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# Inhomogeneous strain relaxation and defect distribution of ZnTe layers deposited on (100)GaAs by metalorganic vapor phase epitaxy

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The structural characterization of ZnTe epilayers grown on (100)GaAs by metalorganic vapor-phase epitaxy is reported. A detailed study of the ZnTe/GaAs heterostructure based on both high-resolution and conventional electron microscopy and ion channeling Rutherford backscattering spectrometry allows correlation of the type and spatial distribution of the extended defects occurring at or close to the ZnTe/GaAs interface with the amount of residual lattice strain into the ZnTe epilayers. Both pure edge Lomer and 60°-mixed misfit dislocations were identified at the interface along with partial dislocations bounding stacking faults, their overall density and distance distribution indicating the occurrence of a residual compressive strain at the heterostructure interface. By comparing this interface strain to the corresponding surface value of the same samples the occurrence of an inhomogeneous strain relaxation along the growth direction is clearly demonstrated. It is shown that such a strain gradient should be entirely ascribed to threading dislocations occurring into the ZnTe epilayers, their distribution being strictly correlated to the amount of residual strain along the epilayer growth direction. The conclusions are further supported by the analysis of the ZnTe surface strain, whose dependence on the epilayer thickness is consistent with that expected on the basis of a phenomenological model for the epilayer residual strain relaxation by threading dislocations. © 1995 American Institute of Physics.

## I. INTRODUCTION

The study of the structural properties of highly lattice mismatched heterostructures is one of the major issues of current researches in the field of the epitaxial growth for both fundamental and technological reasons. Solid-state devices for optoelectronics applications such as light-emitting diodes and lasers based on both III-V and II-VI compound epitaxial heterostructures require the growth of high-crystalline-quality materials on either GaAs or Si substrates. These substrates are preferred as they are available in large single-crystalline wafers, a key feature for the mass industrial production of devices. However, the large lattice and thermal mismatches involved by these materials lead to the generation of a high density of extended defects at the heterostructure interfaces and into the epitaxial layers, which can act as non-radiative recombination centers, thus rapidly degrading the device properties. It is therefore important to investigate the

mechanisms of plastic deformation through which extended defects are generated and propagate into these heterostructures.

It is well known that the growth of a pseudomorphic layer onto a crystalline substrate allows the elastic accommodation of the lattice misfit by matching the materials lattice parameters at the heterostructure interface. In the case of a cubic material grown on the surface of a (100)-oriented substrate the epilayer is tetragonally distorted. Moreover, in the elastic regime the energy stored in the epilayer is proportional to its thickness such that, beyond a certain critical thickness, the generation of extended defects at or close to the heterostructure interface becomes energetically favorable. As the growth proceeds beyond this critical value the epilayer plastic relaxation occurs by the generation of new defects bringing the epilayer to a progressively relaxed state. For heterostructures whose lattice mismatches are well below 1%, the equilibrium model of Matthews and Blakeslee<sup>1</sup> predicts, in most cases with good approximation, the value of the epilayer critical thickness and the strain relaxation rate as a function of epilayer thickness. The model assumes that the

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lattice misfit is relaxed by the generation of a network of noninteracting misfit dislocations (MDs) at the interface. However, in the case of highly mismatched heterostructures (i.e., whose misfit is above 1%) the density of MDs required to relax the initial lattice mismatch is so high that dislocation interaction cannot be neglected. It has been suggested that dislocation interaction<sup>2</sup> and/or work hardening<sup>3</sup> effects could give rise to much lower relaxation rates of the epilayer lattice with respect to the prediction of the Matthews and Blakeslee model. However, the generation of MDs is not the only mechanism that can relax strain. In highly mismatched systems a three-dimensional (3D) nucleation could occur at the beginning of the epilayer growth (Volmer–Weber growth mode) or immediately after the critical thickness has been reached (Stranski–Krastanov growth mode), the consequent 3D islanding being then important for the generation of further defects at the heterostructure interface as well as into the epilayer. These defects can in turn act as sources of plastic relaxation for the epilayers; however, the precise mechanisms by which these defects are generated into the epilayers, their nature, and role on the strain relaxation are all not well understood at present.

