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Effect of In-content on the misfit dislocation interaction in InGaAs/GaAs layers

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Abstract

A previous published model (D. González, D. Araújo, G. Aragón, R. Garcia, Appl. Phys. Lett., 71 (1997) 2477) allows us to predict the plastic relaxation in the saturation regime of epitaxial layers. This model is in agreement with the experimental residual strain for $In_xGa_{1-x}As$/GaAs epilayers below 40% In-content. Above 40% In-content, the predicted values of residual strain become larger than the experimental one. This disagreement takes its origin in the change of growth mode that implies a transition from a 60° misfit dislocation (MD) network to a Lomer MD one. An almost complete relaxation can be reached by a Lomer MD network, which is not possible with 60° MD networks. The difference between both kinds of networks comes from the repulsive interaction of 60° MD that inhibits the lattice relaxation.

Keywords: Computer simulation; Epitaxy; Gallium arsenide; Indium arsenide; Interface; Semiconductors

1. Introduction

During the last years, the synergy between market necessity and the ability to grow new alloys with a high chemical and structural quality make possible the fabrication of new devices. For bandgap engineering, the constituent layers of optoelectronic devices should have restrictions in terms of composition or layer thickness. To obtain high crystalline quality devices, nearly defect-free materials must be grown. This implies the growth of a buffer layer to adjust the reticular parameter of the active layer to that of the commercial substrate. Such improvement has a special importance for the highly mismatched InGaAs /GaAs system used for high velocity applications as HBT or MODFET transistors and the monolithic integration of microelectronic devices with optoelectronic ones.

However, a great difficulty existed up to now; to get a control of the reticular parameter throughout the buffer layer. Indeed, as no complete relaxation can be reached even for very large thickness, some uncontrolled residual strain persists. The prediction of the residual strain is fundamental to the design of strained or well-relaxed devices. To get it, no quantitative models are at present available in the bibliography to describe all the stages of relaxation in heteroepitaxial structures. As a first step, we previously proposed a model based on the interaction of interfacial MD that predicts the residual strain either in simple thick epilayers with constant composition [1] or in step graded structures [2]. Such structures are in the last stage of the relaxation corresponding to the work hardening regime. In this work, we check the interval of the model validity in terms of nominal lattice mismatched, using the previously published strain results of thick epilayers.

2. Work hardening model

The aim of this work is to define the limitation of our previously published work hardening model [1]. The main assumption is based on the energy state of the system during the introduction of a new dislocation in between an array of misfit dislocations located at the interface. Briefly, the energy for the work hardening process, ΔE_{WH}, is described as the difference in energy of the system before, E_1, and after E_2, the introduction of the new dislocation

$$\Delta E_{WH} = E_2 - E_1 = E_s + E_{intm} + E_{intd} \quad (1)$$

where E_s is the self energy of a new dislocation, E_{intm} the interaction energy between the new dislocation and the reticular misfit and E_{intd} the interaction energy between the new dislocation and the fixed dislocation array. For a regularly spaced, 60° mixed dislocation array, the mathematical expressions are given elsewhere [1,3]. The interaction

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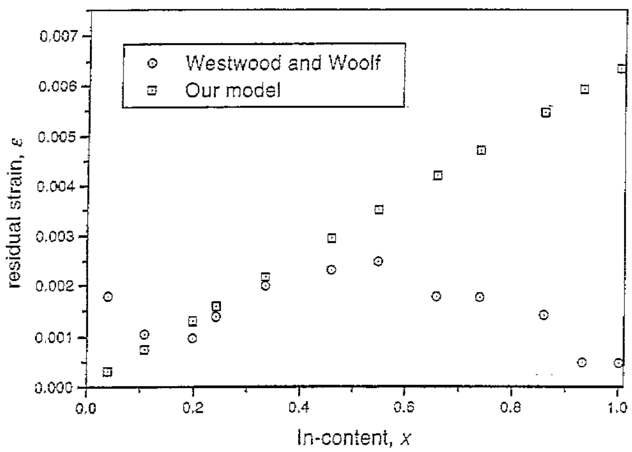

Fig. 1. Experimental and theoretical residual strains versus In-content for low mismatched single InGaAs/GaAs layers. The solid points correspond to experimental data obtained by Maigne [5] and Krishnamoorthy [6], while the open ones are predicted by our model for the corresponding sample.

energy with the array, E_{intd}, increases only with the 60° MD density, while Lomer pure edge MDs do not participate.

