Work-hardening effects in the lattice relaxation of single layer heterostructures

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A modelization of the strain relaxation in single heteroepitaxial layers is presented in this letter. The calculations consider the energetic variations of the heteroepitaxial structure when introducing one new dislocation into the existing interfacial array of fixed misfit dislocations without continuous readjustment of the spacing array. The interaction energy of the new dislocation with both lattice mismatch and dislocation array is shown to be the limiting factor that controls the mechanism of strain relaxation at the saturation stage of relaxation. The model is shown to be in good agreement with the lattice relaxation behavior of previously published strain/thickness data. © *1997 American Institute of Physics.* [S0003-6951(97)04243-5]

The band gap engineering used in semiconductor device fabrication unfortunately also involves, in most cases, lattice parameter variation which introduces misfit dislocations. During the growth of a lattice mismatched layer, next a pseudomorphic phase, three relaxation stages occur.[1] First, when the Matthews and Blakeslee critical thickness is reached,[2] threading dislocations coming from the substrate bend at the interface.[3] Such relaxation is slow. Second, as the epilayer thickens, the stored elastic energy increases making the system unstable. At this point, the situation is energetically favorable for new misfit dislocations (MDs) generation by multiplication[4] and nucleation[5] to allow further strain relaxation. This stage appears as a rapid relaxation. Finally, this relaxation stops before 100% relaxation is achieved.[6] We call this level of relaxation the saturation state. Many authors attribute saturation to dislocations interaction, closely related to a form of work-hardening processes proposed initially by Taylor[7] for bulk materials. These effects will be a limitation of the introduction of new MDs at the interface.

Although many works describe the introduction of the first misfit dislocations, only a few studies on the work-hardening process exist, and all within the experimental field. Dodson[8] was the first to propose strain relaxation inhibition based on dislocation–dislocation interactions. He attributes it to repulsive tensions due to pre-existing dislocations at the interface. Later, Willis *et al.*,[9] Gosling *et al.*[10] and Gillard *et al.*[11] also quantified the effect of dislocation interaction on the limitation of the strain relief. Even though their conclusions show that this effect certainly plays an important role in the lattice relaxation saturation, the available models fail up to now to reproduce the strain/thickness experimental data.

The aim of this contribution is to quantify the influence of a work-hardening phenomenon in a strained epitaxial system during its lattice relaxation. The model estimates the energetic variation of the system when introducing a dislocation in between a fixed array of misfit dislocation. The considered system is a single nominally mismatched layer grown heteroepitaxially on a substrate. To fix the ideas, we apply our calculations to the InGaAs/GaAs (100) system.

Considering a single thermodynamical equilibrium relation, where the sum of the self dislocation array energy (E_{array}), the dislocation interaction with the reticular strain (E_{int}) and the strain energy (E_m) is minimized, the system does not relax totally due to dislocation interactions.[12,13] However, as the latter assumes implicitly that the dislocations are uniformly distributed and rearranged after the introduction of the new dislocation, the resulting strain is lower than experimental published data. In contrast to the work-hardening models commonly used with an adaptable MD array during the lattice relaxation,[8,9] that is to say assuming implicitly a continuous readjustment of dislocation spacing on entry a new MD, we consider here a fixed array of MD in which the new dislocation is inserted. In most fcc heteroepitaxial mismatched systems on substrates (100), edge MD are fixed and 60° MD glide mainly in the {111} planes and are not able to move laterally in the interface plane. To overcome this we assume in the following that a new dislocation coming from the epilayer, with same Burgers vector as those of the interfacial MDs, takes place in the intermediate region between two pre-existing MDs of a fixed array (see Fig. 1).

The energy per unit area for the work-hardening process, ΔE_{WH}, is defined as the difference in energy of the system before, E_1, and after, E_2, the introduction of a new dislocation:

$$\Delta E_{WH} = E_2 - E_1 = E_s + E_{\text{int}m} + E_{\text{int}d}, \tag{1}$$

where E_s is the self energy of a new dislocation, $E_{\text{int}m}$ the interaction energy with the lattice misfit and $E_{\text{int}d}$ the inter-

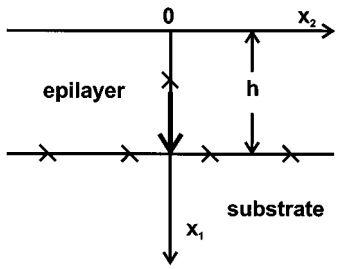

FIG. 1. Scheme of the reference system used in the calculation method. A superficial dislocation is driven to the midpoint between two pre-existing fixed dislocations.

