Critical thickness for the saturation state of strain relaxation in the InGaAs/GaAs systems

D. González,[a)] D. Araújo, G. Aragón, and R. García
Departamento de Ciencia de los Materiales e IM y QI, Universidad de Cádiz, Apartado 40, 11510 Puerto Real, Spain

(Received 8 December 1997; accepted for publication 12 February 1998)

Using previously published relaxation models [D. J. Dunstan, P. Kidd, L. K. Howard and R. H. Dixon, Appl. Phys. Lett. **59**, 3390 (1991) and D. González, D. Araújo, G. Aragón, and R. García, Appl. Phys. Lett. **71**, 2475 (1997)] that predict the strain relaxation in the InGaAs/GaAs system, before and during the stage of relaxation saturation, the critical thickness where dislocation interactions begin to limit the plastic relaxation is estimated. The approximations used to deduce an analytical expression are shown to be appropriate for describing the regime of relaxation considered. A good agreement with experimental data previously published by other authors permits a physical explanation for the different observed regimes of relaxation to be given. © *1998 American Institute of Physics.* [S0003-6951(98)01015-8]

In modern semiconductor technology, different types of alloys are used depending on the application. While telecommunication applications need III-V materials to work in the low absorption bands of optical fibers, other II-VI or III-N alloys are needed for visible applications. By the design of multilayered heterostructures, epitaxial growth has allowed the realization of exciting and useful developments in modern compound semiconductor electronics such as engineering of band structures, quantum phenomena, optical properties and basic material properties. Band-gap engineering of semiconductor materials has permitted in the last decades the fabrication of semiconductor devices such as light-emitting diodes (LEDs), lasers and transistors. Nevertheless, the thermal expansion and lattice parameter of the materials used vary generally within a device structure and can generate defects such as threading dislocation degrading the optoelectronics properties of the device. Therefore, a control of the lattice relaxation between the substrate and the epitaxial layers or within the heteroepitaxial layer structure is necessary to avoid dislocation propagation that can be harmful to device performance. The design involved to achieve this lattice relaxation needs simple rules. Generally, a buffer layer with a high lattice parameter gradient is required, but a limitation of the relaxation occurs when dislocation interaction energy dominates the strain relaxation energy.[1] Such a state of relaxation corresponds to the best strain relief/thickness ratio and is therefore an essential point in the design of well-relaxed structures. Today, several ''critical thicknesses'' have been established to define the change in the regimes of relaxation. Among them, the well-known Matthews and Blakeslee (MB)[2] critical thickness defines the start of plastic relaxation: when an existing dislocation, threading from the substrate, begins to bend at interfaces to become a misfit dislocation. However, more important is the critical thickness of Dunstan *et al.*[3] for the InGaAs/GaAs system. It defines the beginning of the dislocation source activation that allows a fast relaxation of the epilayer.[4] Up to now, no work has been published defining the critical thickness for the end of this fast relaxation regime: when dislocation interactions limit the introduction of new dislocations in the array of misfit dislocation. The latter process is commonly named work hardening by analogy to the work hardening in metals.

In the present contribution, an analytical expression for the critical thickness to reach the saturated state of relaxation for different In content of InGaAs layers grown on the GaAs (001) substrate is presented. The critical thickness corresponds to the transition point between two regimes of relaxation: the first, which follows the Dunstan law[5] (the most accurate for the considered system, other laws should be used for other systems) and depends on the dynamic behavior of dislocation sources and the second, which is governed by work hardening phenomena.[6,7] Figure 1 displays the empirical curve of Dunstan *et al.,* showing experimental relaxation data for the $In_{0.1}Ga_{0.9}As$/GaAs (Ref. 8) and $In_{0.2}Ga_{0.8}As$/GaAs (Ref. 5) systems as well as the calculated strain/thickness behavior in the work hardening regime[6] for 10%, 20%, 30%, and 40% In content of InGaAs/GaAs single layers. The intersection point between the Dunstan curve and the work-hardening model fixes the thickness for a given lattice mismatch i.e., for one alloy composition. We define this critical thickness, h_{WH}, as the thickness needed to saturate the strain relaxation. Equating the Dunstan strain/thickness expression to the work-hardening strain one, the analytical behavior of h_{WH} versus the alloy composition can be obtained.

