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Transmission electron microscopy study of $In_xGa_{1-x}As/GaAs$ multilayer buffer structures used as dislocation filters

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Abstract

To investigate the efficiency of threading dislocation (TD) filtering in multilayer (ML) buffers, $In_xGa_{1-x}As/GaAs$ structures are studied by transmission electron microscopy. The TDs are generated at the first $In_{0.3}Ga_{0.7}As$ thick layer. Different MLs harder and softer on average than this TD generator thick layer are used as filters. The efficiencies of the ML filters are compared with that of a bulk layer with identical average In content. As the individual ML thickness is below the Matthews-Blakeslee critical thickness, no TD bending should occur. However, in contrast with the softer buffer behavior, MLs buffer harder than the TD generator layer are shown to filter. This difference in the TD behavior between the two kinds of structure is attributed to yield strength effects. From a kinetic model, an expression for the TD density vs. the height is deduced. On application of this model to the measured TD densities, filtering parameters are deduced.

Keywords: Transmission electron microscopy; Semiconductors; Gallium arsenide; Superlattices

1. Introduction

Because of the lattice mismatch between $In_xGa_{1-x}As$ and GaAs, strained epitaxial layers or plastically relaxed layers are grown on GaAs substrates. Usually, the strained layers are used to improve the optoelectronic properties of devices. However, to control such strain or to grow unstrained $In_xGa_{1-x}As$ layers, a change in the crystal lattice parameter is necessary. This change is made by plastic relaxation which can induce dislocation propagation in the epitaxial layer structure. To obtain defect-free layers at the top of the structures, buffer layers are introduced between the $In_xGa_{1-x}As$ layers of interest and the GaAs substrate. For this purpose, several dislocation filters have been proposed in the literature up to now. Among them, graded buffer layers [1-3], step-graded buffer layers [4-6] and multilayers (MLs) [7-9] seem to be the most efficient solutions. To interpret the influence of strained MLs on the dislocation behavior, a comparison between the stack of MLs and a bulk layer of equivalent average composition and total thickness is necessary. If this is not done, it will always be unclear whether the MLs have any effect on dislocation recombination. There are many studies in the literature, most of which do not consider this point. Interpretation of results is therefore difficult.

Recently, very strong dislocation filtering effects were noted by Rao and Horikoshi [8], using $(GaAs)_x(Si_2)_{1-x}/GaAs$ MLs. This enhancement in the dislocation filtering was attributed to the elastic modulus effect [8, 9] rather than to strain, although it is likely that both processes make some contribution. In their first paper, Krishnamoorthy et al. [4] explained the behavior of dislocation deeping in the GaAs substrate for x values below 0.18 and above 0.28 based on the effect of the surface force. Moreover, in their second paper [5], they explained the behavior of the threading dislocation (TD) evolution in step-graded structures on the basis of yield strength variations which change the In content of the $In_xGa_{1-x}As$ alloy. The yield strength does not follow Vegard's law from GaAs to InAs [5], but it increases with increasing In content, reaching a maximum at around 50 at.%. In the Ge_xSi_{1-x}/Si system, MLs and constant-composition layers, of the same thickness and average composition, were compared as dislocation filters [10]. It was found that no reduction in TD density occurs between the

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different samples, even when the individual layer thickness is increased above the critical thickness. This result seems to indicate that a difference in strain only produces no change in the TD density.

In this paper, the strain and elastic modulus effects are analyzed by studying the behavior of the dislocation propagation in the $In_xGa_{1-x}As/GaAs$ system using transmission electron microscopy to measure the defect distribution. The cross-sections of the samples are observed by diffraction contrast. Dislocation filters harder and softer on average than the TD generator material are compared.

2. Experimental technique

To analyze the dislocation filtering processes occurring in ML structures, we study different $In_xGa_{1-x}As/GaAs$ MLs working as threading dislocation filters by cross-sectional transmission electron microscopy (XTEM). The sample structures analyzed are shown schematically in Fig. 1. The TD filtering in the ML can be achieved by change in either strain or hardness at the interfaces. Thus two groups of samples are studied.