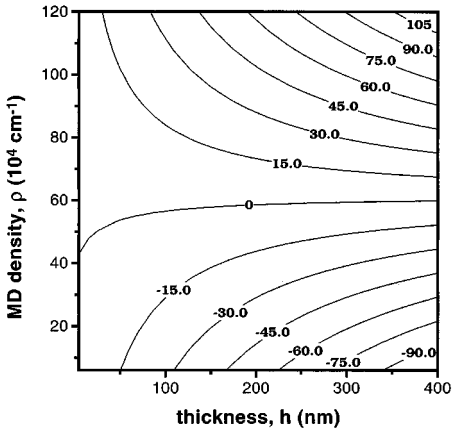

FIG. 2. Contour plot of work-hardening energy (10^{-9} J/m) vs epilayer thickness (x axis) and MD density (y axis) for the $In_{0.2}Ga_{0.8}As/GaAs$ (100) system. This represents the energy necessary to insert a new dislocation in the fixed array of MD dislocations. Below the zero line, this introduction is favorable while above this line the repulsion energy dominates.

action energy between the new dislocation with the stress field of the array of misfit dislocations. In contrast to the usually considered case, where the MDs array adapt its interdislocation spacing to keep the periodicity when the new dislocation is introduced, here we assume that the new dislocation is placed in the midpoint between two dislocations of the fixed array. According to Zhang *et al.*[14] the terms, E_s, $E_{\mathrm{int}m}$ and $E_{\mathrm{int}d}$, are expressed as:

$$E_s=\frac{\mu}{4\pi(1-\nu)}\left[[b_1^2+b_2^2+(1-\nu)b_3^2]\ln\left(\frac{2h}{r_0}\right)+\frac{b_1^2+b_2^2}{2}\right], \tag{2}$$

$$E_{\mathrm{int}d}=\frac{\mu}{4\pi(1-\nu)}\left([b_1^2+b_2^2+(1-\nu)b_3^2]\times\ln[\cosh(2\pi h\rho)]-(b_1^2+b_2^2)\times\frac{4\pi^2h^2\rho^2}{\cosh^2(2\pi\rho h)}\right)+\frac{\mu}{4\pi(1-\nu)}\times[(b_1^2-b_2^2)4\pi\rho h\cdot\tanh(2\pi\rho h)], \tag{3}$$

$$E_{\mathrm{int}m}=\frac{2\mu(1+\nu)}{(1-\nu)}\varepsilon_m b_2 h, \tag{4}$$

where ρ is the linear density of the misfit dislocations array at the interface, all with identical Burgers vector, $\mathbf{b}(b_1,b_2,b_3)$, ν is the Poisson ratio, ε_m the lattice mismatch between the epilayer and the substrate, r_0 the radius of the dislocation core and h the layer thickness. Figure 2 displays a contour plot of the energy differences, ΔE_{WH} (each line is an isoenergetic state) when introducing a new MD in the array versus its MD density ρ and the epilayer thickness h. Two different regions can be distinguished. The upper zone, with positive values of energy differences and the lower with negative ones. For a given thickness, the lower is the MD density, the more favorable is the introduction of a new MD. On increasing the MD density, the process becomes energetically less favorable. The system reaches a saturated state of relaxation when no energy release accompanies the introduction of a new MD. This state (zero line) is the work-hardening limit to the introduction of a new MD. Thus, for low thickness (<100 nm), the predicted MD density increases with the thickness, while for large thickness (>100 nm), saturation occurs and the system reaches a maximal MD density of $61\cdot10^4$ cm^{-1} for the $In_{0.2}Ga_{0.8}As/GaAs$. This value is lower than the estimation obtained by considering an array of mobile misfit dislocations (Zhang *et al.*[13] estimate a MD density of 67×10^4 cm^{-1}).

The zero line defines the maximal MD density, ρ_{WH}, that the system can tolerate. It is obtained by finding the solutions of Eq. (1)

$$\Delta E_{WH}[h,\varepsilon_m;\rho_{WH}(h,\varepsilon_m)]=0. \tag{5}$$

Assuming that the dislocations are all of the 60° type,[15,16] with a Burgers vector $\mathbf{b}=(\sqrt{2}/2,-1/2,1/2)b$ in our coordinate system (see Fig. 1), we deduced the strain reached by the layer at its saturation state by applying:

$$\varepsilon=\varepsilon_m-\rho_{WH}b_{(100)}, \tag{6}$$

ε being the residual strain of the epilayer and $b_{(100)}$ is the projection of the Burgers vector edge component on the interface plane.[17] For 60° dislocation type, $b_{(100)}=b/2$.

The strain-thickness diagram of experimental data previously obtained by Dunstan *et al.*[18] corresponding to $In_{0.2}Ga_{0.8}As/GaAs$[6] and $In_{0.1}Ga_{0.9}As/GaAs$ single layers is compared in Fig. 3 with the values predicted by Eq. (6) as well by other models (Gosling *et al.*,[10] Gillard *et al.*[11] and Dodson[8]). Three different regions that correspond to three different stages of relaxation are distinguished. The first is region A where the misfit dislocation formation follows the Matthews and Blakeslee mechanism[2] that depends on initial density of substrate dislocations.[19,20] In region B of the diagram, the relaxation efficiency depends on other parameters such as dislocation multiplication source availability[4] and activation of new nucleation mechanisms.[1,5] Such mechanisms involve movement of dislocations, depending strongly on kinetic terms such as the activation energy barriers for slip and nucleation, growth temperature, etc..., as well as on the initial density of the dislocation sources.[21–23] The variety of factors that act in this stage of rapid relaxation explains the diversity of results obtained by other workers.[24,25]

Nevertheless, once the saturation density is reached (region C), work-hardening governs the relaxation. The approximations of Gosling *et al.*[10] and of Gillard *et al.*[11] do not explain the inhibition of the relaxation, only our model and that of Dodson[8] are able to predict a change of the strain relief with respect to the B region behavior (i.e., the empirical Dunstan curve[6]). However, only our model is able to predict the experimental soft strain relief behavior of region C.