This article deals with the structural characterization of ZnTe epilayers grown on (100)GaAs substrates. The epitaxial growth of high-crystalline-quality ZnTe layers on GaAs has attracted much efforts in the last few years due to its large number of applications, ranging from the fabrication of blue-green light-emitting devices to the growth of buffer layers in the epitaxy of CdTe,  $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$ , and  $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$  on GaAs substrates. Optimal growth temperatures for molecular-beam epitaxy and metalorganic vapor-phase epitaxy (MOVPE) growth of ZnTe are in the 300–350 °C range,<sup>4,5</sup> giving rise to a lattice mismatch for the ZnTe/(100)GaAs heterostructure  $\sim -7.4\%$ . In a previous letter,<sup>6</sup> we showed by ion-channeling Rutherford backscattering spectrometry (RBS) measurements that relatively thick ZnTe epilayers can still exhibit some residual compressive strain resulting from the superposition of the expected tensile (thermal) strain and a thickness-dependent compressive strain. In Ref. 6 we also demonstrated that the residual compressive strain relaxation of the ZnTe layers proceeds at a slower rate than the one predicted by the equilibrium model. However, no definite conclusions were stated concerning the nature and distribution of the defects responsible of the observed strain relaxation.

In this article we report new results concerning the extended defects occurring at the ZnTe/GaAs heterointerface as well as into the ZnTe epilayers. To this purpose, MOVPE-grown ZnTe/GaAs samples were characterized by both high-resolution and conventional electron microscopy observations and ion-channeling measurements. This allowed us to precisely identify the defects occurring into the ZnTe/GaAs samples and to correlate their distribution with the measured amount of residual strain in the same samples. The contribution of each type of defects to the overall lattice strain relaxation is thus discussed, finally ascribing the observed residual strain relaxation to the occurrence of threading dislocations (TDs) into the epilayers. Our conclusions are

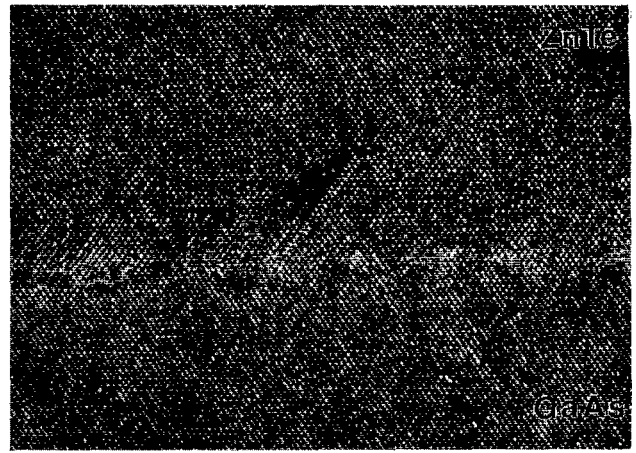


FIG. 1. Typical HRTEM micrograph of a ZnTe/GaAs interface. Bright contrast regions associated with the misfit dislocation cores can be easily identified along the interface line.

further supported by a phenomenological model for the relaxation of strain by TDs in highly mismatched heterostructures.

## II. EXPERIMENT

The present ZnTe epilayers were grown on (100)GaAs substrates by atmospheric-pressure MOVPE, using electronic grade diisopropyl-telluride and dimethyl-zinc as metalorganic precursors, the growth temperature being fixed at 350 °C.<sup>5</sup> The GaAs substrates were  $(100) \pm 0.50^\circ$  oriented and of semi-insulating (resistivity  $>10^7 \Omega \text{ cm}$ ) type. Immediately before the introduction into the reactor chamber, the GaAs substrates were etch treated with a  $\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2:\text{H}_2\text{O}$  solution as specified in Ref. 5, thoroughly cleaned with 18.2 M $\Omega$  de-ionized water and then dried under  $\text{N}_2$  flow. Also, an *in situ* thermal treatment of the substrates was performed in the growth chamber at 460 °C under  $\text{H}_2$  flow. Several samples whose ZnTe thickness ranged between 80 nm and 3.0  $\mu\text{m}$  were grown for the present work at a growth rate of 2.1  $\mu\text{m/h}$ .

Both conventional (TEM) and high-resolution (HRTEM) transmission electron microscopy observations were performed on ZnTe/GaAs sample cross sections by using a Philips EM430ST microscope at a nominal 300 kV accelerating voltage. To this purpose, the samples were thinned by the  $\text{Ar}^+$  milling technique.

Rutherford backscattering spectrometry (RBS) measurements in both random and channeling geometry were performed on the ZnTe/GaAs samples by using a 2.0 MeV  $^4\text{He}^+$  beam, delivered from the AN2000 accelerator of Laboratori Nazionali di Legnaro.

