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Correlation of defect profiles with carrier profiles of InAs epilayers on GaP

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The carrier profile for InAs films grown on GaP is modeled as a first-order approximation which assumes that 90° edge dislocation intersections and the threading dislocation intersections act as shallow donors. Due to dislocation annihilation during growth, the threading dislocation intersection density decreases as the inverse of the distance x from the InAs/GaP interface, $D(x)=D_0x_0/(x_0+x)$, where D_0 and x_0 are dislocation density at the InAs/GaP interface and the first annihilation position from the interface, respectively. The carrier profile in InAs films can be described by a similar equation that is deduced from the threading dislocation intersection profile. The calculated carrier profiles agree well with measured carrier profiles. This correlation supports our hypothesis that both the edge dislocation intersections and the threading dislocation intersections act as shallow donor sources. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1338956]

Owing to its high electron mobility and high electron saturation drift velocity, InAs is a good candidate for both IR photonic and high speed tetrahertz device applications.[1,2] This has motivated our group to pioneer the molecular beam epitaxy (MBE) of high quality InAs on GaP substrates, even though there is an 11% lattice mismatch between GaP and InAs. We have previously reported that such InAs films have unique electronic properties associated with interface misfit dislocation *intersections*, known as ''driedl'' defects,[6] including interface Fermi-level pinning, interface electron generation and scattering, and no carrier freeze out at low temperatures.[1] Here, we report the correlation between the threading dislocation intersection density profile and the carrier profile for InAs films. We have modeled the carrier profiles for these InAs films as a first-order approximation of the observed threading dislocation intersection densities. Due to dislocation annihilation during growth, the dislocation intersection density profile varies with the inverse of distance from the InAs/GaP interface as $D(x)=D_0x_0/(x_0+x)$, where D_0 is threading dislocation intersection density (cm^{-2}) and x_0 is the average height from the interface of the first annihilation point. We then show that the carrier profile in InAs films can be described by a similar equation. This correlation supports the hypothesis that threading dislocation intersections act as shallow donor sources.

Undoped InAs films with various thickness were grown on (001) GaP substrates using MBE. The GaP substrates are thermally cleaned in the growth chamber under a P_2 over pressure. A 100-nm-thick GaP buffer layer was grown followed by the growth of a 20 period superlattice consisting of 5 nm alternating layers of GaP and AlP in order to prevent the out diffusion of background sulfur from the substrate.[3] A 200-nm-thick Be doped *p*-GaP buffer layer was subsequently grown on the superlattice. Undoped InAs films were grown at 350 °C. The first few monolayers of InAs were grown under low V/III beam flux ratios (~1.0) to promote a high nucleation density leading to a smoother interface. A 5-nm-thick undoped $In_{0.8}Al_{0.2}As$ film was grown on the InAs layer as a capping layer. The details of the growth procedure have been reported elsewhere.[1]

A cross-sectional transmission electron microscopy (TEM) image of an 0.5-μm-thick InAs film is shown in Fig. 1. The InAs/GaP interface is indicated in the figure. It is seen that there are dark spots at the InAs/GaP interface and a threading dislocation (TD) network. The dark spots correspond to 90° edge misfit dislocations (MD) at the InAs/GaP interface showing equal spacing of 3.95 nm.[1] Although pairs of 60° misfit dislocations are observed in the high resolution TEM (HRTEM) image,[2] the number is a small fraction

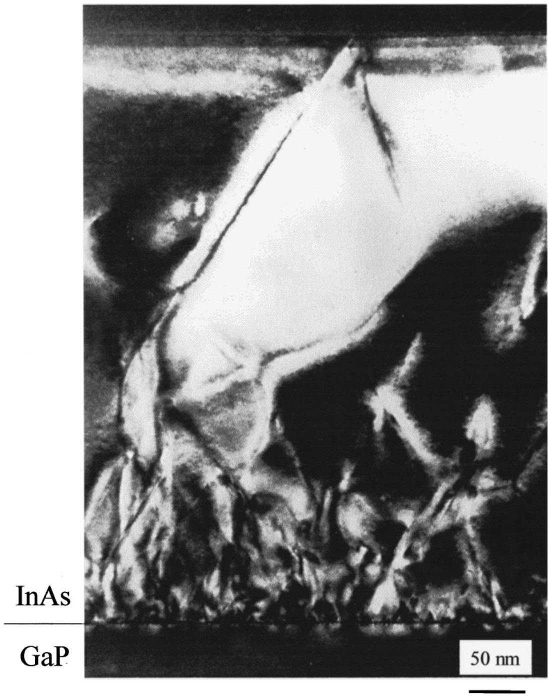

FIG. 1. A cross sectional TEM image of a 0.5 μm InAs film.

