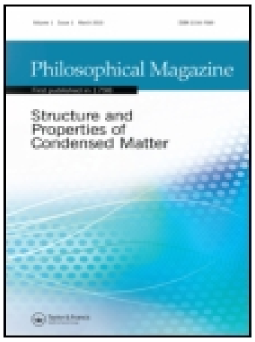

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Critical thickness for dislocation generation in epitaxial piezoelectric thin films

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Abstract

Dislocations form in epitaxial thin films above a critical thickness, when the stress due to the film–substrate mismatch becomes excessive. This phenomenon has been extensively investigated in non-piezoelectric thin films. In piezoelectric films, the mismatch strain field and the electric field are coupled, and the critical thickness depends on an extra physical variable: the electric field. In this paper, the critical thickness for dislocation formation in a piezoelectric film is derived. The dependence of the critical thickness on the piezoelectric properties of the $Al_xGa_{1-x}N/GaN$ system is then discussed.

§ 1. Introduction

Thin films play a pivotal role in modern engineering and technology. Their performance is closely related to the material properties of the film and, in particular, the crystal orientation (or texture for polycrystalline films), and the dislocation density and distribution. As a result of the crystalline misfit with the substrate, a newly deposited film is under stress, independent of whether it is polycrystalline or heteroepitaxial. As the film thickens, the stress builds up and, eventually, the conditions favour the generation of dislocations to relax the stress.

The existence of a critical thickness for dislocation generation in thin films was first proposed by Frank and van der Merwe (1949) and it was subsequently confirmed experimentally. Indeed, if the misfit strain between the substrate material and the film material is sufficiently small, or when the film is very thin, it can be accommodated elastically. However, as the film thickens, the energy required for elastic accommodation increases and eventually becomes excessive, and the dislocations are generated as an alternative means to accommodate the misfit.

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Two approaches are generally followed in the theoretical studies of critical thickness of strained epitaxial films. The first approach involves the comparison of the Gibbs free energy of the two strained systems, with and without the misfit dislocation. In this approach, very thin films would have the lower free energy without the misfit dislocation. As the film thickens beyond a certain critical value, the film with the misfit dislocation would have the lower free energy. By equating the free energies of the two systems, a necessary condition for the critical thickness is obtained. The second approach considers the balance between two driving forces, one originating from the misfit strain that tends to lengthen the misfit dislocation, and the other from the line tension that tends to shorten it. We note that the two approaches are *not* independent of each other and, indeed, Freund (1987) and Nix (1988) showed that the two approaches lead to precisely the same results.

Investigations of the critical thickness based on either one of the foregoing approaches have been reported in the literature. Thus, Matthews and Blakeslee (1974) derived an equation for the critical thickness by assuming a critical balance between the force generated by the lattice mismatch on a segment of a propagating threading dislocation, and the extra line tension associated with a newly created interfacial dislocation. Freund (1987) systematically investigated the driving force for glide of a threading dislocation. The effect of elastic constants on the critical thickness has been investigated by Willis *et al.* (1991), Gosling and Willis (1994) and Zhang (1996). Freund and Nix (1996) and Zhang and Su (1999) extended the analyses on the critical thickness of an epitaxial layer (epilayer) grown on an infinite substrate to an epilayer grown on a compliant substrate.

Ferroelectric thin films are quickly becoming one of the most important components in advanced microelectronic and micromechanical devices, such as high-density nonvolatile random access memories, sensors, microactuators, piezoelectric transducers and pyroelectric detectors. Despite their technological importance and the detrimental effect of dislocation formation in such materials, the theoretical framework for the analysis of the critical thickness for dislocation formation in a piezoelectric film, in relation to its environmental, geometric and materials parameters, has not been formulated. Indeed, for many practical applications, estimations still have to be made extrapolating from the theory of non-piezoelectric elastic films. Nevertheless, the complexity of the formulation involved in such an analysis, due to the crystallographic anisotropy and the coupled elastic and electric fields of piezoelectric materials, makes the problem non-trivial.

In this paper, we make an attempt to formulate the theoretical framework for the aforesaid analyses. In § 2, the coupled elastic and electric fields of a dislocation in a semi-infinite piezoelectric medium is first derived, on the basis of which an explicit expression of the formation energy of the dislocation is obtained in § 3. From equilibrium considerations, a formula to determine the critical thickness for dislocation formation in a piezoelectric thin film is also derived. Finally in § 4, the theory is applied to examine the effect of piezoelectricity on the critical thickness of a thin film.

§ 2. Elastic and electric fields in a piezoelectric semi-infinite space with a dislocation

Consider the half-space $x_2 > 0$ occupied by a piezoelectric material, and a straight dislocation with Burgers vector $\mathbf{b}$. The dislocation and the associated line charge q per unit length trapped by the dislocation core (Im *et al.* 2001) is assumed to