Specifically, the work hardening state ΔE_{WH}, has been defined as the difference in the total energy of the system before (E_1) and after (E_2) the introduction of a new dislocation in the fixed array of misfit dislocations:[6,9]

$$\Delta E_{\mathrm{WH}} = E_2 - E_1 = E_s + E_{\mathrm{intm}} + E_{\mathrm{intd}}, \tag{1}$$

where E_s is the self energy of a new dislocation, E_{intm} the interaction energy between the dislocation and the lattice mismatch and E_{intd} the interaction energy between the new dislocation with the fixed array of misfit dislocations at the interface. For low misfit dislocation (MD) densities, ΔE_{WH} is negative which means the system tends to relax. We defined the saturation state of relaxation as the maximal energetically

a)Electronic mail: david.gonzalez@uca.es

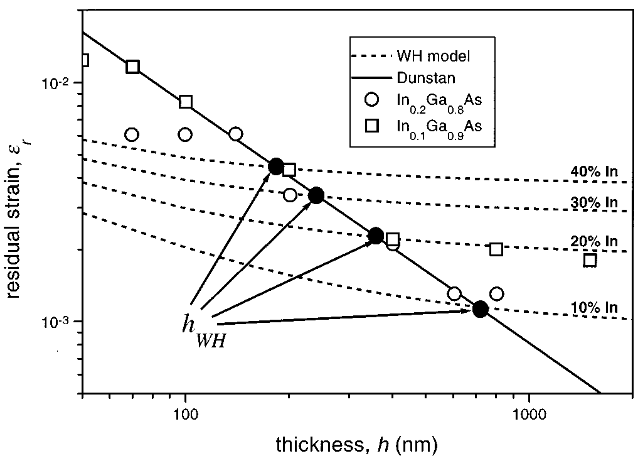

FIG. 1. Residual strain vs layer thickness for the empirical Dunstan law (solid line with accuracy dashed ($k=0.8\pm0.1$ nm) and for the work hardening predictions (dashed-dotted lines for 10%, 20%, 30% and 40% In contents). The intersection of the two models gives the critical thickness for work hardening or strain relief saturation. Experimental data of single InGaAs/GaAs layers with 10% (Ref. 8) and 20% (Ref. 5) In content are also displayed. The relaxation in region I follows Matthews and Blakeslee dislocation bending, while dislocation source kinetics govern the relaxation in region II. The transition to region III where work hardening limits the relaxation is analytically deduced in Eq. (14).

favorable MD density, ρ_{WH}, that the system admits. This state belongs to the zero energy value of ΔE_{WH}. Each term of Eq. (1) can be expressed as:[6,9]

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

$$E_{\mathrm{intm}}=\frac{2\mu(1+\nu)}{(1-\nu)}fb_2h, \tag{3}$$

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

where μ is the shear modulus, ν the Poisson ratio, h the layer thickness, r_0 the radius of the dislocation core, f the lattice mismatch and ρ the linear density of the misfit dislocations array at the interface, that are all assumed to have identical Burgers vectors, $\mathbf{b}$ (b_1,b_2,b_3).

All the hyperbolic terms are functions of $z=2\pi\rho h$. For the considered range of relaxation, the linear dislocation density is in the range of $10^5<\rho<10^6$ cm^{-1} and the thicknesses are greater than 10^2 nm. This means that $z>10$. Therefore, the following assumptions can be made: $\ln[\cosh(z)]\approx z$, $z\tanh(z)\approx z$, $z^2/\cosh^2(z)\approx 0$. Equation (4) is then reduced to:

$$E_{\mathrm{intd}}\approx\frac{\mu}{4\pi(1-\nu)}[[b_1^2+b_2^2+(1-\nu)b_3^2]2\pi\rho h - (b_1^2-b_2^2)4\pi\rho h]. \tag{5}$$

The behavior of misfit dislocation density versus the thickness under work-hardening conditions, ρ_{WH}, can be deduced applying the mentioned approximations and replacing Eqs. (2) and (3) in Eq. (1):

$$\rho_{\mathrm{WH}}=Af+B\frac{\ln\left(\frac{2h}{r_0}\right)}{h}, \tag{6}$$

where A and B are:

$$A=\frac{-4(1+\nu)b_2}{3b_1^2-b_2^2+(1-\nu)b_3^2}, \tag{7}$$

$$B=\frac{-(b_1^2+b_2^2+(1-\nu)b_3^2)}{2\pi(3b_1^2-b_2^2+(1-\nu)b_3^2)}. \tag{8}$$

