Stress relaxation in mismatched layers due to threading dislocation inclination

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A recently observed mechanism of elastic stress relaxation in mismatched layers is discussed. The relaxation is achieved by the inclination of pure edge threading dislocation lines with respect to the layer surface normal. The relaxation is not assisted by dislocation glide but rather is caused by the "effective climb" of edge dislocations. The effective dislocation climb may result from the film growth and it is not necessarily related to bulk diffusion processes. The contribution of the dislocation inclination to strain relaxation has been formulated and the energy release due to the dislocation inclination in mismatched stressed layers has been determined. This mechanism explains recently observed relaxation of compressive stresses in the (0001) growth of $Al_xGa_{1-x}N$ layers.
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It is well known that the processes of stress relaxation in lattice mismatched epitaxy play a crucial role for materials properties and electronic and optoelectronic device performance. The most common mode of misfit stress relaxation is normally related to the formation of misfit dislocations (MDs) at the layer/substrate interface. For layers that grow in a two-dimensional mode (i.e., step flow or layer-by-layer growth), the formation of MDs is usually accomplished by dislocation motion, i.e., by glide.[1] The dislocation gliding can proceed by bending the pre-existing threading dislocations (TDs).[1,2] To operate, this mechanism needs to involve the shear stresses in the dislocation glide plane. This is the standard case for epitaxial growth of (001) oriented semiconductor layers with face centered cubic lattices (e.g., diamond cubic or zinc blende structures), where the biaxial stress state is responsible for shear stresses on the inclined $\langle 111\rangle$ glide planes. The corresponding TDs and their Burgers vectors are inclined with respect to [001] growth direction of the layer.

The different case is realized for (0001) growth of layers with a hexagonal crystal structure, e.g., the group III-nitride semiconductors.[3] For (0001) oriented layers, the TDs usually have pure edge character with [0001] line direction and Burgers vector in the basal plane. The $\{1\bar{1}00\}$ prismatic glide planes of these dislocations are normal to the biaxial stress plane and there is no shear stress in the glide planes. Nevertheless, such edge dislocations may contribute to the misfit stress relaxation by inclining their line direction that corresponds to their effective climb. Recently, such TD behavior was observed in the (0001) growth of compressively stressed $Al_xGa_{1-x}N$ layers.[4]

In the present letter we propose a glide-free mechanism of misfit stress relaxation related to the inclination of the TDs with respect to their original direction. The contribution of TD inclination to the relaxed strain will be determined and the energy change resulting from the dislocation inclination will be found. The critical conditions for dislocation inclination will be established.

Our modeling efforts were motivated by the experimental observations of systematic inclination of TDs in Si-doped 200-nm-thick $Al_{0.49}Ga_{0.51}N$ layers which were grown on relaxed $Al_{0.62}Ga_{0.38}N$ buffer layers on (0001) sapphire, see Ref. 4 for details. The total compressive mismatch for the upper layer at the growth temperature was found $\varepsilon_m \approx 0.003$. It was established that Si doping promoted the relaxation of the elastic stresses caused by the lattice mismatch. The degree of strain relaxation was determined by x-ray diffraction and reached 50%–100% depending on the doping level. It was also found that Si doping enhanced the layer surface roughness during growth. Transmission electron microscopy (TEM) structure investigations proved the presence of high density of TDs with $\rho_{TD} \geqslant 10^{10}$ cm^{-2}. The majority of the observed TDs were edge dislocations with Burgers vectors of the type $\frac{1}{3}\langle 11\bar{2}0\rangle$. The lines of these dislocations were inclined with respect to the [0001] growth direction (see schematics in Fig. 1) with inclination angles α as large as 20°. Cross-section and plane-view TEM studies showed that the TDs inclined toward the $\langle 1\bar{1}00\rangle$ directions. The specific inclination direction is perpendicular to the direction of the Burgers vector, e.g., for TD with $\mathbf{b} = \pm\frac{1}{3}[2\bar{1}\bar{1}0]$ the inclination is in the $\pm[01\bar{1}0]$ direction.