Since the kinetic factors lose importance with respect to purely energetic criteria, the results are easily extrapolable to other systems. The good agreement between experimental data and our model suggests that the third part of the strain-thickness curve (region C in Fig. 3) is controlled by dislocation interaction processes. Inhibition of relaxation is thus attributed to the difficulty of inserting an additional dislocation from the epilayer into the fixed array of MD when the system

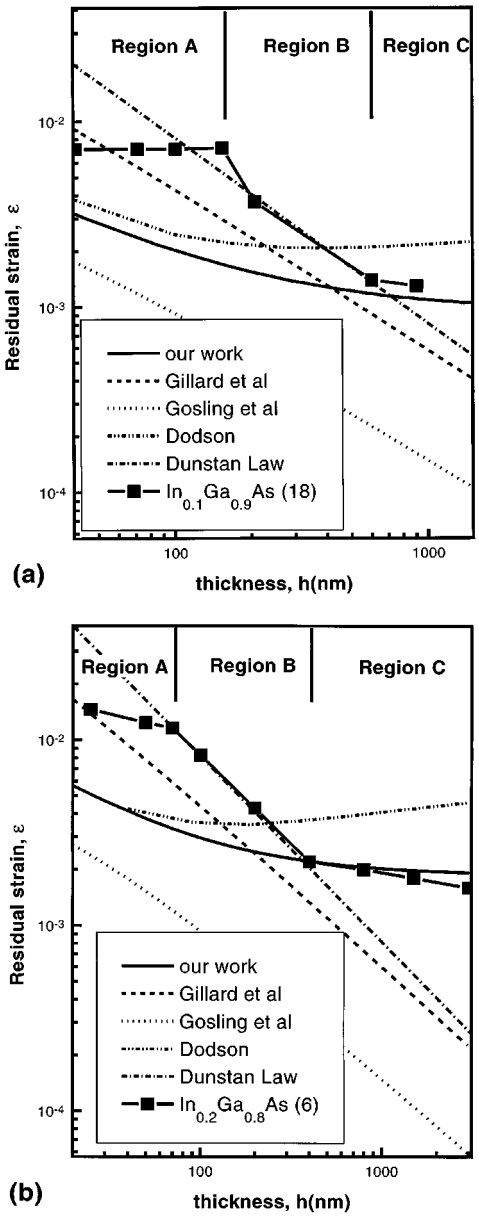

FIG. 3. Strain-thickness diagram where the experimental data for $In_{0.1}Ga_{0.9}As/GaAs$ (a) and $In_{0.2}Ga_{0.8}As/GaAs$ (b) alloys are displayed with our theoretical predictions. Three different regions can be distinguished: the region A, of weak relaxation, limited by nucleation processes, region B with a fast relaxation where dislocation multiplication controls the strain relief, and region C, where the work-hardening process dominates. The latter can be predicted by different models. The Gillard *et al.*, Gosling *et al.* and Dodson models are compared to our formalism. Note that only Dodson and this work are able to predict a change in the behavior of the relaxation respect to region B.

has reached saturation. The key point is the inability that the MDs have to move in its interfacial plane. This increases the repulsion that the new dislocation has to overcome in order to be inserted in the array of MDs.

However, although the results are independent of the select 60° Burgers vector, it is important to note that one limitation of the model is the choice of a single value for the calculations. Indeed, the real array of dislocations is composed of both edge and 60° dislocations. Nevertheless, in low misfit epitaxial systems the fraction of edge dislocations is small and the multiplication process dominant in region B induces zones with identical Burgers vectors that limit the introduction of different types of 60° dislocation.

In summary, a modelization of the strain relief into single epilayers of low lattice misfit allows one to determine at which level work-hardening effects become dominant in the lattice relaxation process. To date, empirical curves were available in the literature[6] to predict the relaxation state of heteroepitaxial mismatched systems, but no theoretically based calculations were able to predict with good accuracy the strain relaxation. This is achieved for the first time by the present model in the strain saturation stage of relaxation. The novelty of the calculation is in considering a fixed array of MD where the new dislocation is inserted at the interfacial plane. The beginning of this stage is indeed of primary importance in the design of the relaxation buffer. It corresponds to the maximal strain/thickness ratio that can be reached by a layer of a defined nominal mismatch.

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