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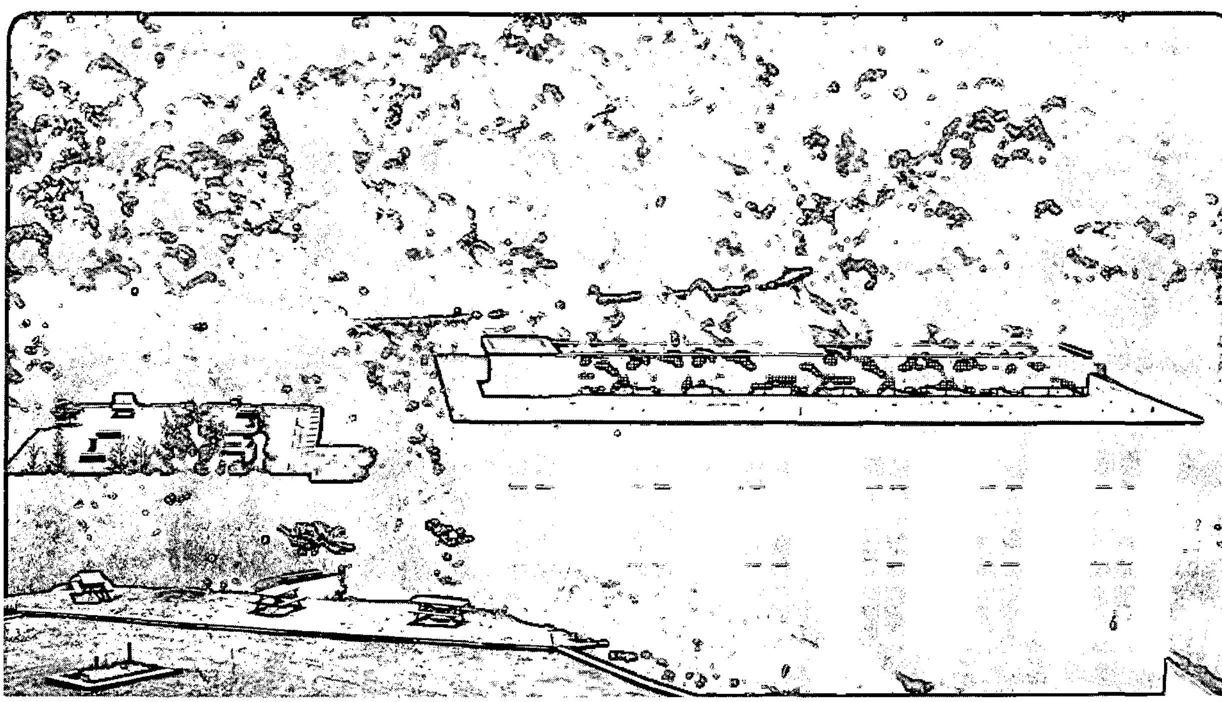

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REORIENTATION OF MISFIT DISLOCATIONS DURING ANNEALING IN InGaAs/GaAs(001) INTERFACES

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ABSTRACT

Transmission electron microscopy is applied to investigate the effect of post-annealing on misfit dislocations in an $In_{0.2}Ga_{0.8}As$/GaAs(001) heterostructure. An orthogonal array of 60° dislocations along [110] and [1$\bar{1}$0] directions was observed in the interfaces of the samples grown by MBE at 520 °C. When the as-grown samples were annealed at temperatures ranging from 600 to 800 °C, the 60° dislocations were gradually reoriented by dislocation reactions occurring at the 90° intersections followed by nonconservative motion driven by dislocation line tension and the residual elastic misfit strain. The final result of this process was a dislocation array lying along [100] and [010] directions. The reoriented **u** =<100> dislocation has a Burgers vector $\mathbf{b}=\frac{a}{2}\langle 101\rangle$, which is the same as that of 60° dislocation, but the edge component of its Burgers vector in the (001) interfacial plane is larger than that of 60° dislocation by a factor of $\sqrt{2}$, resulting in a greater contribution to elastic strain relaxation. This nonconservative reorientation of 60° dislocations to form the **u**=<100> dislocations represents a new strain relaxation mechanism in diamond or zinc blende semiconductor heterostructures.

