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Formation of misfit dislocations during Zn-diffusion-induced intermixing of a GaInAsP/InP heterostructure

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The microstructural degradation of a lattice-matched $Ga_{0.28}In_{0.72}As_{0.61}P_{0.39}$/InP heterointerface induced by Zn diffusion has been investigated using transmission electron microscopy. The localized interfacial stress caused by intermixing appears to create stacking faults in the Ga-mixed InP substrate, and dislocation tangles in the In-mixed GaInAsP layer. The observed results are attributed to the contrasted effect of tensile and compressive stresses upon the nucleation of dislocations from both sides of the GaInAsP/GaInP interface. As an evidence of the interface nucleation, we find a stacking fault at the tensile interface, which is bounded by a pair of partials having opposite Burgers vectors. A model is proposed to explain the strain relaxation in the intermixed region in terms of nucleation and splitting mechanisms of the paired dislocations.

Formation of misfit dislocations at semiconductor interfaces has been a subject of active studies in recent years. The subject has been of particular concern not only for lattice-mismatched heterostructure systems[1] such as GaAs/Si, InGaAs/GaAs, and SiGe/Si, but also for lattice-matched systems in which thermal processing can cause severe intermixing of the layers. The intermixing becomes prominent especially in the presence of impurities and such phenomenon is well documented in the studies of III-V compound semiconductors.[2] Although the destruction of the interface caused by layer mixing is a critical problem in achieving reliable device operations in GaInAsP/InP and InGaAs/InP systems, little effort has been made in the microstructural study of the intermixing process in such systems. In a recent study of transmission electron microscopy (TEM) for a Zn-diffused InGaAs/InP superlattice,[3] it was shown that the intermixing-induced stress can be accommodated by lattice strain without generating misfit dislocations.

In this letter we report on the observation of microstructural degradation of the interface caused by Zn diffusion in a lattice-matched GaInAsP/InP heterostructure. We show, using TEM, that misfit dislocations are generated in the mixed region in varying formations. We also present the features of the dislocations formed at a locally stressed interface.

An undoped $Ga_{0.28}In_{0.72}As_{0.61}P_{0.39}$ epitaxial layer was grown on a S-doped (6×10^{18} cm^{-3}) (001) InP substrate using the liquid-phase epitaxy (LPE) technique as described elsewhere.[4] Prior to the growth of the quaternary layer (1 μm thickness), an undoped InP buffer layer (3 μm thickness) was grown to reduce the influence of predoped S in the substrate upon alloy mixing. Zn diffusion was performed at 600 °C for 1 h in an evacuated silica ampule employing a sintered mixture of Zn_3P_2, InP, and GaAs as diffusion sources. The transmission electron microscopy study was performed for both as-grown and Zn-diffused samples. The samples were cleaved from an LPE-grown sample with a lattice mismatch of $\Delta a/a = -0.08\%$. The samples were examined in a JEOL 2000 EX TEM operating at 200 kV.

Figure 1 shows a set of cross-sectional TEM micrographs of the as-grown [Fig. 1(a)] and Zn-diffused [Fig. 1(b)] samples. The images were taken with an electron beam along the [110] axis. In the as-grown sample, no notable defects such as dislocations or planar defects are observed either in the GaInAsP layer or in the interfacial region of the substrate. (The dark spots scattered on the substrate side are images of indium droplets,[5] which are believed to have formed due to a higher etching rate of phosphorous components during Ar$^+$ ion milling for TEM sample preparation.) In the Zn-diffused sample shown in Fig. 1(b), the crystal around the GaInAsP/substrate interface is heavily destroyed in varying defect formations on both sides of the interface. The Zn diffusion promotes exclusive Ga-In interdiffusion, leaving an abrupt junction for As and P components.[4] Thus, it causes tensile stress in the Ga-mixed InP substrate and compressive stress in the In-mixed quaternary layer.[3] In the tensile region of the Fig. 1(b) sample, a number of stacking faults are grown from the interface. The image of stacking faults at higher magnification is shown in Fig. 2, which displays faults grown on different {111} planes from the interface into the GaInP side. Most of the faults were found in the form of bundles. In the compressive region, no stacking faults are observed. Instead, dislocation tangles are formed nearly parallel to the interface at a distance. The dislocation tangles might be formed to accommodate another misfit boundary at the front of the intermixed region in the quaternary layer. The extent of damages in the interfacial region in Fig. 1(b) is consistent with the depth of interdiffusion measured from Auger electron spectroscopy profiles as reported in the previous work.[4]