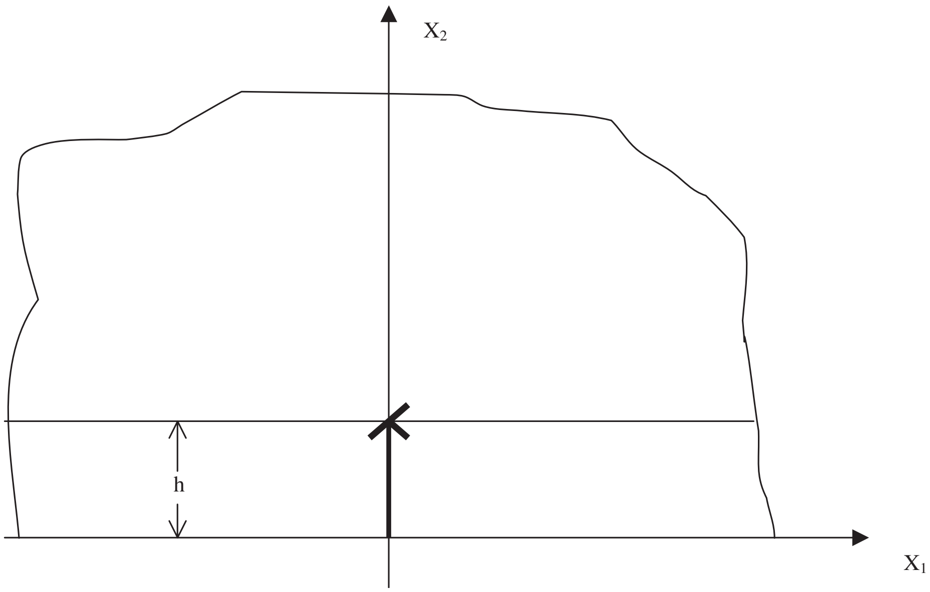

Figure 1. Schematic diagram of a misfit dislocation in the interface between an epilayer and its substrate.

be at $(0, h)$, $h > 0$ (figure 1). In terms of the electrostatic potential φ, the electric field E_i is given by

$$E_i = -\frac{\partial \varphi}{\partial x_i} \equiv -\varphi_{,i}. \tag{1}$$

The constitutive relation of the stress tensor σ_{ij} with the elastic displacement gradients $u_{i,j}$, and that of the electric displacement vector D_i with the electric field E_i respectively are given by

$$\begin{aligned} \sigma_{ij} &= C_{ijkm} u_{k,m} + e_{mij} \varphi_{,m}, \\ D_i &= e_{ikm} u_{k,m} - \alpha_{im} \varphi_{,m}. \end{aligned} \tag{2}$$

Here repeated indices imply summation, a comma stands for differentiation. C_{ijkm} is the elastic stiffness tensor, e_{mij} are the piezoelectric stress constants and α_{im} are the permittivity constants. In the absence of body forces and free charges, the balance laws require that

$$\sigma_{ij,j} = \mathbf{0}, \quad D_{i,i} = \mathbf{0}. \tag{3}$$

Assuming free surface boundary condition for the film, the traction and the electrical displacement both vanish at $x_2 = 0$. Following Barnett and Lothe (1975), we define the $3 \times 4 \times 4 \times 3$ matrix $\mathbf{G}$, the 3×4 matrix $\boldsymbol{\Sigma}$, and the quadruple $\mathbf{u}$ by

$$G_{iJKm} = \begin{cases} C_{ijkm} & (J, K = 1, 2, 3), \\ e_{mij} & (J = 1, 2, 3;\ K = 4), \\ e_{ikm} & (J = 4;\ K = 1, 2, 3), \\ -\alpha_{im} & (J = K = 4), \end{cases} \tag{4}$$

$$\Sigma_{iJ} = \begin{cases} \sigma_{ij} & (J = 1, 2, 3), \\ D_j & (J = 4), \end{cases} \tag{5}$$

$$u_J = \begin{cases} u_j & (J = 1, 2, 3), \\ \varphi & (J = 4), \end{cases} \tag{6}$$

so that equations (2) and (3) can be combined to give

$$G_{iJKm} u_{K,mi} = \mathbf{0}. \tag{7}$$

Here the lower-case indices $i, m = 1, 2, 3$, and the upper-case indices $J, K = 1, 2, 3, 4$. Indices from 1 to 3 refer to the elastic variables, and the index 4 refers to the electric variable. For two-dimensional problems, in which u_K depends on only x_1 and x_2, the general solution of equation (7) is a function of a linear combination of x_1 and x_2. Thus, we can write, without loss of generality,

$$u_J = a_J f(z), \quad z = x_1 + p x_2, \tag{8}$$

where f is an arbitrary function of z, and p and a_J are to be determined in the following.

Substitution of equation (8) into equation (7), and noting that for f to be an arbitrary function, we must satisfy

$$\left[\mathbf{Q} + p(\mathbf{R} + \mathbf{R}^{\mathbf{T}}) + p^2\mathbf{T}\right]\mathbf{a} = \mathbf{0}, \tag{9}$$

where the bold lower-case letters mean quadruples, and the bold capital letters mean 4×4 matrices. $\mathbf{Q}$, $\mathbf{R}$ and $\mathbf{T}$ are defined as

$$\mathbf{Q} = \begin{bmatrix} C_{i1k1} & (e_{11})_i \\ (e_{11}^T)_k & -\alpha_{11} \end{bmatrix},$$

$$\mathbf{R} = \begin{bmatrix} C_{i1k2} & (e_{21})_i \\ (e_{12}^T)_k & -\alpha_{12} \end{bmatrix}, \tag{10}$$

$$\mathbf{T} = \begin{bmatrix} C_{i2k2} & (e_{22})_i \\ (e_{22}^T)_k & -\alpha_{22} \end{bmatrix},$$

$$(e_{ij})_s = e_{ijs}.$$

Introducing the generalized stress function ψ_J,

$$\psi_J = b_J f(z), \quad \mathbf{b} = (\mathbf{R}^{\mathbf{T}} + p\mathbf{T})\mathbf{a} = -\frac{1}{p}(\mathbf{Q} + p\mathbf{R})\mathbf{a}, \tag{11),}$$

one obtains

$$\sigma_{i1} = -\psi_{i,2}, \quad \sigma_{i2} = -\psi_{i,1}, \quad D_1 = -\psi_{4,2}, \quad D_2 = -\psi_{4,1}. \tag{12}$$

It has been shown that p has eight eigenvalues, consisting of four pairs of complex conjugates (Barnett and Lothe 1975, Ting 1996). The four eigenvalues with $\operatorname{Im}(p) > 0$, are denoted by p_α with $\alpha = 1, 2, 3, 4$, and $\bar{p}_\alpha$ with $\operatorname{Im}(p) < 0$ are the complex conjugates of p_α. The corresponding eigenvectors in equation (9) are denoted by $\mathbf{a}_\alpha$.