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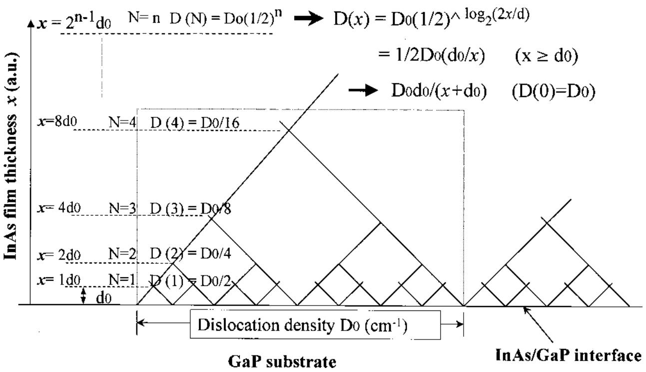

FIG. 2. A schematic diagram of threading dislocation annihilation model.

($<$5%) of the total dislocation density. Another observation is a triangular shape threading dislocation network (TDs), which also originates at the InAs/GaP interface and lies on {111} planes of the InAs films. The TD density is high at the interface and abruptly decreases within approximate 10–20 nm from the interface. It is interesting to note that the number of dislocations decreases with distance from the interface. It can be seen that when two dislocations meet at a point, one is annihilated and one propagates into the upper layer. Taking this dislocation annihilation into account, we modeled the TD density profile as a function of film thickness using a first order simple geometrical structure. Similar work for GaAs/Si structures and for lattice mismatched III–V compound semiconductor structures have been reported by Kroemer *et al.* and Speck *et al.*[4,5]

In order to calculate the dislocation density as a function of film thickness, including MDs and TDs, we use a model shown the schematic diagram of TD annihilation in Fig. 2. We assume that dislocation annihilation occurs repeatedly and each annihilation in Fig. 2. We assume that dislocation annihilation occurs repeatedly and each annihilating position can be expressed with a binary recombination law. At the InAs/GaP interface, the 90° edge MD intersection density is denoted as D_0 (cm^{-2}). By estimating each annihilation distance from the interface (N), the number of dislocation $D(N)$ at a certain position $N=n$ can be written as $D(n)=1/2D_0(1/2)^n$. The position n at $N=n$ is written as $x=2^{n-1}x_0$, where x_0 is the distance of the first annihilation position from the interface, as shown in Fig. 2. We can deduce the following equation:

$$D(x)=1/2D_0(x_0/x), \quad (x>0). \tag{1}$$

For the boundary condition $D(0)=D_0$, we deduce the following:

$$D(x)=D_0x_0/(x_0+x), \quad (x\geqslant 0). \tag{2}$$

These expressions show that TD density abruptly decreases within a thickness x_0 and gradually decreases as the inverse of the distance from the InAs/GaP interface. In our previous work, the spacing of 90° edge MDs were measured to be 3.95 nm using cross-sectional HRTEM analysis; and the MD intersection density D_0 was calculated to be 6.4×10^{12} cm^{-2}.[2] From Fig. 1, we set the first annihilation position at approximately 15 nm from the InAs/GaP interface. The dislocation density curve, $D(x)$, according to Eq. (2) is shown in Fig. 3. This curve shows that the TD density decreases abruptly within a few tens of nanometer from the interface and a high density of TD is localized within a thin layer of thickness x_0 from the interface. The calculated TD intersection density and the measured dislocation density ($\sim1\times10^{10}$ cm^{-2}) for a 1 μm InAs film, using plan-view TEM are indicated in the figure. This value is consistent with the calculated curve. We believe this demonstrates the first-order dynamics of dislocation annihilation. However, for completeness, understanding of the kinetics of dislocation annihilation is needed and is now under investigation.