We investigated the degree of lattice mismatch at the

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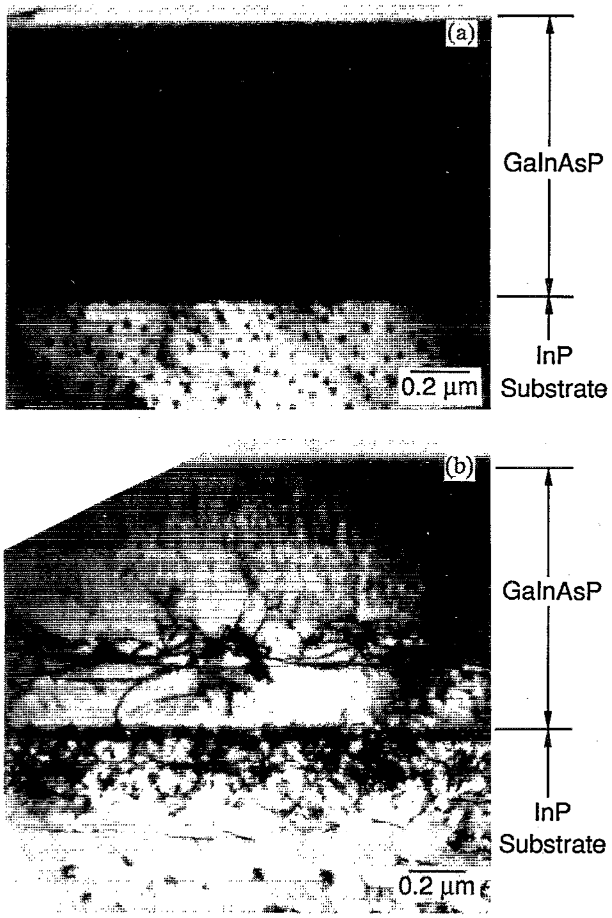

FIG. 1. Cross-sectional TEM images of (a) as-grown and (b) Zn-diffused (600 °C, 1 h) GaInAsP/InP heterostructures. After Zn diffusion, the interface region appears to be heavily destroyed due to intermixing, generating stacking faults on the substrate side and dislocation tangles on the GaInAsP side.

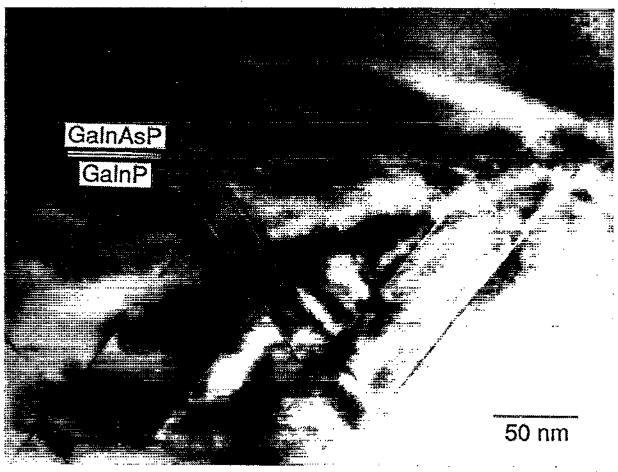

FIG. 2. A magnified view of the interfacial region of Fig. 1(b) showing stacking fault bundles grown on {111} planes into the InP substrate side.

GaInAsP/GaInP heterojunction. From the measurement of average lattice spacings near the junction in the high-resolution lattice images, it was learned that the lattice spacing of the GaInAsP side is 1.6±0.3% greater than the GaInP side along the interface ([$\bar{1}$10] direction). This misfit is that which is accommodated by the dislocations aligned on the junction. The lattice images showed also a distortion to the vertical direction ([001]), indicating a residual strain. Using the data of lattice spacings in the vertical direction and counting the Poisson effect[6,7] on the biaxial lattice deformation, the mismatch of bulk lattice parameters, i.e., a net mismatch before strain relief, was estimated to be 2.9±0.5%.

The different dislocation patterns on both sides of the interface shown in Fig. 1(b) can be explained by the dependence of stress sign on the nucleation of Shockley partial components, as proposed by Maree *et al.*[1] In the gliding of two dissociated partials, i.e., 30° and 90° partials, the resolved shear stress on a {111} slip plane exerts different forces on these partials. In the tensile stress field, the 90° partial, which undergoes a smaller shear stress, nucleates first and the ensuing 30° partial, which requires a higher shear stress, nucleates belatedly, thus allowing extended propagation of a stacking fault. In the compressive stress field, the nucleation order of the partials is reversed, and the stacking fault formed by the first partial nucleation can be annihilated by immediate succession of the second partial, thus forming a 60°-type perfect dislocation. The 60° dislocations usually take the shape of curved lines during their gliding by the cross slip on different {111} planes.[1] The effects of the stress sign on the dislocation morphology have been widely reported in the epitaxial growth of various tensile or compressive films.[1,8] In our system too, as shown in Fig. 1(b), such effects obviously appear with contrast across the intermixed interface, where the stress sign is reversed.