The approximations applied here allows us to deduce an analytical expression for ρ_{WH}. Assuming that the dislocations are of the 60° type, we also deduce an analytical expression for the strain behavior versus the thickness in the work-hardening regime. Indeed, as $\varepsilon=f-\rho b/2$, the strain behavior in the work-hardening regime, $\varepsilon_{\mathrm{WH}}$, becomes:

$$\varepsilon_{\mathrm{WH}}=f(1+Ab_2)+Bb_2\frac{\ln(2h/r_0)}{\hbar}. \tag{9}$$

As shown in Fig. 1, the critical thickness for the work hardening, h_{WH}, is the intersection point between ϵ_{WH} and strain deduced by Dunstan *et al.*,[3] ϵ_{D}. The empirical law of Dunstan can be expressed as:

$$\varepsilon_D=\frac{k}{h}. \tag{10}$$

Equating the expressions (9) and (10), it follows that:

$$f=\frac{C}{h_{\mathrm{WH}}}-\frac{D\ \ln(2h_{\mathrm{WH}}/r_0)}{h_{\mathrm{WH}}}, \tag{11}$$

where C and D are:

$$C=\frac{k}{1+Ab_2} \tag{12}$$

$$D=\frac{Bb_2}{1+Ab_2}. \tag{13}$$

Note that h becomes the critical thickness, h_{WH}, when work-hardening processes begin to govern the strain relaxation. For the $In_xGa_{1-x}As/GaAs$ system with In composition, $x<0.5$, the components of the Burgers vector vary less than 3%. As $k=0.8$ nm, $\nu=0.27$, $b=a/2(-1,-1/\sqrt{2},1/\sqrt{2})$ in the selected coordinate system of Ref. 6 and $r_0=4b$, we deduce the following expression for the InGaAs/GaAs system:

$$f=\frac{7.052\ \mathrm{nm}}{h_{\mathrm{WH}}}-0.185\ \mathrm{nm}\frac{\ln(h_{\mathrm{WH}}/0.81\ \mathrm{nm})}{h_{\mathrm{WH}}}. \tag{14}$$

The solutions of the equation system are graphically displayed in Fig. 1. The experimental data for 10% and 20% In-content show good agreement with the model predictions. The intersection points between the empirical Dunstan curve and the model predictions are the solutions of the equation system [Eqs. (9) and (10)]. The latter are mathematically deduced in Eq. (14) which gives the work-hardening critical thickness versus the lattice mismatch displayed in Fig. 2. The theoretical predictions are compared with the inflection points experimentally observed by Krishnamoorthy *et al.*[10] displaying the percent relaxation versus $(h/h_{\mathrm{MB}})-1$. In the

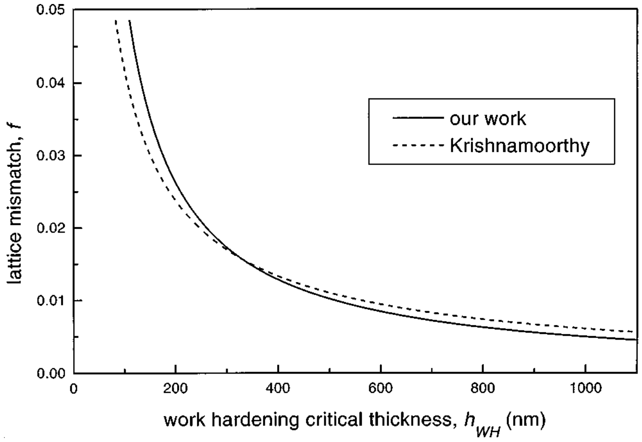

FIG. 2. Graphical representation of the behavior of the work hardening critical thickness, $h_{WH}(f)$, vs the nominal lattice mismatch, f, of the layer for the InGaAs/GaAs system. The solid line corresponds to the model predictions expressed in Eq. (14) and the dashed line to the empirical expression of Krishnamoorthy *et al.* (Ref. 10). Note that the latter is based on experimental data with a lattice mismatch of $f<0.03$. The dashed curve for $f>0.03$ is therefore only an extrapolation and has no experimental validity.