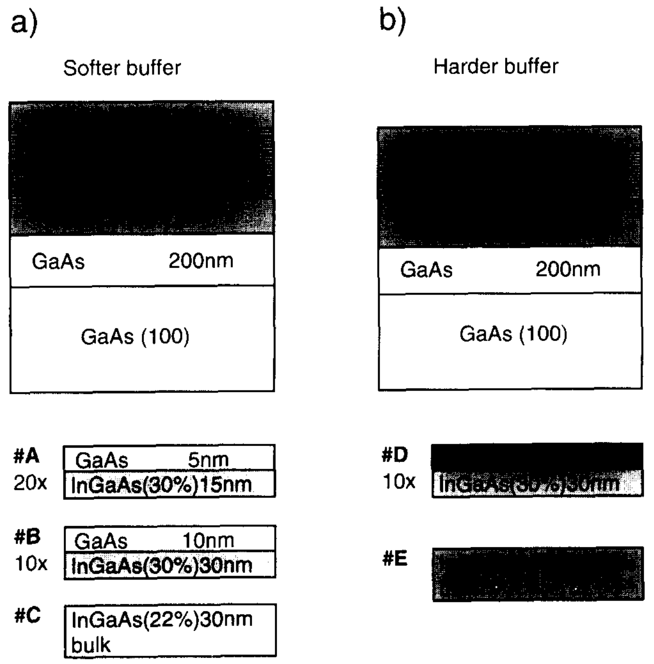

Fig. 1. Schematic diagrams of the sample structures. (a) The structure of the first series of samples. Sample A buffer consists in GaAs(10 nm)/$In_{0.3}Ga_{0.7}As$(30 nm) MLs, sample B consists of an ML buffer with a half individual layer thickness (5 nm/15 nm) and identical total buffer thickness, and sample C contains only a bulk layer of identical medium In content as sample A and B. (b) The structure of the second series of samples. Sample D buffer consists of $In_{0.3}Ga_{0.7}As$(30 nm)/$In_{0.45}Ga_{0.55}As$(10 nm) MLs, and sample E contains only bulk layers of identical total thickness and medium In content as sample D.

First, to analyze the efficiency of the strain assisted mechanisms, two samples (labeled A and B) containing $In_{0.3}Ga_{0.7}As/GaAs$ MLs with an identical total thickness and average In content but with different individual layer thicknesses, and one other sample (labeled C) with a thick layer of identical medium In content and total thickness are compared. Second, to analyze the effect of elastic-modulus-assisted mechanisms, an $In_xGa_{1-x}As/In_yGa_{1-y}As$ ($x=0.3$; $y=0.45$) ML is compared with a bulk layer of identical average composition and total thickness. All the five structures include an $In_{0.3}Ga_{0.7}As$ layer between the MLs and the GaAs substrate that is used as the TD generator. The growth is achieved in a molecular beam epitaxy chamber at 500 °C.

3. Results and discussion

To understand the type and the direction of the TDs generated by the thick layer and propagating in the whole structure, observations by XTEM are performed. In the five samples, three different types of 60° TD are revealed: (i) vertical TDs following the ⟨114⟩-type direction; (ii) quasi-vertical TDs following ⟨216⟩-type direction; (iii) diagonal TDs (the classical TDs, at 54° to the z axis) following ⟨211⟩- and ⟨110⟩-type directions. Similar results were reported by Tamura et al. [11]. Fig. 2 shows a cross-sectional transmission electron micrograph revealing these three types of dislocation.

3.1. Theoretical description of the threading dislocation filtering

In bulk material, the density of TDs depends on the TDs generated in the structure and on the recombination rate that is proportional to the square of the TD density. The kinetics of TD recombination can be expressed as [12]

$$\frac{dD(z)}{dz} = -\lambda_1 D^2 \tag{1}$$

which gives the variation in the TD density $D(z)$ with the height z in the layer [13]

$$D(z) = \frac{D_0}{D_0 \lambda_1 z + 1} \tag{2}$$

with $D_0 = D(0)$ corresponding to the TD density at the first interface. For ML filters, the effect of the interfaces is introduced by a term proportional to the 'interface density' and to the TD density. Therefore, Eq. (1) becomes

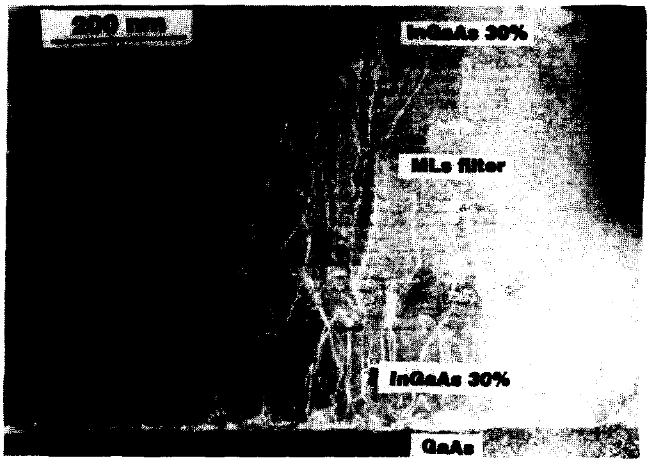

Fig. 2. Cross-sectional transmission electron micrograph of sample A. The three types of dislocation are clearly visible in this (004) weak-beam micrograph.

$$\frac{dD(z)}{dz} = -\lambda_1 D^2 - \lambda_2 DK \tag{3}$$

where the first term of Eq. (3) is proportional to the probability that two TDs meet and recombine with each other and the second term is proportional to the probability that one TD meets an interface and bends. The parameters λ_1 and λ_2 quantify the relative influence of both recombination processes and have the dimensions of a length. D and K are the dislocation density and the interface density respectively.