INTRODUCTION

In the last decade, increasing research focus has been placed upon lattice mismatched semiconductor heterostructures in order to develop high-performance semiconductor devices.[1] The $In_xGa_{1-x}As$/GaAs system has received considerable attention as the band gap of $In_xGa_{1-x}As$ ranges from 0.36 to 1.35 eV. However the lattice mismatch (up to 7%) between the $In_xGa_{1-x}As$ and GaAs can result in misfit dislocations, which have a very deleterious effect on minority-carrier lifetimes and radiative recombination rates. When an epitaxial layer is grown upon a substrate with a different lattice parameter, at some epilayer thickness, generally called the critical thickness, h_c, it becomes energetically favorable to reduce elastic strain energy by introduction of misfit dislocations, which allow the epilayer to relax toward its free lattice parameter. In semiconductor lattices with a diamond or a zinc blende structure, for the interface with (001) orientation, the dislocations usually lie along <110> directions of lowest core energy and slip on {111} planes. The Burgers vectors for perfect misfit dislocations in these structures usually lie at angles of 60° or 90° with respect to the dislocation line and are of the type a/2<110>, where a is the lattice parameter. The 60° dislocation is only 50% effective at relieving lattice mismatch as the 90° dislocation, as only 50% of the magnitude of Burgers vector of 60° dislocation

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projects onto the interfacial plane.[2] However, the 60° dislocations are usually generated at first, since only the dislocation with the Burgers vector of 60° dislocation can glide into the (001) interface on {111} planes.[3] When they come in close proximity, two 60° dislocations react with each other to form a 90° dislocation, e.g., $\frac{a}{2}[101]+\frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{2}[110]$. This reaction is often observed during postgrowth annealing.[4] In our experiment, however, it is observed that an orthogonal array of 60° dislocations along [110] and [1$\bar{1}$0] is reoriented toward [100] and [010] directions after annealing, which represents a new strain relaxation mechanism in semiconductor heterostructures.

EXPERIMENTAL RESULTS

$In_{0.2}Ga_{0.8}As$ layers with a thickness of 40 nm were grown at 520 °C on GaAs buffer layers grown at 600 °C on GaAs (001) substrates, both by molecular beam epitaxy (MBE). In order to investigate the movement of the dislocations during annealing, the as-grown samples were annealed under arsenic overpressure for 30 min. with temperatures at 50 °C intervals from 600 °C to 800 °C. The dislocation structures were examined by both plan view and cross section transmission electron microscopy (TEM) performed in a JEOL 200 CX microscope operated at 200 keV.

An orthogonal array of dislocations along [110] and [1$\bar{1}$0] directions was observed in the as-grown film, as shown in Fig. 1(a). Diffraction contrast experiments indicated that the dislocations were predominantly 60° dislocations. The average interdislocation distance was about 0.5 µm, implying a plastic accommodation of only about 3% of the initial misfit strain in the $In_{0.2}Ga_{0.8}As$/GaAs interface. The cross section lattice image (Fig. 1(b)) revealed that each 60° dislocation shown in Fig. 1(a) in fact consisted of a pair of Shockley partial dislocations resulting from a dissociation of the form $\frac{a}{2}[\bar{1}01] \rightarrow \frac{a}{6}[\bar{1}\bar{1}2]+\frac{a}{6}[\bar{2}11]$.[2] As the average distance between the two partial dislocations is about 5 nm, the two partials cannot be resolved in the plan-view image, and in this letter the dislocations are referred to as perfect 60° dislocations. Fig. 1(a) clearly demonstrates the interactions between pairs of orthogonal 60° dislocations with a common Burgers vector, producing 90° turns at numerous sites along the dislocations. For two 60° dislocations with non parallel Burgers vectors there is also a local reaction, resulting in a short segment of dislocation connecting two three-fold nodes.

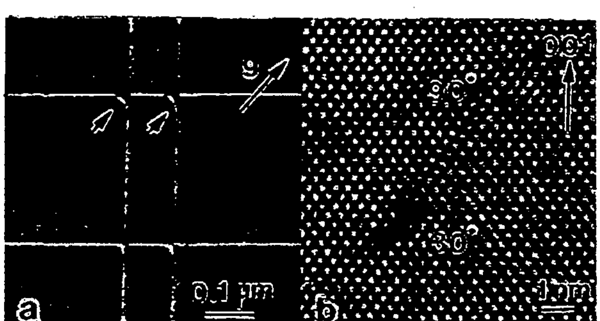

Fig. 1.(a) A plan view TEM image of misfit dislocations in an as-grown specimen with the diffraction vector g=[400]. Note the crossing reactions at nodes, as indicated by arrows. (b) A cross section lattice image viewed along a <110> direction.