Using the solution of the elastic counterpart (Ting 1992), the general solution for equation (7) is given by

$$\mathbf{u} = \frac{1}{\pi}\,\mathrm{Im}\,[\mathbf{A}\,\boldsymbol{\Delta}(z_* - p_* h)\mathbf{q}^{\infty}] + \frac{1}{\pi}\,\mathrm{Im}\left(\sum_{\beta=1}^{4}\left[\mathbf{A}\,\boldsymbol{\Delta}(z_* - \bar{p}_\beta h)\mathbf{q}_\beta\right]\right),$$
$$\boldsymbol{\psi} = \frac{1}{\pi}\,\mathrm{Im}\,[\mathbf{B}\,\boldsymbol{\Delta}(z_* - p_* h)\mathbf{q}^{\infty}] + \frac{1}{\pi}\,\mathrm{Im}\left(\sum_{\beta=1}^{4}\left[\mathbf{B}\,\boldsymbol{\Delta}(z_* - \bar{p}_\beta h)\mathbf{q}_\beta\right]\right), \tag{13}$$

where $\mathbf{A}$ and $\mathbf{B}$ are 4×4 complex matrices defined using $\mathbf{b}_\alpha$ defined by equation (13) for various eigenvalues p_α and eigenvectors $\mathbf{a}_\alpha$:

$$\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4], \quad \mathbf{B} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4], \tag{14}$$

and

$$\boldsymbol{\Delta}(z_* - p_* h) = \mathrm{diag}\,[\log(z_1 - p_1 h),\ \log(z_2 - p_2 h),\ \log(z_3 - p_3 h),\ \log(z_4 - p_4 h)],$$
$$\boldsymbol{\Delta}(z_* - \bar{p}_\beta h) = \mathrm{diag}\,[\log(z_1 - \bar{p}_\beta h),\ \log(z_2 - \bar{p}_\beta h),\ \log(z_3 - \bar{p}_\beta h),\ \log(z_4 - \bar{p}_\beta h)], \tag{15}$$

In equation (13), $\mathbf{q}^{\infty}$ and $\mathbf{q}_\beta$ are complex quantities to be determined next.

The boundary conditions can be written in the following form:

$$\begin{aligned} &\boldsymbol{\psi} = \mathbf{0}, \quad x_2 = 0,\\ &\int_\Omega \mathrm{d}\mathbf{u} = \mathbf{b}, \quad \text{for any closed curve } \Omega \text{ enclosing } (0, h)\\ &\int_\Omega \mathrm{d}\boldsymbol{\psi} = \mathbf{r}, \quad \text{for any closed curve } \Omega \text{ enclosing } (0, h)\\ &\sigma_{ij} \to 0; \quad D_i \to 0, \quad \text{when } |Z| = \infty. \end{aligned} \tag{16}$$

In equation (16), $\mathbf{b} = (b_1, b_2, b_3, b_4)$, $\mathbf{r} = (0, 0, 0, -q)$, b_i, $i = 1, 2, 3$, are the components of the Burgers vector. The quantity $b_4 \neq 0$ corresponds to an electric dipole layer along the cut plane. Note the distinction between $\mathbf{b}$ and the eigenvectors $\mathbf{b}_1, \mathbf{b}_2$, etc., in equation (14). q is the line charge per unit length. Equation (16) is in a general form that contains all the relevant boundary conditions for the dislocation problems in epilayers. Substitution of equation (14) into equation (16) gives

$$\mathbf{q}^{\infty} = \mathbf{A}^{\mathbf{T}}\mathbf{r} + \mathbf{B}^{\mathbf{T}}\mathbf{b},$$
$$\mathbf{q}_\beta = \mathbf{B}^{-1}\bar{\mathbf{B}} I_\beta \bar{\mathbf{q}}^{\infty}, \tag{17}$$

where

$$\mathbf{I}_1 = \mathrm{diag}\,[1, 0, 0, 0],\ \mathbf{I}_2 = \mathrm{diag}\,[0, 1, 0, 0],\ \mathbf{I}_3 = \mathrm{diag}\,[0, 0, 1, 0],\ \mathbf{I}_4 = \mathrm{diag}\,[0, 0, 0, 1]. \tag{18}$$