## III. RESULTS

Figure 1 shows a HRTEM micrograph of a ZnTe/GaAs cross section imaged along a  $\langle 110 \rangle$  zone axis. The heteroepitaxial interface can be readily identified in the micrograph by the bright contrast regions associated to the MD cores along the interface. These dislocations remove half-planes on the ZnTe side of the interface as expected for the lattice-mismatch relaxation of the ZnTe/GaAs heterostructure. In-

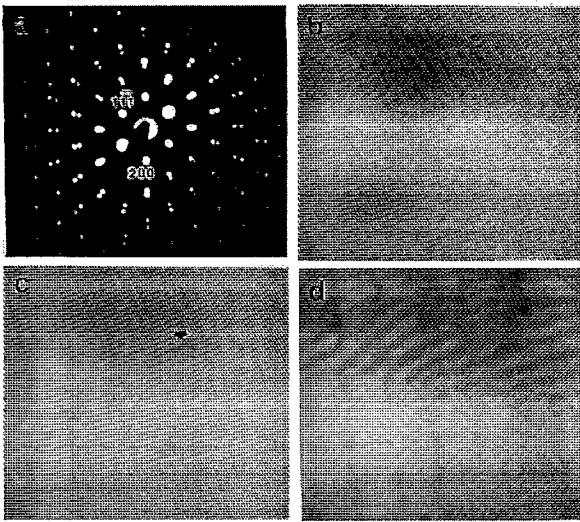


FIG. 2. The results of the FFT filtering method applied to the HRTEM micrograph in Fig. 1 are shown. The digitized images were obtained by selecting different diffraction spots in the FFT pattern. In (a) the corresponding  $\langle 110 \rangle$  zone axis diffraction pattern is shown for comparison. The selected diffraction pattern for each digitized image is: (b) (002), (002), (111), (111), (111), and (111); (c) (111) and (111); (d) (111) and (111). Images (c) and (d) are used to identify GaAs half-planes terminating at the interface along opposite  $\{111\}$  glide directions. The arrow in (c) shows a  $60^\circ$ -mixed dissociated dislocation.

deed, electron-diffraction patterns of the interface region [see Fig. 2(a)] result from the superposition of diffraction patterns belonging to ZnTe and GaAs crystals having different lattice parameters. Moreover, the occurrence of a stacking fault terminating at the ZnTe/GaAs interface is shown in the HRTEM micrograph, indicating that partial dislocations are present at the interface along with perfect ones.

In order to perform a precise structural characterization of MDs, HRTEM images of the ZnTe/GaAs interface were digitized and their fast Fourier transform (FFT) obtained. By selecting different diffraction spots of the FFT pattern, a filtered digitized image of the interface region can be obtained after inverse transformation. Figures 2(b), 2(c), and 2(d) show the result of the FFT image filtering method when applied to the HRTEM micrograph presented in Fig. 1. In particular, Figs. 2(c) and 2(d) were obtained by selecting diffraction spots corresponding to symmetric  $\{111\}$  glide planes with respect to the interface. Therefore, GaAs half-planes parallel to these glide directions terminating at the interface can be easily identified. When two such planes end at the same point a pure edge Lomer dislocation occurs at that point, whereas a single half-plane indicates the presence of a  $60^\circ$ -mixed dislocation.<sup>7</sup> Filtered HRTEM images of our samples show that both pure edge Lomer and  $60^\circ$ -mixed dislocations occur at the ZnTe/GaAs interface. Also, a few partial dislocations can seldomly be identified at the interface and into the ZnTe epilayer, as indicated in Fig. 2(c). These partials are clearly associated to the stacking faults observed in the HRTEM micrographs, possibly resulting from the dissociation of a  $60^\circ$ -mixed dislocation into two Schokley and/or Frank partial dislocations.<sup>7,8</sup> We estimate that only about 1% of all interface dislocations are of partial type, in fairly good agreement with Ref. 8. Therefore, only Lomer

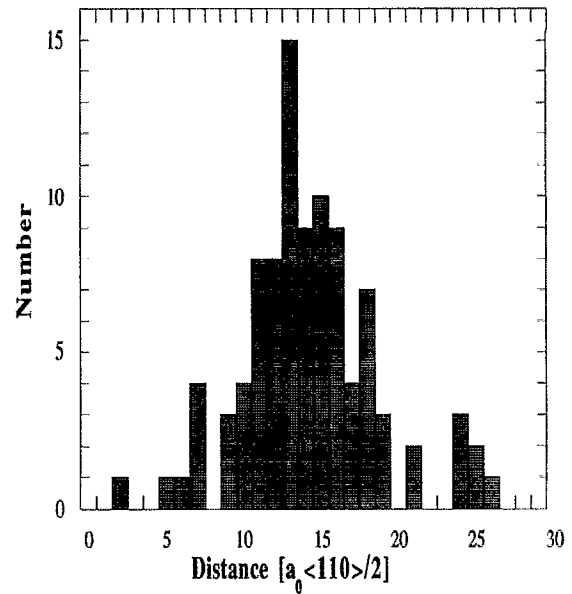


FIG. 3. Histogram of the distance distribution (in units of  $a_0\langle 110 \rangle/2$ ) between GaAs  $\{111\}$  half-planes lying along the same glide direction which terminates at the ZnTe/GaAs interface.

and  $60^\circ$  mixed dislocations effectively contribute to the interface misfit relaxation.