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After the as-grown samples were annealed at 600 °C for 30 min., the average interdislocation distance decreased to the order of 0.1 μm, which means the dislocation density increased from a value corresponding to relaxation of ~3% of the original misfit strain in the as-grown structure to relaxation of ~15% of the misfit strain after annealing. Our observations did not reveal the mechanism of formation of these additional misfit dislocations. The original right-angle bends as shown in Fig. 1 (a) were also gradually replaced by obtuse angle bends (Fig.2 (a)), and, correspondingly, segments of original 60° dislocation were replaced by the segments of dislocations bent away from <110> directions toward <100> directions (Fig.2 (a)). Fig. 2(b) is a cross section lattice image for the annealed sample shown in Fig. 2(a). The reoriented dislocations were still located at the interface but less obviously dissociated into two partials. The dislocations no longer lie on a {111} plane.

It is well known that two close parallel 60° dislocations may react with each other after annealing to form a single 90° dislocation, e.g., $\frac{a}{2}[101]+\frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{2}[110]$.[4] However, at the dislocation densities in these heterostructures this reaction would be expected to have a low probability. A few such cases were observed, but dislocation segments with Burgers vector $\mathbf{b}=\frac{a}{2}<110>$ were predominantly formed by the reactions between two orthogonal 60° dislocations. After annealing, it was observed that the original node of two crossing 60° dislocations with opposite screw and surface-normal Burgers vector components moved apart, forming segments of dislocation with $\mathbf{b}=\frac{a}{2}<110>$ of increasing length between the node pair (Fig. 2(a)). Usually, the dislocations near the node were also bent away from <110> directions (Fig. 2(a)). This type of reaction has a high probability because the original 60° dislocation segments are long and many intersections occur along each dislocation.

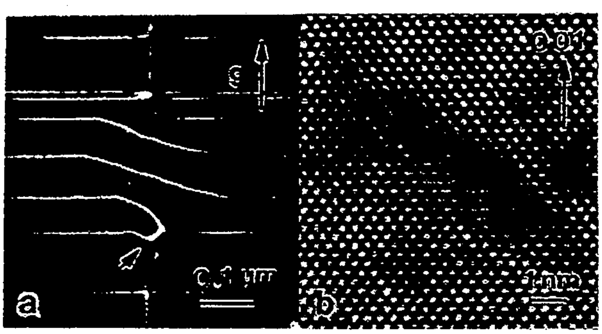

Fig. 2. TEM images of a sample annealed at 600°C for 30 min. (a) A plan view image with g=[220]. A segment of dislocation with $\mathbf{b}=\frac{a}{2}[110]$ was observed between two nodes (marked by arrow). (b) A cross section lattice image viewed along a <110> direction.

Fig. 3 is a plan view TEM images of the samples annealed at 800 °C for 30 min. The average interdislocation distance did not change significantly for samples annealed above 600 °C, but the 60° dislocation segments were annealed out by 800 °C, and an alternative dislocation network was formed. From TEM diffraction contrast analysis using diffraction vectors in the (001) interfacial plane, it was found that the network is composed of two orthogonal arrays of dislocations: one along [100] and [010] directions, and the other along [110] and [$1\bar{1}0$] directions (Fig. 3) The segments of the dislocations with line directions **u**=[100] and **u**=[010] were out of contrast respectively for diffraction vectors g=[400] or g=[040] (Fig. 3(a) and (b)). The cross section lattice images with the electron beam projected along the relevant directions of the dislocation lines, for example [100], revealed that the Burgers vector of the dislocation is $\frac{a}{2}[01\bar{1}]$

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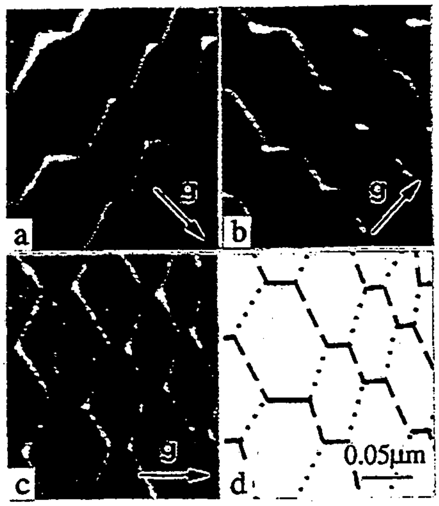

Fig. 3. TEM images of a dislocation network in a sample annealed at 800°C for 30 min. The images were taken in the same region under different diffracting conditions (a) g=[400], (b) g=[040], and (c) g=[220]. The dislocations with Burgers vectors $\mathbf{b}=\frac{a}{2}[01\bar{1}]$, $\mathbf{b}=\frac{a}{2}[\bar{1}0\bar{1}]$, and $\mathbf{b}=\frac{a}{2}[\bar{1}10]$ are out of contrast in (a), (b), and (c), and are illustrated by solid, dotted, and dashed lines in (d), respectively.

