Dislocation behavior in InGaAs step- and alternating step-graded structures: Design rules for buffer fabrication

D. Araújo, D. González, and R. García
Dpto. de Ciencia de los Materiales e IM y QI, Universidad de Cádiz, Apartado 40, 11510 Puerto Real, Spain

A. Sacedón and E. Calleja
Departamento de Ingeniería Electrónica, E. T. S. I. Telecomunicación, Universidad Politécnica de Madrid, Ciudad Universitaria, 28040 Madrid, Spain

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A comparison between compositionally stepped and alternating step-graded structures used in the production of a relaxation buffer layer is carried out by means of transmission electron microscopy. The latter shows higher efficiency in relieving the strain. A simple balance force model permits us to understand the reason for a higher generation of threading dislocations observed in the alternating step-graded structures. The presented results can be applied as new design rules for buffer fabrication that contrast in some key points with previous published rules as, for example, the "zero-net-strain" precept [D. Dunstan, P. Kidd, P. F. Fewster, N. L. Andrew, L. González, Y. González, A. Sacedón, and F. González-Sanz, Appl. Phys. Lett. **65**, 845 (1994)]. © *1995 American Institute of Physics.*

During the last decade, special attention has been dedicated to plastic relaxation in heteroepitaxial structures either for the fabrication of devices grown in novel materials or for its fundamental understanding. Some of the most important materials in this field are the InGaAs alloys. Their efficient optoelectronic properties (carrier mobility, relaxation lifetimes,...) and a photon emission in the range of the minimum absorption of light guides (1.55 and 1.3 μm) are essential in the field of the modern opto- and microelectronic technologies. However, their lattice mismatch with commercial substrates (GaAs,...) makes crystal relaxation through dislocation necessary. For this purpose, several buffer structures have been proposed in the literature, amongst which graded buffer layers,[1–4] step-graded buffer layers,[5–7] and multilayers (MLs)[8,9] seem to be the most efficient solutions. The high growth control and quality of III–V compounds and their high dislocation mobilities also make such buffers good candidates to obtain lattice matched II–VI substrates for visible optoelectronics applications.

Although few in number, some very interesting results have been previously reported on compositional graded buffer layers. From experimental data, Krishnamoorthy *et al.*[5] proposed a criterion based on the yield strength relating the interfacial misfit to the threading dislocation creation. Furthermore, a simple balance force model explained the dislocation deepening in the substrate.[11] Finally, Dunstan *et al.*,[1,7,12,13] Tersoff,[3] and Sacedón *et al.*[14] have presented models for the average strain behavior of single, graded, and step-graded structures, respectively.

One of the advantages of step-graded layers is the possibility to probe the relaxation state layer by layer either by double crystal x-ray diffraction (DCXRD) up to three layers and/or by transmission electron microscopy (TEM).[10] In this letter, the lattice relaxation is studied by TEM on step- and alternating step-graded structure. The correspondence between the strain and the misfit dislocation density in such structures has been shown elsewhere.[9,10] Two samples (labeled A and B, respectively) were grown by molecular beam epitaxy (MBE) to compare the misfit and threading dislocation behavior between both types of structures. A schematic description of each sample structure is shown at the left-hand side of the electron micrograph presented in Fig. 1 and as dashed lines in Fig. 2. The multilayer structure consists of 5% step composition in an increasing order for sample A and as alternating steps for sample B.

The samples are observed in cross-sectional and planar view orientations. The general dislocation behavior described here is in agreement with results obtained on other samples with different average grading rates, layer thicknesses, and steps of composition. To guide the reader with simple concepts and to have an exact comparison between the two types of structure, results are presented here from samples with identical grading rates, layer thicknesses, and cap layer compositions and thicknesses.

Figure 1 shows (220) bright field TEM micrographs of both structures in cross sectional orientation. A mean value of misfit dislocation density at interfaces is statistically deduced upon observation of several specimens. This value allows us to determine the relaxation and the strain for each layer of both stacks using a precalibration of edge and 60° dislocations proportions.[10] The dislocation density at the top of the buffer is deduced from planar view observations.

The strain dependence versus the thickness of both samples is reported in Fig. 2. The linear increase in the strain observed for sample A is in contrast with the Dunstan *et al.*[1] prediction. For sample B, in addition to the well-relaxed alternating step second layers, a similar increase in strain for each of the two layers is also observed. Such behavior is attributed to a work hardening process in sample A that distributes, in a nearly constant way, the misfit dislocation between the layer interfaces ($8–10\times10^{8}$ cm^{-2}) and to a relaxation blocking process due to the alternating step in sample