The solution for the half-space in equation (13) is made up of the two parts. The first terms on the right-hand sides are the solution for the infinite space with a line charge of q per unit length along the dislocation line at $(x_1, x_2) = (0, h)$. The second terms represent 16 one-component images for the infinite space whose singularities are located outside the half-space. The first terms can be expressed in real form using the following relations (Ting 1996):

$$
\begin{aligned}
\operatorname{Im}[\mathbf{A}\,\boldsymbol{\Delta}(z_* - p_*h)\mathbf{q}^{\infty}] &= \operatorname{Im}\left[\mathbf{A}\,\boldsymbol{\Delta}(z_* - p_*h)(\mathbf{A}^{\mathrm{T}}\mathbf{r} + \mathbf{B}^{\mathrm{T}}\mathbf{b})\right] \\
&= -\frac{1}{2}\log(\hat{r})\,\mathbf{h} - \frac{\pi}{2}\mathbf{S}(\hat{\theta})\cdot\mathbf{h} - \frac{\pi}{2}\mathbf{H}(\hat{\theta})\cdot\mathbf{g}, \\
\operatorname{Im}[\mathbf{B}\,\boldsymbol{\Delta}(z_* - p_*h)\mathbf{q}^{\infty}] &= \operatorname{Im}\left[\mathbf{B}\,\boldsymbol{\Delta}(z_* - p_*h)(\mathbf{A}^{\mathrm{T}}\mathbf{r} + \mathbf{B}^{\mathrm{T}}\mathbf{b})\right] \\
&= -\frac{1}{2}\log(\hat{r})\,\mathbf{g} + \frac{\pi}{2}\mathbf{L}(\hat{\theta})\,\mathbf{h} - \frac{\pi}{2}\mathbf{S}^{\mathrm{T}}(\hat{\theta})\,\mathbf{g},
\end{aligned}
\tag{19}
$$

where $\mathbf{h} = \mathbf{S}\cdot\mathbf{b} + \mathbf{H}\cdot\mathbf{r}$, and $\mathbf{g} = \mathbf{S}^{\mathrm{T}}\cdot\mathbf{r} - \mathbf{L}\cdot\mathbf{b}$. The generalized Barnett–Lothe tensors $\mathbf{S}(\theta)$, $\mathbf{H}(\theta)$ and $\mathbf{L}(\theta)$ are defined as

$$
\mathbf{S}(\theta) = \frac{1}{\pi}\int_0^{\theta}\mathbf{N}_1(\omega)\,\mathrm{d}\omega, \quad \mathbf{H}(\theta) = \frac{1}{\pi}\int_0^{\theta}\mathbf{N}_2(\omega)\,\mathrm{d}\omega, \quad \mathbf{L}(\theta) = \frac{1}{\pi}\int_0^{\theta}\mathbf{N}_3(\omega)\,\mathrm{d}\omega, \tag{20}
$$

with

$$
\begin{aligned}
\mathbf{N}_1(\theta) &= -\mathbf{T}^{-1}(\theta)\mathbf{R}^{\mathrm{T}}(\theta), \\
\mathbf{N}_2(\theta) &= \mathbf{T}^{-1}(\theta), \\
\mathbf{N}_3(\theta) &= \mathbf{R}(\theta)\mathbf{T}^{-1}(\theta)\mathbf{R}^{\mathrm{T}}(\theta) - \mathbf{Q}(\theta),
\end{aligned}
\tag{21}
$$

$$
Q_{JK}(\theta) = n_i G_{iJKm} n_m,\ R_{JK}(\theta) = n_i G_{iJKm} m_m,\ T_{JK}(\theta) = m_i G_{iJKm} m_m.
$$

$\vec{n}^{\mathrm{T}} = [\cos\theta, \sin\theta, 0]$; $\vec{m}^{\mathrm{T}} = [-\sin\theta, \cos\theta, 0]$ are the respective unit vectors, normal and tangential, to a circle with its centre at $r = 0$, and $\mathbf{S}$, $\mathbf{H}$ and $\mathbf{L}$ are the corresponding values of $\mathbf{S}(\theta)$, $\mathbf{H}(\theta)$ and $\mathbf{L}(\theta)$ at $\theta = \pi$. In equation (19), $(\hat{r}, \hat{\theta})$ is the polar-coordinate system with origin at $(0, h)$. The second terms in equation (13) can be written as

$$
\begin{aligned}
\frac{1}{\pi}\operatorname{Im}\left(\sum_{\beta=1}^{4}\{\mathbf{A}\,\boldsymbol{\Delta}(z_* - \bar{p}_\beta h)\mathbf{q}_\beta\}\right) &= \sum_{\alpha=1}^{4}\sum_{\beta=1}^{4} U^{\alpha\beta}, \\
\frac{1}{\pi}\operatorname{Im}\left(\sum_{\beta=1}^{4}\{\mathbf{B}\,\boldsymbol{\Delta}(z_* - \bar{p}_\beta h)\mathbf{q}_\beta\}\right) &= \sum_{\alpha=1}^{4}\sum_{\beta=1}^{4} \psi^{\alpha\beta},
\end{aligned}
\tag{22}
$$

with

$$
\begin{aligned}
U^{\alpha\beta} &= \frac{1}{\pi}\operatorname{Im}\left[\log\left(z_\alpha - z^{\alpha\beta}\right) q_{\alpha\beta}\mathbf{a}_\alpha\right], \\
\psi^{\alpha\beta} &= \frac{1}{\pi}\operatorname{Im}\left[\log\left(z_\alpha - z^{\alpha\beta}\right) q_{\alpha\beta}\mathbf{b}_\alpha\right],
\end{aligned}
\tag{23}
$$

$$
z^{\alpha\beta} = \bar{p}_\beta h = x_1^{\alpha\beta} + p_\alpha x_2^{\alpha\beta} \tag{24}
$$

and where $q_{\alpha\beta}$ is the αth component of $\mathbf{q}_\beta$, that is $q_{\alpha\beta} = (\mathbf{q}_\beta)_\alpha$, and $\mathbf{a}_\alpha$ and $\mathbf{b}_\alpha$ are the eigenvectors of equations (9) and (11) defined earlier.