In the cases when there is a reduced number of layers and/or when bending forces are absent, the first term of Eq. (3) dominates and $D(z)$ follows a law in $1/z$. However, in the case of MLs with high interface density the second term of Eq. (3) becomes important if the mechanisms involving strain and/or elastic modulus force the TDs to bend at interfaces. Then the solution is

$$D(z) = \frac{\lambda_3 \exp^{(-\lambda_3 Z + C)}}{1 - \lambda_1 \exp^{(-\lambda_3 Z + C)}} \tag{4}$$

with the integration constant λ_3 and C corresponding to $\lambda_2 K$ and $[(\lambda_1 D_0 + \lambda_3)/D_0]$ respectively.

3.2. The effect of strain

Fig. 1 displays the five multilayer structures studied. Samples A, B and C have identical average In contents. Samples A and B have only different interface densities and sample C is a bulk layer used as a reference to probe the filtering effect of structures A and B. The multilayers used in samples A and B are on the average softer [4] than the $In_xGa_{1-x}As$ ($x = 0.3$) first layer used as TD generator. Bending forces induced by the increase in strain and hardness are present in the $In_xGa_{1-x}As$ layers. Fig. 2 displays one XTEM (004) weak-beam micrograph corresponding to sample A. The TD densities are measured from similar micrographs for the five structures. No difference between the three structures in TD filtering is observed (see Fig. 4(a) later for the measured TD densities along the whole structures). No significant filtering effects between the samples A, B and C are revealed. The layers are thinner than the Matthews–Blakeslee [14] critical thickness. Their model determines the thickness necessary to bend TDs at strained interfaces by equating the force exerted by the misfit stress to the line tension in the dislocation. Therefore, in our case, TDs will not bend if only a strain-related process occurs. Moreover, to bend dislocations, another condition must be considered: the energy state of two TDs with a misfit segment joining the two TDs must be lower than that of a simple TD. El-Masry et al. [15] described such a model. In our case, the layer thickness is lower than the El-Masry et al. critical thickness. Therefore to bend dislocations an additional force is necessary. As in this case the average hardness is lower than that in the TD generator layer, additional forces involving hardness to not affect the TD bending.

3.3. Effect of the hardness

Fig. 3 displays two (004) weak-beam cross-sectional transmission electron micrographs of samples D and E. Sample D corresponds to the ML filtering structure that is grown with a higher average In content and therefore higher hardness than the TD generator $In_xGa_{1-x}As$ layer. Sample E has an identical In content as sample D and is used as a reference to check the efficiency of the TD filtering. In sample E, the majority of the TDs are shown to reach the top surface. This contrasts with the behavior of TDs in sample D. TD bending is shown to occur frequently in sample D. In Fig. 4, the TD density vs. the height in the structure for samples E and D is shown. Assuming a TD behavior following Eq. (2) in sample E, we deduce $\lambda_1 = 7.0 \times 10^{-6}$ nm and $D_0 = 5 \times 10^9$ cm^{-2}. Introducing these values in the fit of sample D (Eq. (4)), i.e. assuming an identical probability that two TDs recombine without the effect of interfaces in the ML sample, we determine the value of $\lambda_3 = 3.83 \times 10^4$ nm. Such structures with a higher average hardness than the TD generator are shown to filter significantly TDs even for layer thicknesses below the El-Masry et al. or the Matthews–Blakeslee critical thickness. Therefore an additional force acting on the TDs must be considered. Moreover, this force is able to bend dislocations only in harder materials. As the hardness increases with