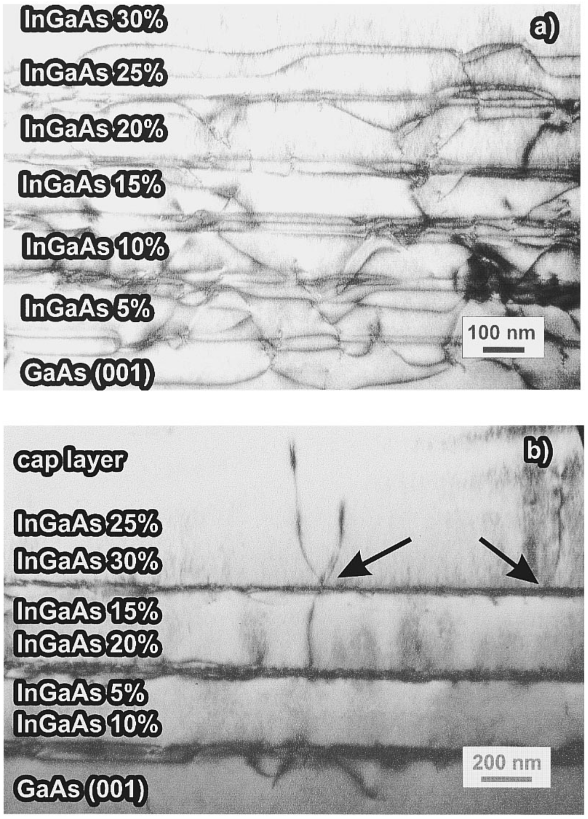

FIG. 1. Bright field (220) TEM micrographs of samples A and B, respectively. In sample B, the arrows show threading dislocations contaminating the cap layer.

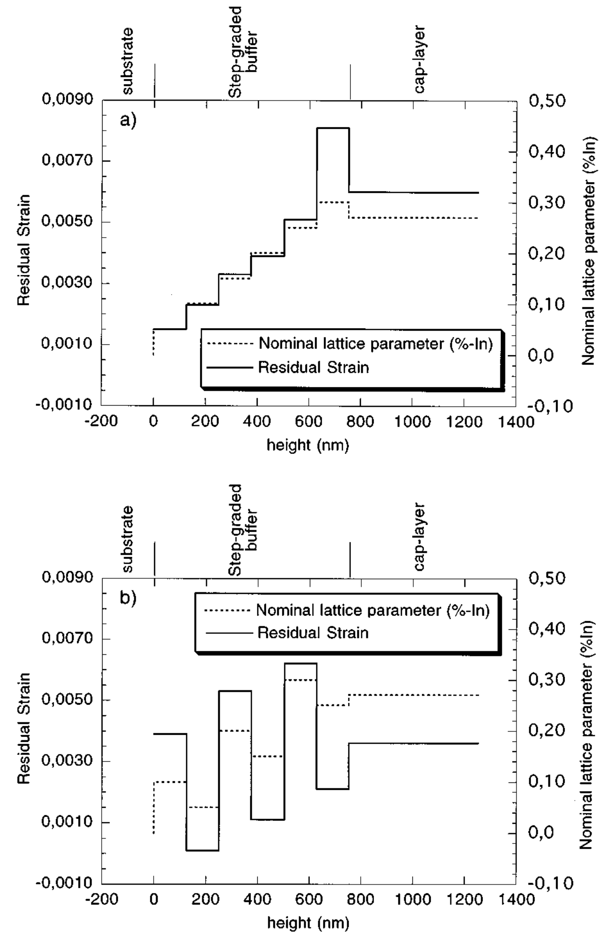

FIG. 2. Residual strain determined using the TEM observed misfit dislocation density vs the thickness for samples A and B. The dashed curve corresponds to the layer composition and is used as a guide for the eye.

B. Photoluminescence spectra measurements confirmed the high strain values deduced by TEM measurements at the top of the structure and also the better relaxation of the top layer of sample B ($\epsilon=0.0036$) compared to that of sample A ($\epsilon=0.0060$).

In sample A, some misfit dislocations relaxing the structure are shown to thread from interface to interface. The distribution of these threading dislocations versus the thickness is shown in Fig. 3. A maximal density of threading dislocations is observed at the center of the structure and a lower density is observed at the first/last layers of the stack.

In sample B, nearly no threaders are observed between the interfaces up to the 15%–30% In interface [see Fig. 1(b)]. Since a high step of 15% In occurs every two layers, these highly strained layers push dislocations down to their previous interface. Indeed, the elastic forces have high values in these layers. This leads to the observed dislocation free layers in the whole step structure.

Dislocation densities in the cap layers lower than 10^5 cm^{-2} and nearly 10^8 cm^{-2} are measured by plan view TEM observation in samples A and B respectively. This result contrast with the threading dislocation behavior in the bottom layers, where absence of threading dislocations is clearly observed in sample B [Fig. 1(b)]. This difference is basically due to the generation of threading dislocations at the last interface, as shown by arrows in Fig. 1(b), that occur only in sample B. Indeed, a large number of dislocations are shown to begin to thread from this last high step interface (15%–30%), some of which bend at the upper alternating step (30%–25%). However, a still larger number of threading dislocations follows into the cap layer [see arrows in Fig. 1(b)].