§3. Critical thickness for dislocation generation

Dislocation formation in an epilayer is energetically favourable when the strain energy that can be relieved by the dislocation is larger than its self-energy. The thickness for the generation of a dislocation in an epilayer is thus at least equal to that marked by the balance point of the misfit energy and the dislocation self-energy, which is also the point of zero Gibbs free-energy change when the dislocation forms in the piezoelectric film. Although this condition is well accepted, it should be noted that this is only a lower-bound condition, and the nucleation energy of the dislocation has not been taken into account. This may be a reason for the frequently found under-prediction of the critical thickness by this criterion. In the absence of a better alternative, we use the usual energy balance criterion to estimate the critical thickness of the piezoelectric thin film in our present analysis, within this understanding.

Neglecting the line charge (Im *et al.* 2001), the formation energy of a dislocation in an originally stress-free epilayer–substrate system can be written as

$$E_{\mathrm{f}} = \frac{1}{2}\iiint_V \Big[\Big(\sigma_{ij}^{\mathrm{m}} + \sigma_{ij}^{\mathrm{d}}\Big)\Big(\varepsilon_{ij}^{\mathrm{m}} + \varepsilon_{ij}^{\mathrm{d}}\Big) - \Big(D_j^{\mathrm{m}} + D_j^{\mathrm{d}}\Big)\Big(\varphi_{,j}^{\mathrm{m}} + \varphi_{,j}^{\mathrm{d}}\Big)\Big]\,\mathrm{d}v$$

$$- \frac{1}{2}\iiint_V \big(\sigma_{ij}^{\mathrm{m}}\varepsilon_{ij}^{\mathrm{m}} - D_{,j}^{\mathrm{m}}\varphi_{,j}^{\mathrm{m}}\big)\,\mathrm{d}v. \qquad (25)$$

Here quantities with the superscript m and d represent the fields produced by the mismatch and the dislocation respectively. The integration domain encloses the entire solid of unit thickness except the dislocation core. For convenience, the plane obtained from a cut along the x_2 axis is taken to be the glide plane (figure 1). Applying the divergence theorem to equation (22) yields

$$E_{\mathrm{f}} = \frac{1}{2}\iint_S \Big[\Big(\sigma_{ij}^{\mathrm{m}} + \sigma_{ij}^{\mathrm{d}}\Big)\Big(u_i^{\mathrm{m}} + u_i^{\mathrm{d}}\Big) - \Big(D_j^{\mathrm{m}} + D_j^{\mathrm{d}}\Big)\Big(\varphi^{\mathrm{m}} + \varphi^{\mathrm{d}}\Big)\Big] n_j\,\mathrm{d}s$$

$$- \frac{1}{2}\iint_S \big(\sigma_{ij}^{\mathrm{m}} u_i^{\mathrm{m}} - D_j^{\mathrm{m}}\varphi^{\mathrm{m}}\big) n_j\,\mathrm{d}s$$

$$= \frac{1}{2}\iint_S \Big[\Big(\sigma_{ij}^{\mathrm{d}} u_i^{\mathrm{d}} - D_j^{\mathrm{d}}\varphi^{\mathrm{d}}\Big) n_j\,\mathrm{d}s\Big] + \iint_S \Big(C_{ijkl}\varepsilon_{kl}^{\mathrm{m}} u_i^{\mathrm{d}} - \alpha_{ij}\varphi_i^{\mathrm{m}}\varphi^{\mathrm{d}}\Big) n_j\,\mathrm{d}s$$

$$= E_{\mathrm{s}} + E_{\mathrm{int}}, \qquad (26)$$

where E_{s} and E_{int} denote the self-energy of the dislocation and the interaction energy between the dislocation and the mismatch strain respectively. The integration boundary S includes the upper and lower sections with side planes ($x_1 \to \pm\infty$; $x_2 = 0$; $x_2 \to \infty$), and two sides of the cut. In deriving equation (26), we have used the constitutive relation (2). The integration of the lower and upper planes cancel each other and on $x_2 = 0$, $x_1 \to \pm\infty$ or $x_2 \to \infty$, $\sigma_{ij} = 0$ and $D_j = 0$. Therefore, the only non-zero contributions come from the two sides A^+ and A^- of the cut plane, and the contour of the dislocation core.

In the following, we also omit the contribution from the dislocation core. Therefore

$$E_{\mathrm{s}} = \frac{1}{2}\int_0^{h-r_0} \sigma_{ij}^{\mathrm{a}} n_j [u_i]\,\mathrm{d}x_2 - \frac{1}{2}\int_0^{h-r_0} D_j^{\mathrm{a}} n_j [\varphi]\,\mathrm{d}x_2, \\ = \frac{1}{2}\int_0^{h-r_0} \sigma_{ij}^{\mathrm{a}} n_j b_i\,\mathrm{d}x_2 - \frac{1}{2}\int_0^{h-r_0} D_j^{\mathrm{a}} n_j b_4\,\mathrm{d}x_2, \tag{27}$$

where

$$[u_i] = u_i(A^-) - u_i(A^+), \\ [\varphi] = \varphi(A^-) - \varphi(A^+), \tag{28}$$

$$E_{\mathrm{int}} = -\int_0^h C_{ijkl}\varepsilon_{kl}^{\mathrm{m}} n_j [u_i]\,\mathrm{d}x_2 + \int_0^h \alpha_{ij}\varphi_{,i}^{\mathrm{m}} n_j [\varphi]\,\mathrm{d}x_2 \\ = -\int_0^h C_{ijkl}\varepsilon_{kl}^{\mathrm{m}} n_j b_i\,\mathrm{d}x_2 + \int_0^h \alpha_{ij}\varphi_{,i}^{\mathrm{m}} n_j b_4\,\mathrm{d}x_2. \tag{29}$$