For an initial small density of MD, the work hardening energy is negative and the introduction of new dislocations is favored. However, the higher MD density, the lower ΔE_{WH} is. Finally, the MD introduction process stopped when the work hardening energy reaches a zero value. The corresponding MD density, ρ_{WH}, for the work hardening regime is obtained by solving $\Delta E_{WH}(h,f,\rho(h,f)) = 0$ where h is the layer thickness and f is the lattice mismatch.

This saturated relaxation begins at a defined critical thickness above that at which the work hardening process governs. Such thickness, h_{WH}, can be expressed as [4]

$$f = \frac{7.052\ \text{nm}}{h_{WH}} - 0.185\ \text{nm}\frac{ln(h_{WH}/0.81\ \text{nm})}{h_{WH}} \quad (2)$$

for the InGaAs/GaAs system.

Furthermore, the residual strain corresponding to work hardening stage follows

$$\varepsilon = f - \rho_{WH}\frac{b}{2} \quad (3)$$

where b is the modulus of the Burgers vector of the dislocation array (in this case 60°). In the following, we verify the validity range of the present model applying it to InGaAs epilayers whose thickness exceeds h_{WH}.

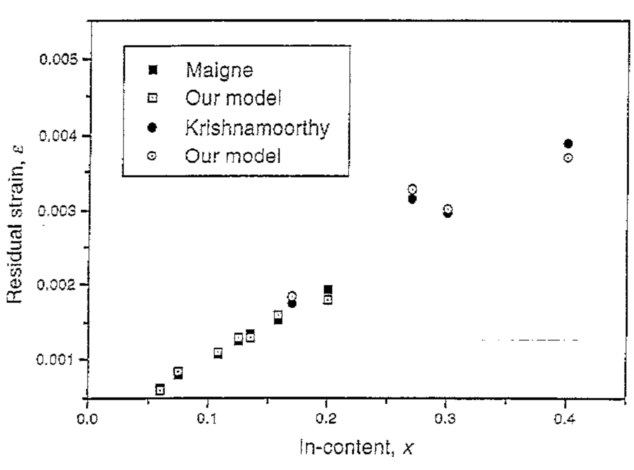

Fig. 2. Experimental residual deformation in 2.8 μm thick $In_xGa_{1-x}As$ epilayers versus the In-content (open circles) [10], compared with theoretical values calculated using the work hardening model (open squares).

3. Results

In a low lattice mismatch epitaxial system, a layer by layer or 2D growth usually occurs. The relaxation by a 60° MD network takes places forming an orthogonal array. Edge MD dislocations may result from the recombination of two 60° dislocations, but this represents a small percentage of the total density. In Fig. 1, experimental data from the bibliography [5,6] are compared with their respective numerical predictions applying the work hardening model. The experimental and theoretical data are in excellent agreement for low misfit systems, with In-content lower than 40% ($f < 3\%$).

However, the systems with a lattice mismatch larger than 2–3% ($x > 0.3$–0.4 for $In_xGa_{1-x}As$/GaAs) undergo a transition from two-dimensional to three-dimensional growth [7,8], before the generation of the MD [9]. Such a transition drastically affects the relaxation process. To investigate the relation between the growth mode and the work hardening efficiency, we use the previously published data obtained by Westwood and Woolf [10]. The latter data correspond to 2.8 μm thick single layers and we assume then that the epilayers have reached the work hardening regime. The comparison of experimental published data with the calculated ones is displayed in Fig. 2.