(Fig. 4), the same as that of the original 60° dislocations. As the dislocation lines were along <100> directions instead of the <110> directions of a 60° dislocations, the invisibility criterion $\mathbf{g}\cdot\mathbf{b}=0$ and $\mathbf{g}\cdot\mathbf{b}\mathrm{x}\mathbf{u}=0$ were satisfied simultaneously and thus the dislocation lines were completely out of contrast when g=[400] and g=[040] (Fig. 3(a) and (b)). For diffraction vectors g=[220] and $g=[2\bar{2}0]$, the segments of dislocations with line directions $\mathbf{u}=[110]$ and $\mathbf{u}=[1\bar{1}0]$ were out of contrast respectively (as shown in Fig.3(c) with g=[220]). This standard "invisibility condition" illustrated that the dislocations along <110> directions are 90° edge dislocations with Burgers vector $\mathbf{b}=\frac{a}{2}[\bar{1}10]$ and $\mathbf{b}=\frac{a}{2}[110]$. The dislocation network formed by all of the dislocations is illustrated diagrammatically in Fig.3 (d).

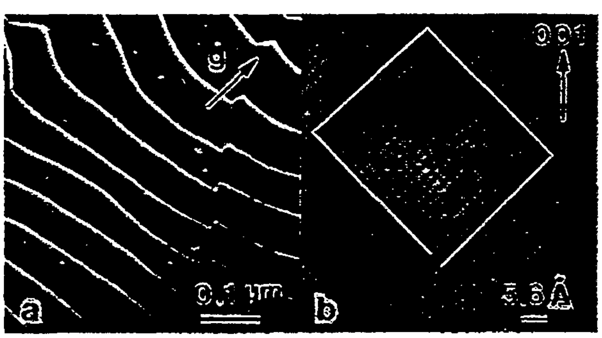

Fig. 4. TEM images of a sample annealed at 800°C for 30 min. (a) A plan view image with g=[040]. (b) A cross section image viewed along the [100] direction showing that the dislocation has a Burgers vector $\mathbf{b}=\frac{a}{2}[01\bar{1}]$, as indicated on the Burgers circuit.

The commonly observed 90° and 60° misfit dislocations are along <110> directions as a result of low core energy in these orientations.[2] A 90° dislocation can relieve a misfit strain of $\frac{a}{\sqrt{2}}$ and is the most effective strain-relieving dislocation. The 60° dislocation is less effective in strain relief, with each relieving a misfit strain of $\frac{a}{2\sqrt{2}}$. However, the 60° dislocation is usually formed at first, since only the 60° dislocation can glide into the (001) interface on {111} planes after it has formed as a half loop from the surface, or as a loop from a defect near the interface.[3] Two 60° dislocations may react with each other to form a 90° dislocation to reduce the total dislocation density, however, we have found that, in $In_{0.2}Ga_{0.8}As/GaAs(001)$ interfaces, long segments of 90° dislocations are hardly ever formed even after high temperature annealing, and that the elastic misfit strains are mainly relieved by dislocations along <100> directions. Although the Burgers vector of the **u**=<100> dislocation is the same as the 60° dislocation, as the dislocation line lies along the <100> direction, each **u**=<100> dislocation can relieve a strain of a/2 in the (001) interface, which is $\sqrt{2}$ times that of the 60° dislocation (Fig. 5). When the dislocation line is reoriented from <110> toward <100>, the strain relieved by the dislocation increases from $\frac{a}{2\sqrt{2}}$ to a/2. The dislocation thus experiences a climb force produced by the high residual elastic misfit strain. In the as-grown sample, the 60° dislocations formed first and glided into the interface. In the annealing process the climb force causes the dislocations to move nonconservatively toward <100> directions to further relieve the residual strain.