Each Lomer dislocation can be considered as the sum of two  $60^\circ$ -mixed dislocations having different edge components,<sup>7</sup> such that the entire MD distribution can be regarded as equivalent to a set of  $60^\circ$ -mixed dislocations whose edge component have only two possible values. The distances between adjacent  $60^\circ$ -mixed dislocations with equal edge components can be measured by taking successive GaAs  $\{111\}$  half-planes terminating at the interface along the same glide direction. This procedure allows one to precisely determine the distance distributions of  $60^\circ$ -mixed dislocations along both glide directions. These distributions turn out to be practically identical, therefore the overall distribution obtained by combining both sets of data can be considered for a better statistics. Figure 3 shows the result obtained from the HRTEM analysis of a 300-nm-wide interface region of a 486-nm-thick ZnTe epilayer. It appears that the dislocation separation follows a Gaussian distribution, whose average value in units of  $a_0\langle 110 \rangle/2$  (where  $a_0$  is the GaAs lattice parameter) is  $14.2 \pm 0.4$ . This gives an equivalent  $60^\circ$ -mixed dislocation density  $\sim 1.76 \times 10^6 \text{ cm}^{-1}$ .

The value of the MD average spacing can be used to derive the amount of residual in-plane lattice strain  $\epsilon_{\parallel}$  at the interface. The relationship between  $\epsilon_{\parallel}$  and the MD contribution to the relaxation of the misfit  $f$  is given by

$$f = \epsilon_{\parallel} + \frac{b_{\text{eff}}}{d}, \quad (1)$$

where  $b_{\text{eff}}$  is the edge component of the MD Burgers vector parallel to the interface and  $d$  is the average MD distance. For the 486-nm-thick epilayer, Eq. (1) gives a MD contribution to the lattice misfit relaxation of  $-(7.05 \pm 0.22)\%$ , the misfit value at the actual growth temperature (estimated to be  $613 \pm 10 \text{ K}$ ) being  $f = -7.45\%$ . Therefore, the interfacial re-

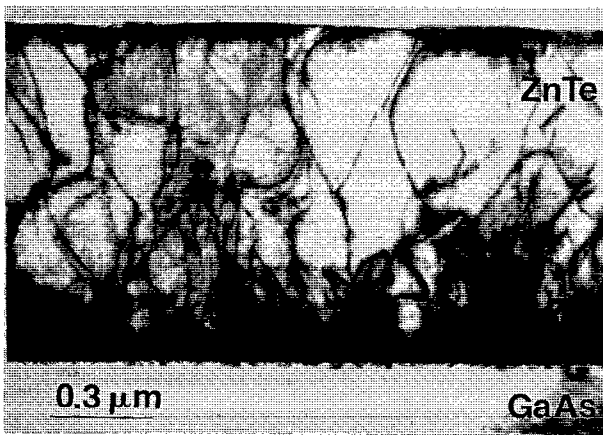


FIG. 4. Bright-field TEM micrograph of a 1.0- $\mu\text{m}$ -thick ZnTe/GaAs sample cross section observed along the  $\langle 110 \rangle$  zone axis. Dark contrast regions reveal the spatial distribution of extended defects into the ZnTe epilayer.

sidual in-plane lattice strain at the growth temperature is  $\epsilon_{\parallel} = -(0.40 \pm 0.22)\%$ . This value differs from the corresponding surface residual in-plane strain as previously determined for the same sample by reflectance spectroscopy and ion-channeling measurements,<sup>6</sup> the latter being  $-(0.07 \pm 0.03)\%$ , thus clearly pointing out that a strain gradient occurs into the ZnTe epilayer.