The behavior of the dislocations at the last interface and in the rest of the structure can be understood through a simple balance force model. The result of the growth of the forces governing the dislocation behavior at the interface in the epilayer is the following[11]

$$F_R=F_s-F_l-F_e-F_i+F_{dd}, \quad (1)$$

where F_R, F_s, F_l, F_e, F_i, and F_{dd} are the resultant, surface, lineal, elastic, interface, and dislocation interaction forces, respectively. Between the two sample structures, assuming a constant elastic modulus, only two of these forces vary as the average grading and the thickness are identical for both samples: F_{dd} and F_e. Due to relaxation blocking processes, the misfit dislocation density at the interfaces is lower in sample B at the alternated steps and higher at the high composition steps [Fig. 1(b)]. Therefore, F_{dd} is weaker than in sample A at the inverted interfaces ($F_{dd,\mathrm{A}}>F_{dd,\mathrm{B}}$) and larger at high steps ($F_{dd,\mathrm{A}}<F_{dd,\mathrm{B}}$). Moreover, due to high steps occurring every second layer in sample B, the

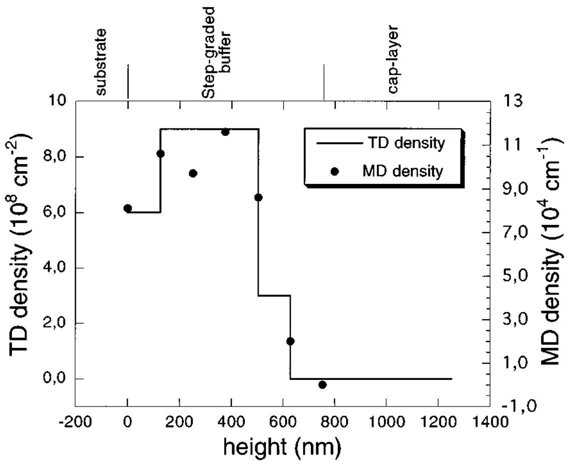

FIG. 3. Threading and misfit dislocation densities determined by cross sectional TEM observation vs the thickness of sample A. In sample B, threading dislocations are observed only at the top of the stack with a density just at the detection limit of cross sectional TEM observations (10^8 cm^{-2}).

strain stays at higher values, keeping the elastic force F_e also at high values in the high step layers of sample B and in the 30% layer of sample A ($F_{e,\mathrm{A}} < F_{e,\mathrm{B}}$; in sample A, $\epsilon = 0.0015$ to 0.005 until the 30% layer and $\epsilon = 0.0081$ in this layer; in sample B, $\epsilon = 0.0039$, 0.0053, and 0.0062 in high step layers and below 0.002 in alternating step layers). This pushes the dislocation down more strongly.

By comparing the forces that curb dislocations to thread at the 30% layer interfaces between the two samples, it appears that these two forces act in the same direction, i.e., $F_{dd,\mathrm{A}} < F_{dd,\mathrm{B}}$ and $F_{e,\mathrm{A}} > F_{e,\mathrm{B}}$:

$$\text{Top of the grading:} \quad F_{dd,\mathrm{A}} - F_{e,\mathrm{A}} < F_{dd,\mathrm{B}} - F_{e,\mathrm{B}}. \quad (2)$$

This means that, in sample A 30% layer, less dislocations are generated by the repulsive force F_{dd} and the dislocations are submitted to a higher bending force F_e; i.e., the probability of having dislocations in the cap layer is much higher in the alternating step type of structure. Indeed, threading dislocations are revealed by XTEM observations only in such structures [see Fig. 1(b)].

In the bottom layers (<30%), F_e is much lower in sample A than in sample B and F_{dd} is slightly lower than in the 30% layer for both samples. This means that Eq. (2) becomes

$$\text{Below the 30\% layers:} \quad F_{dd,\mathrm{A}} - F_{e,\mathrm{A}} > F_{dd,\mathrm{B}} - F_{e,\mathrm{B}}. \quad (3)$$

As a result, nearly no threading dislocations are observed in the sample B layers below the 30% layer.

As shown in Fig. 3, in sample A, the density of threading dislocations increase slightly in the first steps and decrease strongly in the last ones. The first increase is attributed to the slight increase of the density of misfit dislocation (8–10 $\times 10^4$ cm^{-1}), which in turn increase F_{dd}, while the decrease is attributed to the strong increase of the strain that makes the elastic force much more important.

In summary, the residual strain has been estimated by TEM measurements on samples with direct and alternating step buffers. We show with a simple balance force model that compositional inverse step structures becomes highly defective at the top of the buffer while relatively clean layers are obtained in direct step buffers. Indeed, threading dislocations are observed in the cap layer with a density around 10^8 cm^{-2}, while this value is below the detection limit on the direct step sample. However, a tight control of the extent of relaxation can be achieved in an inverse step buffer due to the relaxation blocking process, while in the direct step structure, the residual strain of the underlying layer cannot be properly predicted. Moreover, the alternating step structure is shown to relax the strain more efficiently. Therefore, as design rules for buffer fabrication, we recommend beginning the growth up to half of the total thickness by an inverse step structure to achieve a good control of the strain relaxation, and then to follow up with a rather simple direct step structure in order to limit the TD propagation (bearing in mind not to overpass the critical effective step composition of 18%).

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