latter, two regimes of relaxation were observed. First, a fast relaxation was shown to occur growing up to $h \approx 30 h_{MB}$ (where h_{MB} is the critical thickness of Matthews and Blakeslee.[2]) Then, in the second regime, a strong slowing of the relaxation was observed. The intersection point of these two empirical behaviors can be deduced from the Krishnamoorthy curve fits and can be expressed as $\epsilon(h_{WH})$. The latter is compared to Eq. (14) in Fig. 2. The good agreement between both curves can be used to explain Krishnamoorthy's data: dislocation interactions slow the introduction of new dislocations into the array of misfit dislocations and this induces the observed inflection point. Also note that for very low lattice mismatch, the critical thickness tends towards infinity as usually observed. For highly mismatched layers, the discrepancy between the two curves results from the low accuracy of the empirical expression of Krishnamoorthy,[1] which is based on experimental data of InGaAs compositions of low lattice mismatch ($f<0.03$).

This result allows us to complete the description of the several stages of relaxation in mismatched heterostructures. The different stages of relaxation are defined by the different critical thicknesses obtained through the expressions of Matthews and Blakeslee,[2] Dunstan[3] and our work-hardening expression [Eq. (14)]. The latter expressions delimit areas of different states of relaxation. For a given nominal lattice mismatch and thickness, the final state of relaxation of the layer can be predicted. Stage I correspond to the relaxation through pre-existing dislocation bending. Stage II is the well-known dynamic stage of relaxation where the sources of dislocation multiplication become active. Finally, stage III corresponds to the strain relaxation saturation state, where work-hardening processes limit the strain relief. Deep in stage III, a small additional relaxation, due to the presence of a high threading dislocation density, could be considered[11] (neglected here).

In summary, an analytical expression of the strain relief in the work-hardening regime is obtained. The critical thickness for work-hardening strain relief saturation is analytically deduced by equating the strain behavior in the dynamic and saturation stages. The theoretical values are shown to correspond very well with experimental data from the literature. Thus a physical explanation for the different strain relief regimes observed by different authors can be given. A slowing of the relaxation at the end of the second regime is usually observed which is attributed here to dislocation interactions. The beginning of this relaxation regime occurs at a thickness named the critical thickness for work hardening, h_{WH}. This critical thickness corresponds to the best relief/thickness ratio and is therefore of fundamental interest in the design of well-relaxed heteroepitaxial structures.

This work was supported by the Spanish Interministerial Commission for Science and Technology CICYT (MAT Project No. 94/0538) and of the Andalucian government (Group No. TEP 0120).

[1] B. W. Dodson, Appl. Phys. Lett. **53**, 37 (1988).
[2] J. W. Matthews and A. E. Blakeslee, J. Cryst. Growth **27**, 118 (1974).
[3] D. J. Dunstan, S. Young, and H. Dixon, J. Appl. Phys. **70**, 3038 (1991).
[4] R. Beanland, J. Appl. Phys. **72**, 4003 (1992).
[5] D. J. Dunstan, P. Kidd, L. K. Howard, and R. H. Dixon, Appl. Phys. Lett. **59**, 3390 (1991).
[6] D. González, D. Araújo, G. Aragón, and R. García, Appl. Phys. Lett. **71**, 2475 (1997).
[7] D. González, D. Araújo, G. Aragón, and R. García, Appl. Phys. Lett. **71**, 3099 (1997).
[8] D. J. Dunstan, P. Kidd, P. F. Fewster, N. L. Andrew, L. González, Y. González, A. Sacedón, and F. González-Sanz, Appl. Phys. Lett. **65**, 841 (1994).
[9] T. Y. Zhang, J. E. Hack, and L. J. Guido, J. Appl. Phys. **75**, 2358 (1994).
[10] V. Krishnamoorthy, Y. W. Lin, L. Calhoun, H. L. Liu, and R. M. Park, Appl. Phys. Lett. **61**, 2680 (1992).
[11] K. Durose and H. Tatsuoka, Inst. Phys. Conf. Ser. **134**, 581 (1993).