Moreover, considering that our ion-channeling strain measurement was obtained from the epilayer surface region (around 200 nm thick) and taking into account the epilayer thickness (486 nm), most of the residual in-plane strain difference (about 0.33%) occurring between the epilayer surface and the interface should relax in an almost 300-nm-thick region close to the ZnTe/GaAs interface. This indicates that extended defects different from MDs at the interface must occur into the ZnTe epilayers, thus contributing to the overall ZnTe lattice relaxation. In this respect, although the presence of stacking faults at the interface could contribute to such strain relaxation through the occurrence of partial dislocations (typically of Shockley type<sup>7</sup>) into the epilayer, their relatively low density cannot account for the observed 0.33% strain relaxation above. Indeed, we estimate that if only 30° Shockley partial dislocations occur into the epilayer, as in the case of extrinsic<sup>9</sup> stacking faults, these partials cannot relax more strain than  $b_{\text{eff}}\delta_{\text{sf}} \approx 0.03\%$  (where  $b_{\text{eff}}$  is the Burgers vector edge component parallel to the interface of the 30° Shockley partial dislocation and  $\delta_{\text{sf}} \approx 1.8 \times 10^4 \text{ cm}^{-1}$  is the linear density of stacking faults along the interface), whereas if only 90° Shockley partials associated to intrinsic<sup>9</sup> stacking faults are taken into account the corresponding contribution to the lattice relaxation is less than 0.06%. Therefore, other types of defects should occur into the epilayer to account for the 0.33% strain relaxation.

Figure 4 shows a bright-field micrograph of a ZnTe/GaAs sample cross section viewed along one of the  $\langle 110 \rangle$  zone axis. The occurrence of a high density of extended defects into the ZnTe epilayer can be inferred by the presence of dark contrast regions in the micrograph. Although a quantitative estimate of the defect distribution close to the interface cannot be afforded by TEM observations, it appears that

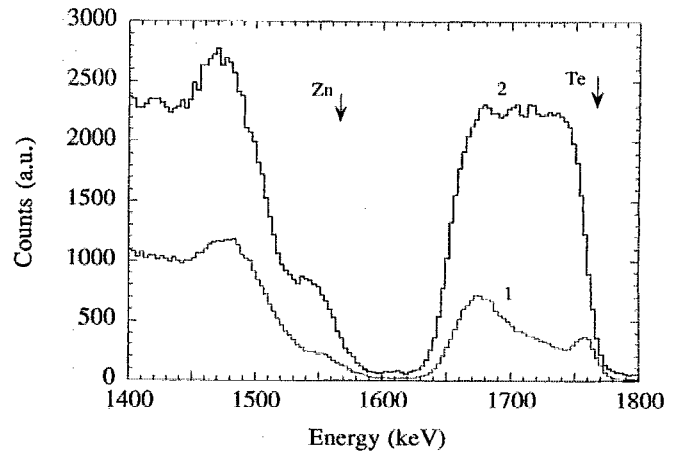


FIG. 5. 2.0 MeV  $^4\text{He}^+$  beam RBS spectra in (1)  $[100]$  aligned and (2) random geometry are shown for a 182-nm-thick ZnTe epilayer.

their density varies within the epilayer, such that a  $\sim 300$ -nm-thick strongly defected region close to the interface is observed. Within this defected region a highly defected zone, extending for about 100 nm or less from the interface, can be further identified. Finally, a residual distribution of threading dislocations (TDs) is found into epilayer regions far from the interface, their density being lower than the overall defect density observed within 300 nm from the interface and slowly decreasing towards the epilayer surface. In the case of a 1- $\mu\text{m}$ -thick epilayer the density of TDs below the ZnTe surface was estimated to be  $\sim 10^9 \text{ cm}^{-2}$ .

A quantitative appreciation of the defect distribution close to the heterostructure interface was obtained by the ion-dechanneling analysis of RBS spectra recorded from samples having ZnTe layer thickness below 300 nm. Figure 5 shows the  $[100]$ -aligned and the random RBS spectra of a 182-nm-thick ZnTe/GaAs sample. The aligned spectrum shows a fairly strong increase in the dechanneling rate with increasing the beam penetration depth into the ZnTe layer, indicating that a highly defected region is present close to the ZnTe/GaAs interface. For epilayer thicknesses below about 300 nm, the Te signal in the RBS spectra is well separated from the Zn as well as from the Ga and As ones, allowing us to analyze the epilayer dechanneling rate without spurious effects due to RBS signal overlapping. Thus, useful informations can be obtained on the distribution and evolution of the defects occurring into the ZnTe epilayers by comparing the epilayer normalized channeling yield  $\chi_D$  (i.e., the  $[100]$ -aligned RBS yield normalized to the random yield) to the corresponding yield  $\chi_V$  of a perfect crystal. To this purpose, the dechanneling probability<sup>10</sup>

$$P_D(z) = \ln \left( \frac{1 - \chi_V(z)}{1 - \chi_D(z)} \right) \quad (2)$$

can be used, where  $z$  is the distance from the ZnTe surface. Although our TEM observations show that TDs occur below the ZnTe surface even for relatively thick epilayers, we found<sup>6</sup> that the values of the minimum yield  $\chi_{\text{min}}$  (i.e., the  $[100]$ -aligned yield behind the Te surface peak) measured for epilayers thicker than 300 nm compare well with the semi-empirical estimate expected for an ideal ZnTe crystal. This