When viewed down the growth direction [see Fig. 1(b)], the inclined TDs have an average projected length L. The Burgers vectors of the dislocations are projected on the layer/substrate interface without any distortion. Therefore, in the far field, the projected dislocation segments are equivalent to the sections of misfit dislocations. The MD segments can be hypothetically combined to form straight line MD arrays with the distance l between MDs. Assuming that the total treading dislocation density ρ_{TD} is evenly distributed between the three families [as it is for the case of (0001) growth of nitrides], we find that the distance between effective MDs in each of the $\langle 11\bar{2}0\rangle$ directions will be $l = 3/\rho_{TD}L$. The plastic relaxation associated with the array of effective MDs is given as $\varepsilon^1_{pl} = b/l$, where b is the magnitude of the dislocation Burgers vector. The total biaxial far

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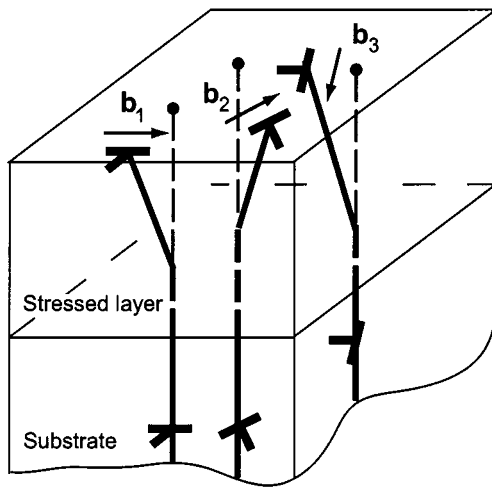

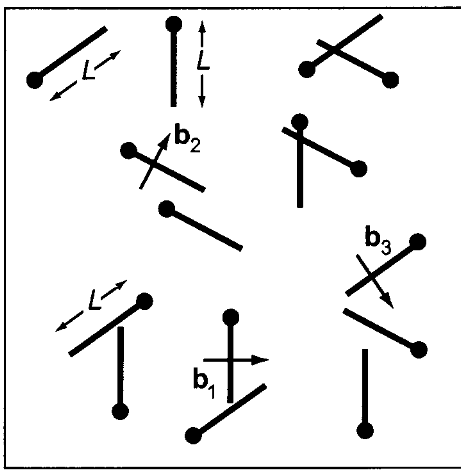

FIG. 1. Inclined pure edge dislocations in a stressed layer. (a) Three families of edge dislocations corresponding to three possible orientations of the Burgers vector in the (0001) plane of the layer with a hexagonal crystal structure. (b) Plan-view showing the average dislocation projected length L.

field plastic relaxation at the top layer surface resulting from the triangular MD grid $\varepsilon_{\rm pl}^{\rm top}$ is given by

$$\varepsilon_{\rm pl}^{\rm top}=\tfrac{3}{2}\varepsilon_{\rm pl}^{1}=\tfrac{1}{2}b\rho_{\rm TD}L. \tag{1}$$

The projected length L is directly related to the layer thickness h and the inclination angle α by $L=h\tan\alpha$. This also means that the projected length varies linearly with layer depth. Therefore, the average plastic relaxation for the layer of the thickness h is

$$\bar{\varepsilon}_{\rm pl}=\tfrac{1}{4}b\rho_{\rm TD}h\tan\alpha. \tag{2}$$

For $\rho_{\rm TD}=3\times10^{10}\,{\rm cm}^{-2}$, $h=200\,{\rm nm}$, $\alpha=17°$, and $b=0.318\,{\rm nm}$ (corresponding to the observations in Ref. 4), Eq. (1) gives the plastic relaxation at the layer surface $\varepsilon_{\rm pl}^{\rm top}=0.0029$ that is comparable with the initial misfit $\varepsilon_m\approx0.003$.

To understand the conditions for TD inclination in a stressed layer, we consider the energy balance similar to those used in the "energy approach"[5,6] for deriving the critical thickness for the introduction of MDs in strained films. The energy release ΔE due to dislocation inclination can be formulated as