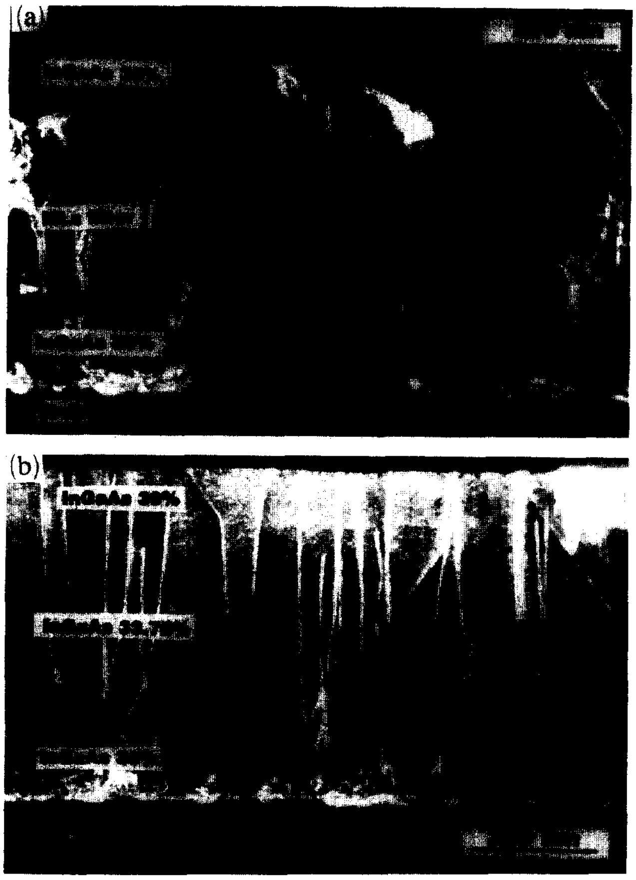

Fig. 3. Cross-sectional transmission electron micrographs of (a) sample D and (b) sample E. The difference in the TD filtering is visible. More TDs bend in sample D.

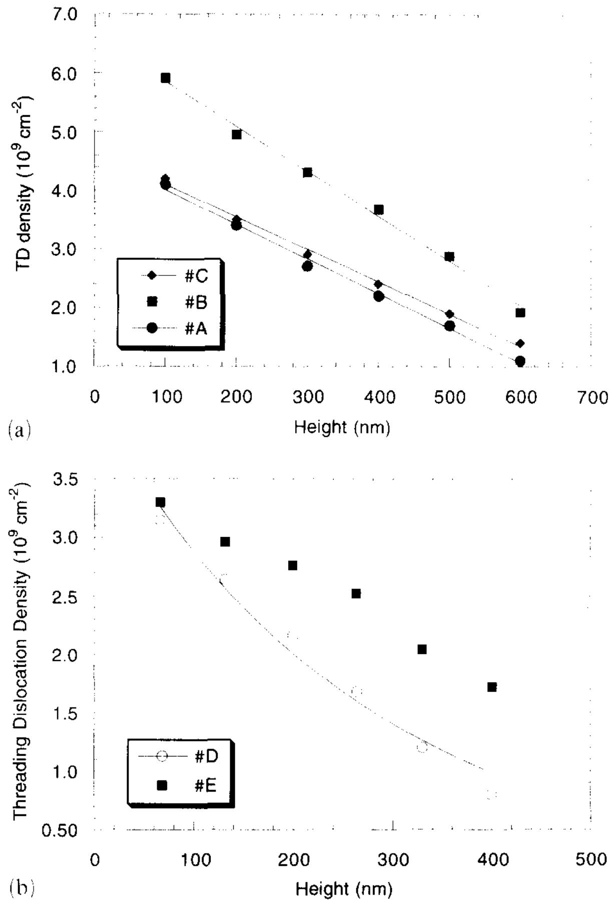

Fig. 4. (a) TD density vs. the height in the first series of samples (sample A, B and C). The lines corresponds to fits following Eq. (2). Using Eq. (2), the fitted values deduced for samples A, B and C gives 5×10^9 cm^{-2} for D_0 and 5×10^{-6} nm for λ_1. (b) TD density vs. the height for the second series of samples. Fitting Eq. (2) to sample E, $\lambda_1=7\times10^{-6}$ and $D_0=4\times10^9$ cm^{-2} are deduced. On the assumption of an identical bulk recombination effect in the ML of sample D, $\lambda_3=3.83\times10^4$ nm is deduced from fitting Eq. (4).

increasing In content up to values of roughly 50 at.%, the competition between the force-associated with the strain that acts on the dislocation bending (the linear dislocation energy, the surface force and threading effects such as Frank–Read mechanisms) produces different main contributors changing the In content of the layer. As the energy associated with the dislocation is proportional to μb^2 (where μ is the elastic modulus and b the dislocation Burger's vector), the second series of buffer layers is less stable than the first and TD bending can occur easily at interfaces.

4. Conclusion

The TD filtering between layers of different hardnesses is compared. Bulk layers of identical average In content permit probing of the effects of interfaces on the TD filtering. Buffer layers harder on average are shown to be efficient filter structures. In contrast, MLs softer on average than the TD generator do not show a significant effect of TD filtering compared with that of bulk layers. This shows the important role played by the yield strength in TD bending. Finally, a kinetic model of dislocation filtering in MLs is presented. The TD behavior with the height of the structure is found to follow that predicted by the model. Parameters related to the probability that a dislocation bends at an interface are determined.

Acknowledgments

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