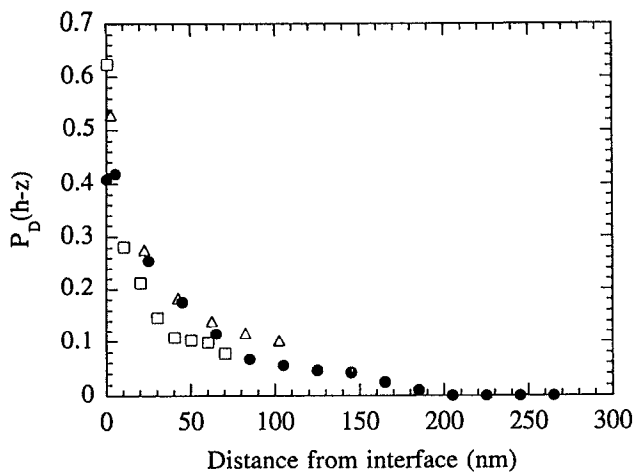


FIG. 6. Dechanneling probability as a function of the distance from the ZnTe/GaAs interface for three epilayers of different thicknesses, namely: (□) 80 nm; (△) 182 nm and (●) 285 nm.

fact indicates that the dechanneling caused by TDs is low so that in our calculations we assumed  $\chi_V(z)$  to coincide with the normalized yield of a 3.0- $\mu\text{m}$ -thick epilayer.

In Fig. 6 the values of  $P_D(h-z)$  are shown as a function of the distance from the ZnTe/GaAs interface for three samples whose thicknesses  $h$  are 80, 182, and 285 nm. At any distance from the interface no distinctive evolution of the dechanneling probability with increasing the sample thickness appears from our data. Moreover, two different regions can be distinguished in the  $P_D(z)$  profile for all of the analyzed samples. In the first region, extending up to about 60 nm from the interface, a sharp decrease of the dechanneling probability with increasing the distance from the interface can be observed, whereas a much slower decrease of  $P_D(z)$  is observed between about 60 and 200 nm from the interface (second region). As the derivative of the dechanneling probability is proportional to the local defect concentration in the layer, the above result points out that most of the defects occurring into the ZnTe epilayers are located in a  $\sim 60$ -nm-thick region close to the interface and that outside this region their density slowly decreases toward the epilayer surface, also qualitatively in accordance with our TEM observations. In this respect the integral dechanneling probability, i.e., the value of the area below  $P_D(h-z)$ ,<sup>10</sup> calculated in the first highly defected region of the epilayers, turns out to be constant (within the experimental uncertainties) for all of the analyzed samples, although a slight increase of the width of the high dechanneling region is observed with increasing the epilayer thickness. Finally, the apparent lack of further increase of the total disorder obtained when integrating the  $P_D(h-z)$  profile over 200 nm or more from the interface can be only ascribed to the approximation used in Eq. (2), where the normalized yield of a thick ZnTe epilayer has been substituted for the actual  $\chi_V(z)$ .

#### IV. DISCUSSION

In the previous section we pointed out the occurrence of a strain gradient into the ZnTe epilayers, suggesting that part of the observed interface residual lattice strain is actually

relaxed by extended defects generated into the ZnTe lattice. An inhomogeneous strain relaxation along the growth direction of thin (below  $\sim 10$  nm) ZnTe epilayers on (100)GaAs was reported by Patrat *et al.*<sup>11</sup> and Etgens *et al.*;<sup>12</sup> however, this effect was attributed to the free surface elastic deformation of ZnTe islands resulting from 3D nucleation after the critical thickness of ZnTe epilayers on (100)GaAs is exceeded.<sup>12</sup> On the contrary, the strain gradient measured in our relatively thick samples can only be ascribed to plastic relaxation. Indeed, the presence of an inhomogeneous distribution of defects close to the heterostructure interface was observed by TEM observations. Moreover, most of the measured excess strain between the epilayer surface and the heterostructure interface appears to relax within about 300 nm from the interface, where the highest concentration of these defects can be observed by both TEM and ion-channeling measurements, further confirming their role in the ZnTe strain relaxation. It is also important to point out that the interface residual strain value obtained from the HRTEM analysis of the MD distribution for the 486-nm-thick sample of Fig. 1 coincides, within the experimental error, with values reported in the literature<sup>7,8</sup> for thicker (around 2  $\mu\text{m}$ ) ZnTe epilayers, suggesting that after the growth of a layer a few tenths of a micron thick, interfacial defects no longer contribute to the epilayer strain relaxation. MD interaction<sup>2</sup> and/or work hardening<sup>3</sup> involved by the relatively high dislocation densities at the ZnTe/GaAs interface could well explain this effect.