Under the boundary condition $D_j = 0$ on the surface of the epilayer, one obtains from the second equation of the constitutive equations (2),

$$\alpha_{ij}\varphi_{,j}^{\mathrm{m}} = e_{ikl}\varepsilon_{kl}^{\mathrm{m}}, \tag{30}$$

from which the interaction energy can be obtained:

$$E_{\mathrm{int}} = -(C_{i1kl}\varepsilon_{kl}^{m} b_i - e_{1kl}\varepsilon_{kl}^{m} b_4)h. \tag{31}$$

Here we have used $\mathbf{n} = (1, 0, 0)$. The self-energy can be obtained from equation (27):

$$E_{\mathrm{s}} = -\frac{1}{4\pi}(b_1 g_1 + b_2 g_2 + b_3 g_3 - b_4 g_4)\log\left(\frac{h}{r_0}\right) \\ -\frac{1}{2\pi}\sum_{\alpha=1}^{4}\sum_{\beta=1}^{4}\mathrm{Im}\left\{\log\left[\left(1-\frac{p_\alpha}{\bar{p}_\beta}\right)+\frac{p_\alpha}{\bar{p}_\beta}\frac{r_0}{h}\right]q_{\alpha\beta}\mathbf{b}_\alpha\right\}\cdot\mathbf{b} \\ +\frac{1}{2\pi}\sum_{\alpha=1}^{4}\sum_{\beta=1}^{4}\mathrm{Im}\left\{\log\left[\left(1-\frac{p_\alpha}{\bar{p}_\beta}\right)+\frac{p_\alpha}{\bar{p}_\beta}\frac{r_0}{h}\right]q_{\alpha\beta}b_{\alpha 4}\right\}\cdot \mathrm{b}_4, \tag{32}$$

where $b_{\alpha 4}$ is the fourth component of the eigenvector $\mathbf{b}_\alpha$, g_i is the ith component of $\mathbf{g}$, which is defined after equation (19), and $\mathbf{b}$ is the Burgers vector as defined before. If there are no electric dipoles along the cut, $b_4 = 0$. Equation (32) can be simplified accordingly. Finally, substituting equations (31) and (32) into equation (26) yields the following equation for the critical thickness h_{c} of the piezoelectric epilayer for dislocation generation:

$$\frac{1}{4\pi}(b_1 g_1 + b_2 g_2 + b_3 g_3 - b_4 g_4)\log\left(\frac{h}{r_0}\right) + \frac{1}{2\pi}\sum_{\alpha=1}^{4}\sum_{\beta=1}^{4}\mathrm{Im}\left\{\log\left[\left(1-\frac{p_\alpha}{\bar{p}_\beta}\right)+\frac{p_\alpha}{\bar{p}_\beta}\frac{r_0}{h}\right]q_{\alpha\beta}\mathbf{b}_\alpha\right\}\cdot\mathbf{b} \\ -\frac{1}{2\pi}\sum_{\alpha=1}^{4}\sum_{\beta=1}^{4}\mathrm{Im}\left\{\log\left[\left(1-\frac{p_\alpha}{\bar{p}_\beta}\right)+\frac{p_\alpha}{\bar{p}_\beta}\frac{r_0}{h}\right]q_{\alpha\beta}b_{\alpha 4}\right\}\cdot \mathrm{b}_4 = -(C_{i1kl}\varepsilon_{kl}^{\mathrm{m}} b_i - e_{1kl}\varepsilon_{kl}^{\mathrm{m}} b_4)h_{\mathrm{c}}. \tag{33}$$

§4. Application

$Al_xGa_{1-x}N/GaN$ heterostructure field-effect transistors are being developed for high-power high-temperature microwave applications. Owing to the large piezoelectric constants of $Al_xGa_{1-x}N$ materials, and the sizeable lattice mismatch between $Al_xGa_{1-x}N$ and GaN, misfit dislocations are common defects in such structures. In the following, we use the theory developed in the foregoing to calculate numerically the critical thickness for dislocation formation in this system and explore the dependence of this thickness on the piezoelectric properties of the epilayer.

Consider $Al_xGa_{1-x}N$ with a wurtzite crystal structure to grow in the (0001) orientation on GaN, with the same crystal structure. We use the lattice constants of the $Al_xGa_{1-x}N$ film obtained using the linear interpolation of Ambacher *et al.* (2000):

$$\begin{aligned} a_0(x) &= (-0.077x + 3.189) \times 10^{-10}\,\mathrm{m}, \\ c_0(x) &= (-0.203x + 5.189) \times 10^{-10}\,\mathrm{m}. \end{aligned} \qquad (34)$$

When $x = 0$, one can obtain the lattice constants for GaN. The elastic constants are from Shimada *et al.* (1998):

$$\begin{aligned} &C_{11} = C_{33} = 350\,\mathrm{GPa},\ C_{22} = 376\,\mathrm{GPa},\ C_{13} = 140\,\mathrm{GPa}, \\ &C_{12} = 104\,\mathrm{GPa},\ C_{44} = C_{66} = 101\,\mathrm{GPa}. \end{aligned} \qquad (35)$$