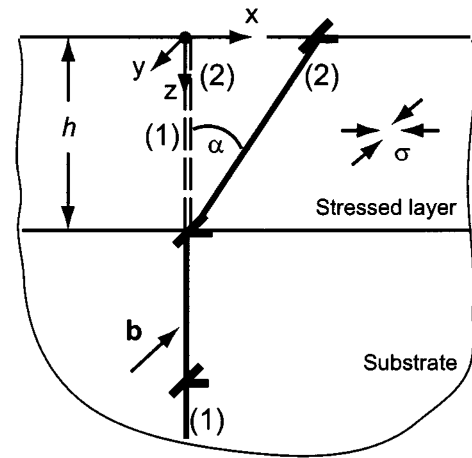

FIG. 2. Representation of the inclined dislocation as a superposition of straight dislocation (1) and angular dislocation (2). The dislocation Burgers vector b is in the yz plane. There is a compressive biaxial stress $\sigma_{xx}=\sigma_{yy}=\sigma=2G\,\varepsilon_m(1+\nu)/(1-\nu)$ in the layer.

$$\Delta E=E_{\rm inclined}-E_{\rm straight}-W_{\rm int}, \tag{3}$$

where $E_{\rm inclined}$ is the self-energy of the dislocation in the inclined configuration, $E_{\rm straight}$ is the self-energy of the dislocation in the initial configuration with the line direction normal to the surface, $W_{\rm int}$ is the work done by the biaxial misfit stress σ (see Fig. 2) in the process of dislocation inclination. To find $E_{\rm inclined}$, we use the representation of the inclined dislocation as the superposition of the straight dislocation (1) and an angular dislocation (2) as shown in Fig. 2. In this case, $E_{\rm inclined}$ can be found as

$$E_{\rm inclined}=E_{\rm straight}+E_{\rm angular}+W_{\rm straight}^{\rm angular}, \tag{4}$$

where $E_{\rm angular}$ is the self-energy of the angular dislocation and $W_{\rm straight}^{\rm angular}$ is the interaction energy with the initial dislocation. Exact calculations[7] of the energy $E_{\rm angular}$ include the contribution of the dislocation core region which is proportional to the change in dislocation length. Numerical estimates show that the interaction contribution $W_{\rm straight}^{\rm angular}$ cancels in the first approximation the dislocation core contribution. As a result the energy balance takes the simpler form

$$\Delta E=E_{\rm angular}-W_{\rm int}. \tag{5}$$

The interaction part is calculated as

$$W_{\rm int}=b\sigma S_{\rm angular}=G\frac{1+\nu}{1-\nu}bh^2\varepsilon_m\tan\alpha, \tag{6}$$

where $S_{\rm angular}$ is the area bounded by the angular dislocation, G is shear modulus, and ν is Poisson ratio.

The first step in the calculation of the self-energy of the angular dislocation involves the determination of the elastic fields of the dislocation in the presence of the free surface. Subsequently, integration of the elastic fields yields the elastic self-energy term in the Eq. (5). The results of these calculations will be presented elsewhere.[7] Here we use the approximate expression for $E_{\rm angular}$ based on the physical arguments of varying screening for the dislocation elastic field in the process of TD inclination. Actually, for very

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small inclination angles, the angular dislocation is equivalent to the dipole with the separation of the order $h \sin\alpha \approx h\alpha$. For large inclinations ($\alpha \rightarrow \pi/2$), the dislocation acquires a parallel orientation with respect to the layer surface and the characteristic screening length becomes the layer thickness h. Accordingly, the dislocation length changes as $h/\cos\alpha$ with inclination α. These observations permit to propose the following dependence for E_{angular}:

$$E_{\text{angular}} = \frac{Gb^2}{4\pi(1-\nu)} \frac{h}{\cos\alpha} \log\left[\left(\frac{h}{b}-1\right)\sin\alpha + 1\right], \qquad (7)$$

where we assume the value of b for the dislocation core radius. The developed approximation fits closely to numerical solutions of E_{angular} for a wide range of film thicknesses and inclination angles.[7]

Finally, we analyze the following dependence for the energy release:

$$\Delta E(\tilde{h},\alpha) = \frac{Gb^3}{(1-\nu)} \left\{ \frac{\tilde{h}}{4\pi\cos\alpha} \log[(\tilde{h}-1)\sin\alpha + 1] - (1+\nu)\tilde{h}^2 \varepsilon_m \tan\alpha \right\}, \qquad (8)$$

where $\tilde{h} = h/b$ is the normalized film thickness.