The occurrence of a 3D nucleation during the early stages of growth is still expected in our samples. Indeed, surface reflection high-energy electron-diffraction patterns taken along the  $\langle 110 \rangle$  zone axis of thin ZnTe epilayers are invariably spotty,<sup>5</sup> this feature being currently considered as a signature of the 3D epitaxial growth mode. As the growth proceeds beyond the onset of 3D nucleation, segments of misfit dislocations form at the interface between the islands and the substrate as a consequence of the ZnTe lattice relaxation.<sup>12</sup> A substantial part of the initial lattice misfit turns out to be relaxed for  $\sim 25$ -nm-thick ZnTe epilayers,<sup>11</sup> giving rise to the high misfit dislocation density observed at the interface. At this stage, interaction between segments of misfit dislocations can result into the generation of a dense network of TDs, some of which propagate into the epilayer. Also, TDs could be generated into epilayer regions close to the heterostructure interface as the coalescence of adjacent islands takes place. Indeed, the occurrence of TDs into the ZnTe epilayers appears from the cross-section TEM observations of our samples.

Although our ion-channeling measurements confirm that an inhomogeneous distribution of defects occurs within 300 nm from the interface, the identification of these defects as being TDs only is not straightforward, in consideration of their expected low ion-dechanneling efficiency. For instance, the high dechanneling yield observed within 60 nm from the ZnTe/GaAs interface (the first highly defected region of Sec. III) could also be ascribed, at least partly, to the high density of dislocations at the interface. In fact, the lattice deformation field they induce extends also into the epilayer. In any case, the amount of dechanneling occurring within  $\sim 60$  nm

from the interface does not change by increasing the epilayer thickness, indicating that no further defects are generated in this region when the epilayer grows thicker. On the contrary, beyond the 60-nm-thick region, the dechanneling rate indicates that further defects occur in the epilayers, whose density slowly decreases by increasing the distance from the heterostructure interface.

The decreasing density of TDs with increasing the distance from the interface strongly suggests that these defects play a role in relaxing the ZnTe epilayer residual strain. A phenomenological model describing the residual strain relaxation of highly mismatched heterostructures by TDs occurring into the epilayers was recently proposed by Durose and Tatsuoka.<sup>13</sup> The model correlates the epilayer residual strain gradient along the growth direction to the inhomogeneous distribution of TDs along the same direction. It considers that as a TD inclined with respect to the growth direction passes through each monolayer, its contribution to the monolayer strain relaxation can be taken as that of a misfit dislocation segment having the same effective Burgers vector  $b_{\text{eff}}$  of the TD and a length equal to the projected length  $l$  (in unit of length) of the TD on the (100) plane. Therefore  $l/l$  dislocations that thread the same monolayer equal one misfit dislocation and the total number of equivalent misfit dislocations per unit length in the  $n$ th monolayer is  $N_n = lD_n/2$ , where  $D_n$  is the areal density of TDs in the monolayer. The amount of residual strain occurring in the  $(n+1)$ th monolayer is therefore

$$\epsilon_{n+1} = \epsilon_n - N_n b_{\text{eff}}. \quad (3)$$

Following Durose and Tatsuoka<sup>13</sup> we assume  $N_n$  as being proportional to the amount of residual strain in the  $n$ th monolayer,

$$N_n = A \epsilon_n, \quad (4)$$

where  $A$  is a suitable constant. Combining Eqs. (3) and (4) gives for the residual strain in the  $n$ th monolayer

$$\epsilon_n = \epsilon_1 (1 - A b_{\text{eff}})^{n-1} \approx \epsilon_1 (1 - A b_{\text{eff}})^n, \quad (5)$$

where  $\epsilon_1$  is the residual lattice strain at the interface. Finally, writing Eq. (5) in terms of the epilayer thickness gives for the surface residual parallel strain of the epilayer

$$\epsilon_{\parallel}(h) = \epsilon_1 (1 - A b_{\text{eff}})^{2h/a_0}, \quad (6)$$

where  $a_0$  is the bulk lattice parameter of the epilayer. Equation (6) predicts that  $\ln(\epsilon_{\parallel})$  is a linearly decreasing function of the epilayer thickness.

