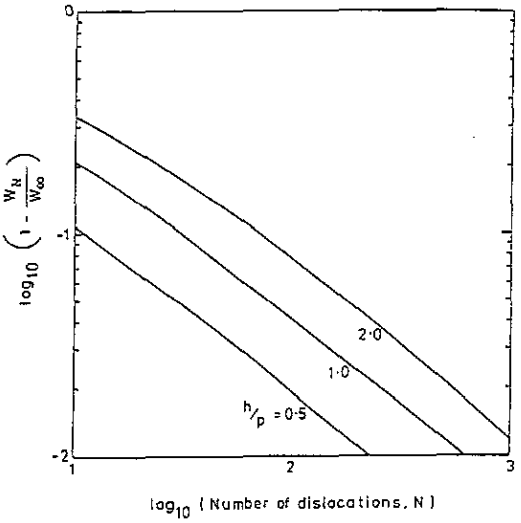

Figure 2. The energy per unit area of a two-dimensional finite array of $N \times N$ edge dislocations, $W(N)$, compared with that of an infinite array [10]. The curves correspond to different values of h/p.

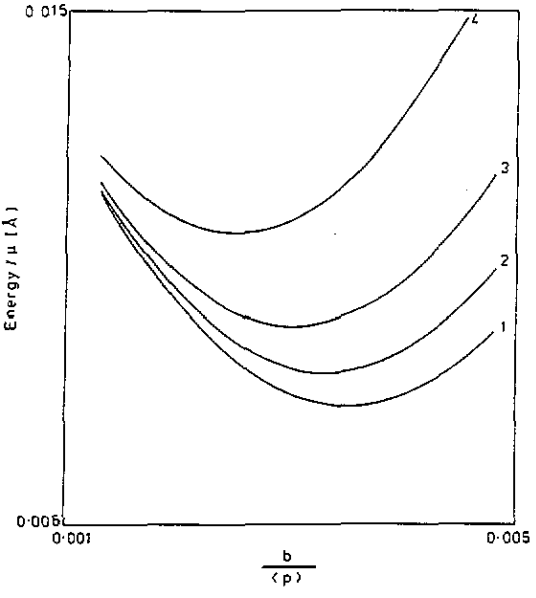

Figure 3. The energy per unit area calculated for edge dislocations of irregular spacing [11]. The film thickness was taken to be 255 Å, which is approximately $2h_c$ for the parameters chosen. The different curves correspond to different values of the standard deviation in dislocation spacing relative to the mean. These values are: curve 1, 0; curve 2, 0.3; curve 3, 0.45; curve 4, 0.6.

For the special case of a two-dimensional array of *regularly* spaced dislocations equation (7) may be simplified to give the energy per unit area as

$$\frac{W}{L^2} = \frac{W_0}{L^2} - \frac{2}{p}\sigma_0 b_y h + \frac{2}{p}\mu\frac{h}{p}\left(b_y^2\frac{\nu}{(1-\nu)} - \frac{b_z^2}{2}\right) + \frac{2}{p}E_D + \frac{2}{p}\sum_{i=1}^{N-1}\frac{(N-i)}{N}E_I(ip) \qquad (15)$$

where p is the nearest neighbour distance and is a constant. In a regular array interdislocation distances, d_{ij}, are integer multiples of the periodic spacing, p; hence the appearance of the product, ip, in the summation of dislocation–dislocation interaction energies. We have used a less general form of (15), applicable only to so-called 90° dislocations having

$b = (0, b_y, 0)$, to calculate the energy per unit area when the number of dislocations is finite [10]. The results (figure 2) show that the energy per unit area of a finite system of dislocations is lower than that of an infinite system by a percentage that increases as the ratio h/p increases [10]. Also, the present method gives identical results to those of the theory of Willis *et al* as N tends to infinity (i.e. for infinite regular dislocation arrays).

Equation (7) has been used to calculate the effect of non-uniformity of nearest neighbour dislocation spacing on the energy of the system [11]. The results (figure 3) show that the effect of increasing non-uniformity, while maintaining constant average nearest neighbour dislocation spacing, is to increase the energy of the system. These results are of particular importance for the relaxation of strain in layers thicker than the critical thickness. They explain the experimental observation that, even for layers grown or annealed at high temperature and thus expected to be close to equilibrium, strain relaxation in $Si_{1-x}Ge_x$ layers is always much less than predicted by equilibrium theory assuming uniformly spaced dislocations.

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