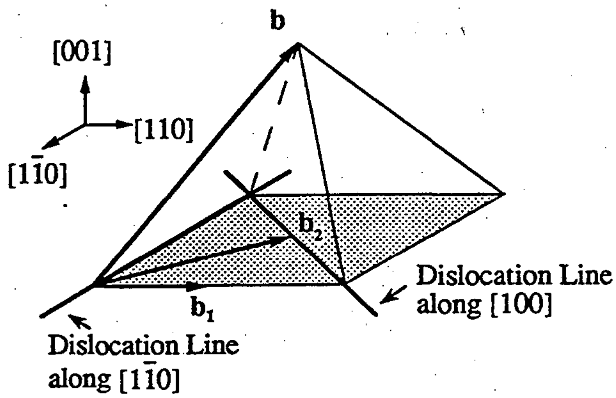

Fig. 5. When a dislocation with Burgers vector $\mathbf{b}=\frac{a}{2}[011]$ is bent from the [1$\bar{1}$0] toward the [100] direction, the edge component of the Burger vector in (001) interfacial plane changes from $\mathbf{b_1}=\frac{a}{4}[110]$ to $\mathbf{b_2}=\frac{a}{2}[010]$.

It has been suggested that **u**=<100> dislocations can form by glide on the {110} planes in $(Al)GaAs/In_xGa_{1-x}As/GaAs(001)$ heterostructures which are highly strained ($x \geq 0.40$).[5] In the $In_{0.2}Ga_{0.8}As/GaAs(001)$ system, however, the **u**=<100> dislocations were formed gradually by the climb of the 60° dislocations in (001) interfaces rather than the glide of the **u**=<100> dislocations on {110} glide planes. During annealing, two crossing orthogonal 60° dislocations react with each other differently depending on the relations between their Burgers vectors.

Two orthogonal 60° dislocations with the same Burgers vectors form a pair of L-shaped dislocations by annihilation at the node in the as-grown specimen (Fig. 1). During annealing, the original right-angle jogs are blunted and the dislocation lines are bent away from the <110> directions by the remaining residual elastic misfit stress and dislocation line tension forces (Fig. 2). The dislocations are finally straightened and reoriented into the <100> directions after higher temperature annealing (Fig. 4). As this operation may not be completed even after annealing at 800 °C for 30 min., the observed dislocation lines are not absolutely straight, nor do they always lie precisely along <100> directions (deviating at most by ~10°).

On the other hand, two orthogonal 60° dislocations with opposite screw and surface-normal components of the Burgers vectors undergo a similar reorientation as

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described in (i), but as these two dislocations can react to form a dislocation with a resultant Burgers vector $\mathbf{b}=\frac{a}{2}\langle 110 \rangle$, a segment of dislocation with $\mathbf{b}=\frac{a}{2}\langle 110 \rangle$ must be generated to connect two nodes (Fig. 2). After high-temperature annealing, these short segments of dislocation are formed in addition to the $\mathbf{u}=\langle 100 \rangle$ dislocations (Fig. 3).

In summary, in our TEM study of $In_{0.2}Ga_{0.8}As$/GaAs(001) heterostructures, a 60° dislocation array along [110] and [$1\bar{1}0$] directions was observed in the interfaces of the samples grown at 520 °C. After the as-grown samples were annealed for 30 min. at temperatures ranging from 600 °C to 800 °C, the 60° dislocation segments were gradually annealed out, and replaced by an array of dislocations along [100] and [010] directions. Cross section TEM observations show that these dislocations have Burgers vectors $\mathbf{b}=\frac{a}{2}\langle 101 \rangle$ which are the same as that of the original 60° dislocation, but as the edge component in the (001) interfacial plane is $\sqrt{2}$ that of the 60° dislocation, they can relieve the elastic misfit strain more effectively. The $\mathbf{u}=\langle 100 \rangle$ dislocations were formed by non-conservative motion of the 60° dislocations in the (001) interfacial plane. They originate, in the as-grown samples, from orthogonal 60° dislocations with parallel Burgers vectors that have crossed and reacted with each other at nodes to form right-angle bends. During annealing, the right-angle bends gradually straightened, and the dislocations reoriented into $\langle 100 \rangle$ directions by residual misfit stresses and dislocation line tension. Formation of these $\mathbf{u}=\langle 100 \rangle$ dislocations by non-conservative reorientation of two orthogonal 60° dislocations represents a new strain relaxation mechanism in diamond or zinc blende semiconductor heterostructures.

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