The experimental residual strain increases until it reaches a maximum for an In-content near $x \sim 0.5$, falling then quickly down toward the InAs binary compound. As the thickness remains constant, the behavior predicted by our model is linear and the higher than 40% In-content, the stronger the discrepancy with experimental values is. Thus, the model predictions fit the experimental values between $x = 0.04$ and $x = 0.4$ Below $x < 0.04$ the work hardening regime has not been reached. Indeed, for such layers, a high residual strain (64% of its reticular misfit) is induced that is away from the work hardening stage.

As we have described previously, the beginning of 3D growth from an In-content $x > 0.3$–0.4 modifies the relaxation kinetics and induces changes in dislocation distribution and type.

4. Discussion

In heterostructures with In-content around $x = 0.3$–0.4, an island growth transition occurs that modifies drastically the structure and formation of MD. The edge MD begins to prevail and progressively substitutes for the 60° dislocations as the In-content increases. In epitaxies of InAs on GaAs growth, edge dislocations are the main constituents of the MD array [10]. In our work hardening model, we have considered a perfectly spaced network of 60° mixed dislocations. When the edge dislocation proportion increases, the term E_{intd} that depends on the interaction between 60° MD diminishes progressively. Furthermore, the term E_{intd} tends to zero in a network containing only Lomer dislocations. This result takes place because the out of growth plane Burgers vector component contributes most to the repulsive interactions, while the misfit component scarcely participate in the repulsive effect.

The increment of edge dislocation proportion for $In_xGa_{1-x}As/GaAs$ when $x > 0.4$ produces a reduction of work hardening effect because: first, the total MD density diminishes and second, the interaction between the dislocation array and the new dislocations is much smaller. As a result, in heterostructures where the edge dislocation proportion increases, the residual strain diminishes with respect to the theoretical results obtained by our model considering only 60° mixed dislocations The relaxation is not inhibited by the interaction between edge dislocations and can reach values close to 99% [11] for an edge dislocation array. This result suggests that the work hardening observed in heteroepitaxies is exclusively due to the interaction among 60° MD.

5. Conclusions

In conclusion, the validity range of a previously published strain relaxation model is estimated. The model has been proposed for the last relaxation stage and is based on the interaction between 60° MD. This model predicts correctly the residual strain for $In_xGa_{1-x}As/GaAs$ epilayers with an In-content below 40%. For higher In-content, the model predictions are larger than the experimentally observed strain values. The increase in the edge dislocation proportion, due to a change in the growth mode, can explain this result. Therefore, the relaxation inhibition results only from the interaction between 60° MD present at the interface. The relaxation through edge dislocations diminishes the work hardening effect in epitaxies and allows the system to reach an almost complete relaxation of the lattice mismatch.

Acknowledgements

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References

[1] D. González, D. Araújo, G. Aragón, R. Garcia, Appl. Phys. Lett. 71 (1997) 2477.
[2] D. González, D. Araújo, G. Aragón, R. Garcia, Appl. Phys. Lett. 71 (1997) 3099.
[3] T.Y. Zhang, J.E. Hack, J. Guido, J. Appl. Phys. 75 (1994) 2363.
[4] D. González, D. Araújo, G. Aragón, R. Garcia, Appl. Phys. Lett. 72 (1998) 1875.
[5] P. Maigné, J. Vac. Sci. Technol. A 15 (1997) 43.
[6] V. Krishnamoorthy, Y.W. Lin, L. Calhoun, H.L. Liu, R.M. Park, Appl. Phys. Lett. 61 (1992) 2680.
[7] J.Y. Yao, T.G. Anderson, D. L Dunlop, J. Appl. Phys. 69 (1991) 2224.
[8] K.H. Chang, R. Gibala, D.S. Srolovitz, P.K. Bhattacharya, S.F. Mansfield, J. Appl. Phys. 67 (1990) 4093.
[9] C.W. Snider, B.G. Orr, D. Kessler, L.M. Sander, Phys. Rev. Lett. 66 (1991) 3032.
[10] D.A. Woolf, D.I. Westwood, A. Vila, A. Cornet, J.M. Morante, J. Appl. Phys. 74 (1993) 1731.
[11] A. Trampert, E. Tournié, K.H. Ploog, Appl Phys. Lett. 66 (1995) 2265.