The piezoelectric and dielectric constants from Ambacher *et al.* (2000) are

$$\begin{aligned} &e_{22} = 1\,\mathrm{C\,m}^2,\ e_{21} = e_{23} = -0.36\,\mathrm{C\,m}^{-2},\ e_{16} = e_{34} = -0.3\,\mathrm{C\,m}^{-2}, \\ &\alpha_{11} = \alpha_{33} = 9.5\varepsilon_0,\ \alpha_{22} = 10.4\,\varepsilon_0. \end{aligned} \qquad (36)$$

Here, we note that, in our coordinate system, the axis of symmetry of transversely isotropic (or hexagonal) materials is the x_2 axis, instead of the x_3 axis, as is usually the case. For single-crystal $Al_xGa_{1-x}N$, with a wurtzite structure, grown on the basal plane of sapphire or GaN, a high density of threading dislocations parallel to the **c** axis crossed the film from the interface to the film surface (Ning *et al.* 1996, Shen *et al.* 2000). They have a predominantly edge character with a $\frac{1}{3}\langle 11\bar{2}0\rangle$ Burgers vector. In our coordinate system, the components of Burgers vector can be expressed in the form

$$\mathbf{b} = [a_0, 0, 0]. \qquad (37)$$

To obtain the solution, one needs to derive the eigenvalues and eigenvectors through equations (9) and (11). The wide range of material constants (from about 10^{-10} to about 10^{10}) presents considerable difficulties in the numerical calculation. To solve this problem, we rewrite the constitutive equations (2) in the forms

$$\begin{aligned} \sigma_{ij} &= \frac{1}{\alpha_0}(\alpha_0 C_{ijkm} + e_{mij}\widehat{\varphi}_{,m}), \\ D_i &= e_{ikm}u_{k,m} - \alpha^r_{im}\widehat{\varphi}_{,m}, \end{aligned} \qquad (38)$$

where $\widehat{\varphi}_{,m} = \alpha_0\varphi_{,m}$ and α_0, α^r_{im} are the vacuum dielectric constant and the relative dielectric constant respectively. By substituting equation (38) into equation (7), one can dispose of the parameter $1/\alpha_0$ before the parentheses. Then using the material matrixes (10), one can establish the matrix **N** and derive the eigenvalues and eigenvectors as follows:

$$\begin{bmatrix} \mathbf{N}_1 & \mathbf{N}_2 \\ \mathbf{N}_3 & \mathbf{N}_1^{\mathbf{T}} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = p \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \tag{39}$$

where

$$\mathbf{N}_1 = -\mathbf{T}^{-1}\mathbf{R}^{\mathbf{T}}, \quad \mathbf{N}_2 = \mathbf{T}^{-1}, \quad \mathbf{N}_3 = \mathbf{R}\mathbf{T}^{-1}\mathbf{R}^{\mathbf{T}} - \mathbf{Q} \tag{40}$$

and **T**, **Q** and **R** are given by equations (10), replacing C_{ijkm} with $\alpha_0 C_{ijkm}$, and α_{im} with the relative dielectric constants.

Assuming that $b_4 = 0$, the mismatch strain then becomes

$$\varepsilon_{11}^{\mathrm{m}} = \varepsilon_{33}^{\mathrm{m}} = \frac{a}{a_0} - 1 \approx 0.005\,31. \tag{41}$$

We are now ready to consider the effect of the piezoelectric properties of the epilayer on the critical thickness, by considering the $Al_xGa_{1\text{-}x}N$ material system, whose material constants are given by equations (35) and (36). There are three independent piezoelectric constants, and their effects on the critical thickness are shown respectively in figures 2–4. The piezoelectric constants e_{21} and e_{16} assume negative values. The relations between the critical thickness and the mismatch strain, with and without the piezoelectric effect respectively are compared in figure 5. It is interesting to note that the piezoelectric properties affect the critical thickness significantly, by an increase of about 10–50%. The case where the piezoelectric constant equals zero corresponds to the non-piezoelectric anisotropic elastic materials.

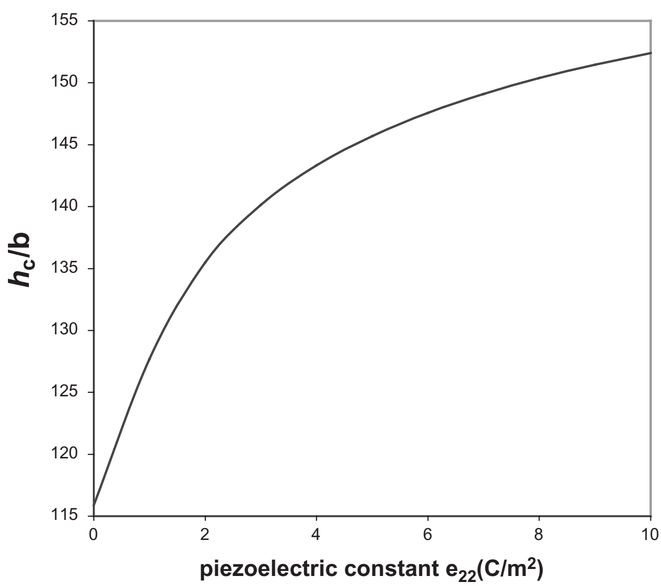

Figure 2. The critical thickness h_c/b versus the piezoelectric constant e_{22} of the epilayer, where the index 2 corresponds to the direction of the c axis.