However, since the misfit stress is localized around the mixed region in this system, the GaInAsP/GaInP interface is expected to be the nucleation site of the partials. This situation is in contrast to that of a growing thin film, in which case the film surface is a favorable nucleation site.[1] The homogeneous nucleation of dislocations inside a crystal produces paired dislocations with opposite Burgers vectors.[9] Thus, the nucleation and gliding of a leading 90° partial from the tensile interface entails the end of the fault as another 90° partial at the interface. Figure 3 shows a short single fault found at the interface, in which the Burgers circuit around the partials is completely closed, indicating that it is homogeneously nucleated. From the compressive interface, on the other hand, a pair of perfect dislocations of the 60° type may be generated by the stress field effect mentioned before. However, we could not find the paired 60° dislocations in the compressive side. Instead, in the tensile side we observed occasionally two 60° dislocations, which exist adjacently with opposite edge components. An example is seen in Fig. 3 (two 60° dislocations marked by arrows). These dislocations seem to be split afresh after the homogeneous nucleation, although the nucleation of perfect dislocations is unfavorable under a tensile stress field.

The paired dislocations, once nucleated from either compressive interface or tensile interface, are separated to relax interfacial strain, constituting appropriate configura-

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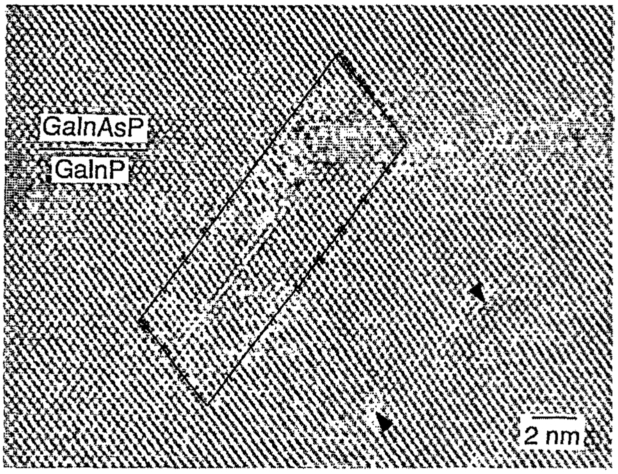

FIG. 3. A high-resolution TEM micrograph of a single stacking fault. The completely closed Burgers circuit on the transverse section indicates that the faults are homogeneously nucleated. Two 60° perfect dislocations which have opposite edge components are observed on the right side of the fault.

tions of the Burgers vectors, as illustrated in Fig. 4. Dislocations, marked as 2 and 3 in Fig. 4, which have extra half-planes aligned to the tensile side remain stable at the interface, and the opposite dislocations, marked as 1 and 4 in Fig. 4, are expelled from the interface. The actions of shear stresses inducing such splitting are depicted in Fig. 4. The dislocations released from the interface can nestle to the front of the intermixing region, accommodating the misfit stress existing at the front. The dislocation tangles found near the intermixing front in the compressive side in Fig. 1(b) are speculated to be formed by these dislocations.

We also observed sessile-type 90° (pure edge) dislocations on the GaInAsP/GaInP interface of the Fig. 1(b) sample. The extra half-planes of these dislocations were aligned to the tensile side in all. These dislocations comprised about 40% of total number of perfect dislocations located at the interface. The sessile edge dislocations might be produced by the reaction between two 60° dislocations during their gliding,[10] and be introduced by a climb process.[10] We expect that the climb reaction is very active during intermixing.[11] However, it should be noted here that the edge dislocation, produced from those 60° types (such as dislocation 1 or 4 in Fig. 4) which released from the interface, has an extra half-plane to the compressive side; thus, it should climb toward the intermixing front. The sessile edge dislocations observed at the interface might be supplied by the reaction between alternative 60° types which remained near the interface (such as dislocation 2 or 3 in Fig. 4) or which nucleated heterogeneously from pre-existing dislocations. We speculate that the climb reaction in this system takes place by the precipitation of interstitials, which may be generated by a kick-out mechanism.[2–4,11] The evidence to support the climb reaction or the diffusing species has not yet been observed in cross-sectional TEM. Further microstructural investigations are required for the study of diffusing species and their role on the dislocation generation.

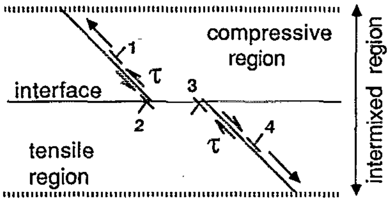

FIG. 4. Schematic sketch illustrating the nucleation and splitting of the paired dislocations from the tensile or compressive interface in the intermixed region.

In summary, the preliminary results we presented and discussed in this letter suggest several intriguing features for the formation of misfit dislocations in the intermixing layers. First, the interface dislocation nucleation is favorable due to the localized interfacial stress. Second, the rich formation of stacking faults in the tensile stress field and the virtually nonexistent stacking fault in the compressive stress field pose a strong contrast across the intermixed interface. Third, the apparently active atomic interdiffusion may promote dislocation climb processes.

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