A typical dependence for ΔE is given in Fig. 3(a). It is clear that for sufficiently large thickness or angle α, ΔE becomes negative and gives the favorable parameters for plastic relaxation via dislocation inclination. By applying the requirement $\Delta E = 0$, we can map the regions for favorable dislocation inclination in coordinates layer thickness-inclination angle as shown in Fig. 3(b). The plots define the energetic conditions for dislocation inclination for the given misfit strain. For $\alpha \rightarrow \pi/2$, the plots demonstrate the usual critical thickness behavior for MD formation in mismatched layers.

The other important feature of $\Delta E(\tilde{h},\alpha)$ dependence is the existence of the energy barrier to dislocation inclination at finite values of the layer thickness h. The typical heights for this barrier are of the order of $5-10\ \text{Gb}^3$, which lead to reasonable values of the order up to 10 eV per dislocation. Such barriers can be overcome when additional factors come into play. We believe that surface roughness helps to diminish the energy barrier. The last statement is supported by the models proposed for dislocation nucleation during the development of morphological instabilities at stressed surface of crystals.[8,9] Once inclined, the TDs may maintain their orientation. Typically, the TD line direction becomes frozen-in and thus demonstrates that dislocation climb does not occur in the bulk of the material. The possible mechanism of the crystal growth with inclined dislocations may then include directional surface diffusion and the incorporation of adatoms at the intersection of pre-existing TDs with the growing crystal surface. Therefore, we may refer this mechanism as "effective climb." We suppose that actual inclination angle is determined by the growth conditions, such as temperature, reactor pressure, precursor flow ratios, etc. To check this proposal, additional experiments must be performed. The other important experiments may include the growth of the samples with inclined dislocations to larger thickness, where the layers become fully relaxed or the layer strain *reverses* due to the inclined TDs.

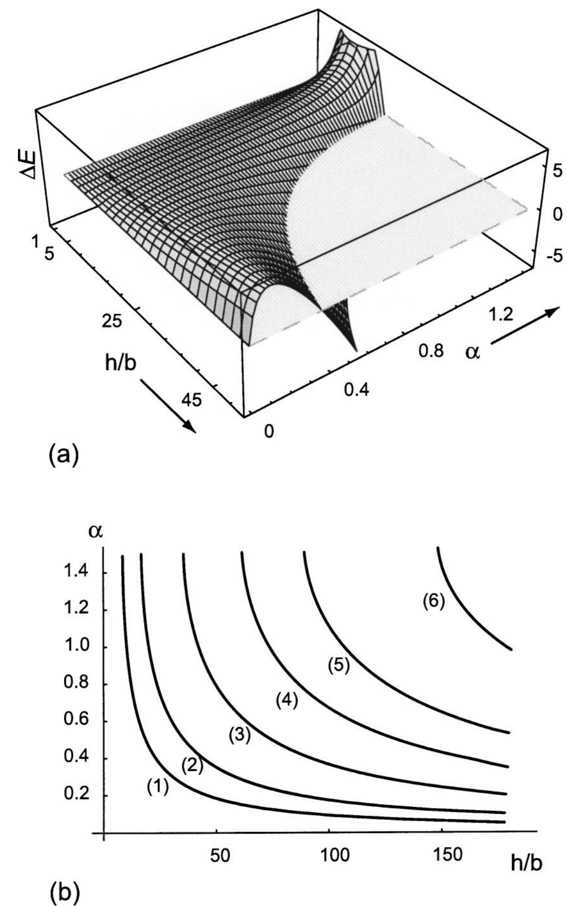

FIG. 3. Critical conditions for edge dislocation inclination in stressed layer. (a) Energy release due to the inclination of the initial straight dislocation. Parameters used for the plot: misfit strain in the layer $\varepsilon_m = 0.01$, dislocation core radius $R_c = b$, Poisson ratio $\nu = 1/3$. The energy change ΔE is in the units of Gb^3. (b) Inclination stability diagram in coordinates layer thickness h—inclination angle α for the misfit strain $\varepsilon_m = 0.015$ (1), 0.010 (2), 0.006 (3), 0.004 (4), 0.003 (5), and 0.002 (6), correspondingly.

In conclusion, a mechanism of elastic stresses relaxation in growing mismatched layers has been considered. The mechanism involves the TD lines inclination and their effective climb. The energetically favorable conditions for the operation of this mechanism have been determined.

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