Figure 7 shows the values of the surface residual parallel strain  $\epsilon_{\parallel}$  obtained by ion-channeling measurements as a function of the ZnTe epilayer thickness.<sup>6</sup> Below  $\sim 0.5 \mu\text{m}$  our strain data closely follow the expected  $\ln(\epsilon_{\parallel})$  vs  $h$  dependence, whereas a marked departure appears for thicker layers. The use of Eq. (6) for the best fit of strain data belonging to epilayers thinner than 500 nm gives  $\epsilon_1 = (0.227 \pm 0.012)\%$  and  $A b_{\text{eff}} = (7.79 \pm 0.83) \times 10^{-4}$ . It is noteworthy that our HRTEM-derived value of the residual interface strain [i.e.,  $(0.40 \pm 0.22)\%$ ] coincides fairly well, within its experimental uncertainties, with the best-fit value of  $\epsilon_1$  above. Furthermore, our value of  $A b_{\text{eff}}$  approaches (within about a factor 2)

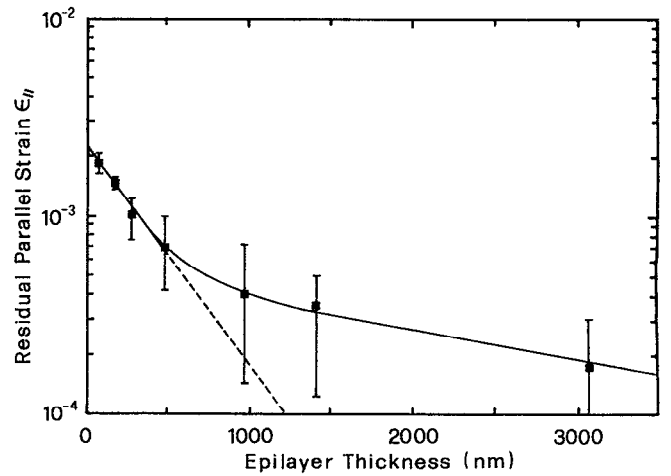


FIG. 7. Values of the epilayer surface residual in-plane strain  $\epsilon_{\parallel}$  obtained from ion-channeling measurements (see Ref. 4) are shown, along with their experimental uncertainties, as a function of the ZnTe thickness. The dashed line represents the result of the best fit of strain data belonging to epilayers thinner than 500 nm with Eq. (6). The solid line is only a guide for the eyes.

the  $3.8 \times 10^{-4}$  value reported by Durose and Tatsuoka<sup>13</sup> for MOVPE-grown ZnTe/GaAs heterostructures, the latter being obtained by cross-section TEM observations of the TD fall-off along the [100] growth direction. These numeric consistencies support our assumption that TDs are responsible for the ZnTe residual strain relaxation, although this relaxation mechanisms seems to hold only for epilayers thinner than  $\sim 500$  nm. For thicker layers the relaxation rate slows down markedly until for epilayer thicknesses around  $\sim 3 \mu\text{m}$  the ZnTe lattice appears substantially relaxed. Interestingly, such a lower relaxation rate belongs to regions of the epilayers far from the interface where an approximately constant density of TDs was observed by TEM. As the residual strain into the epilayers is the driving force of the TD annihilation in the model of Durose and Tatsuoka, a constant background density of TDs is indeed expected for nearly relaxed layers, in further agreement with our conclusions.

## V. CONCLUSIONS

We reported on a detailed interface structural characterization of ZnTe epilayers grown on (100)GaAs by atmospheric-pressure MOVPE. The ZnTe/GaAs heterostructures were characterized by both conventional and high-resolution TEM observations as well as by RBS measurements in channeling conditions. MDs were observed at the interface by HRTEM and identified as Lomer and  $60^\circ$ -mixed dislocations after FFT digital image filtering of the HRTEM micrographs. In a few cases partial dislocations were also identified at the interface, bounding stacking faults occurring into the ZnTe epilayers, the latter possibly resulting from the dissociation of  $60^\circ$ -mixed dislocations. In order to derive the amount of ZnTe residual lattice strain at the interface, a statistical analysis of the distance distribution between equivalent  $60^\circ$ -mixed dislocation cores was performed. By comparing the interface residual strain with the corresponding ZnTe surface value, the occurrence of a strain gradient into the epilayers was clearly demonstrated for the first time. More-

over, most of the excess strain appeared to relax within about 300 nm from the interface, where both TDs and stacking faults occur. We proved that the stacking fault contribution to the strain relaxation is negligible, suggesting that the epilayer strain gradient should be entirely ascribed to the presence of TDs into the ZnTe. Indeed, most of the TDs were found close to the ZnTe/GaAs interface, their distribution being rather inhomogeneous and strictly correlated to the amount of residual strain relaxation along the epilayer growth direction. This conclusion is further supported by the analysis of the epilayer surface strain whose dependence on the epilayer thickness is consistent with what expected on the basis of a phenomenological model for the residual strain relaxation of highly mismatched heterostructures by TDs.

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