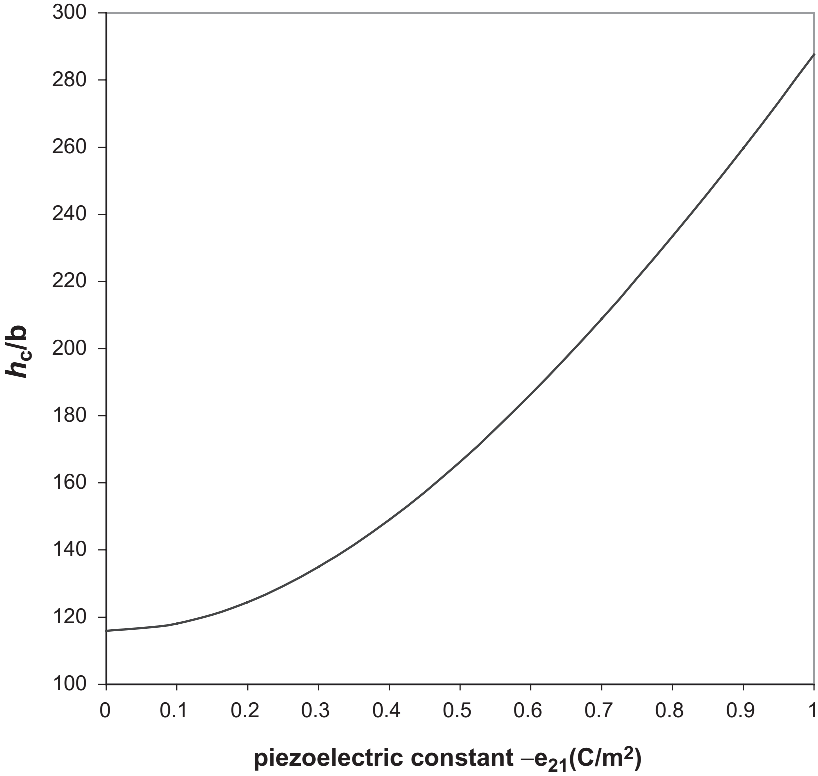

Figure 3. The critical thickness versus the piezoelectric constant $-e_{21}$.

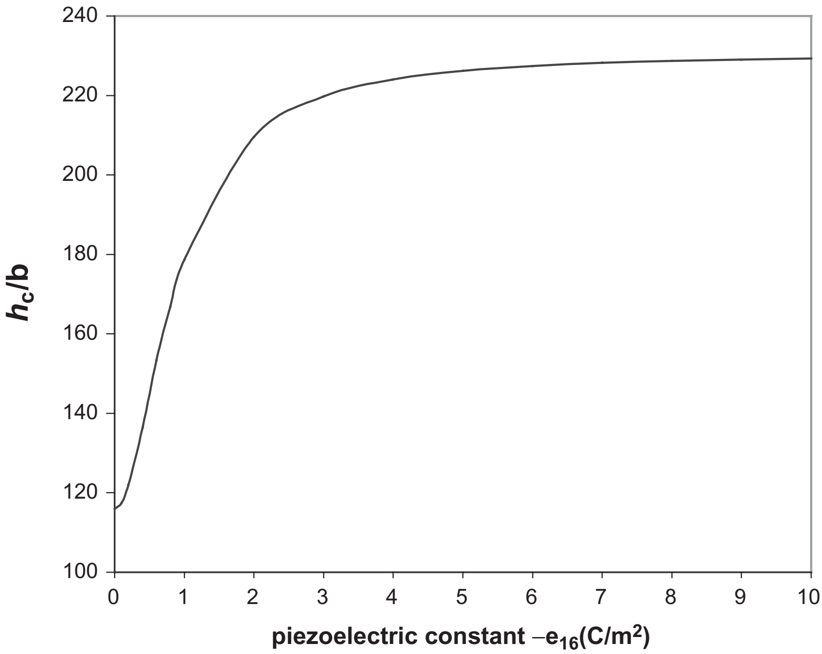

Figure 4. The critical thickness versus the piezoelectric constant e_{16} of the epilayer.

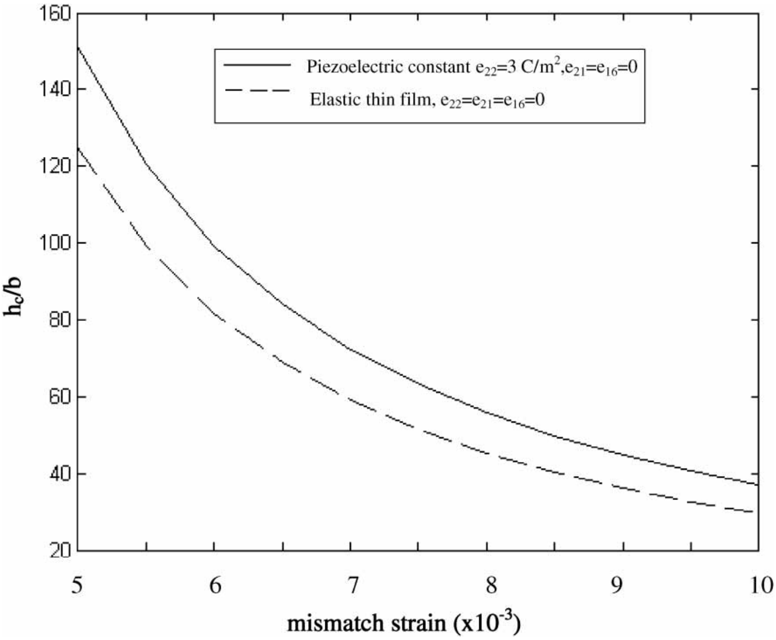

Figure 5. The critical thickness versus the mismatch strain.

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