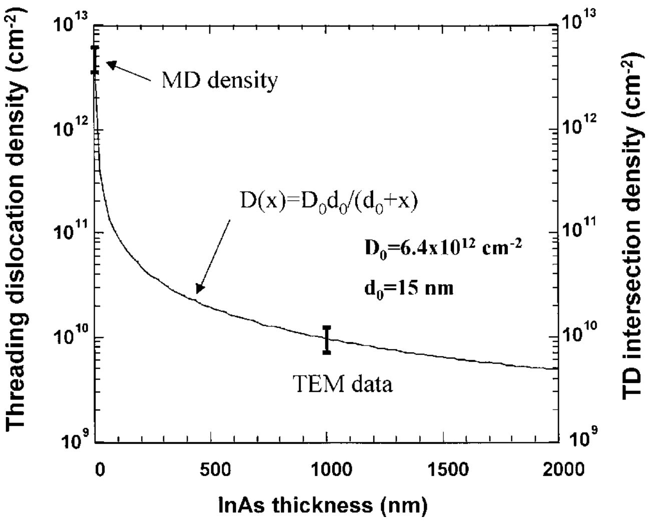

FIG. 3. A calculated dislocation density curve, which corresponds to the threading dislocation intersection density.

It has been reported that a high sheet carrier density is localized at InAs/GaP interface.[2] It has been reported that most of the sheet carriers are generated by a high density of MD intersections, known as driedl defects which act as shallow donor ‘‘dopants’’.[6] The magnitude of the sheet carrier density ($\sim1\times10^{13}$ cm^{-2}) is quite close to the MD intersection density ($\sim6.4\times10^{12}$ cm^{-2}). This carrier density is the result of Fermi-level pinning 0.2 eV above the conduction band edge of InAs at the InAs/GaP interface[2] due to the MD intersections. This causes a spike in the carrier density at the interface. An electrochemical capacitance–voltage (ECV) carrier profile (N_d-N_a) of a 1 μm InAs film is shown in Fig. 4. The carrier profile shows an initial spike in the carrier density at the interface that gradually decreases with increasing distance from the InAs/GaP interface. It has been suggested that the bulk carriers could be provided by charges associated with the TDs. However, the carrier density estimated by supposing each atomic site along TDs being singly charged is one order of magnitude larger than the measured carrier density.[1] We propose a model in which both TD intersection and MD intersections can be donor sources. In this model, the carrier profile is expressed in terms of both MD and TD intersection densities. The equation for the carrier profile $N(x)$, expressed as a function of the distance from an InAs/GaP interface, is derived from Eq. (2) by dividing Eq. (2) with x_0 and adding a constant background carrier density N_0:

$$N(x)=N_0+N_s/(x_0+x), \tag{3}$$

where $N_s=D_0$, which is the sheet carrier density (cm^{-2}) at an InAs/GaP interface. x_0 is an effective triangular well

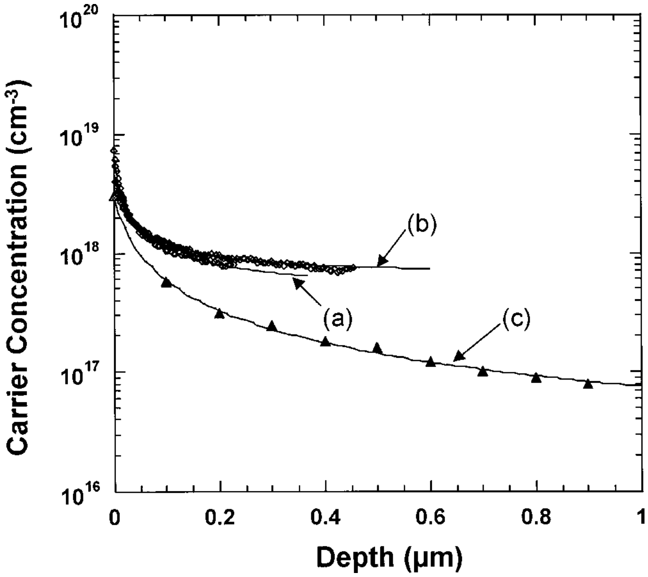

FIG. 4. ECV carrier profiles of 0.25, 0.5, and 1.0 μm InAs films and the calculated carrier profiles. The average background carrier density N_0 of 0.25, 0.5 μm InAs films was $4-6\times10^{17}$ cm^{-3}. The calculated carrier profiles for 0.25 (a), 0.5 (b), and 1.0 μm (c) show good agreement with the measured carrier profiles. For InAs films of 0.25, 0.5, and 1.0 μm, N_s and x_0 are $N_s=7.4\times10^{12}$ cm^{-2}, and $x_0=12$ nm, $N_s=6.2\times10^{12}$ cm^{-2} and $x_0=15$ nm, $N_s=6.3\times10^{12}$ cm^{-2} and $x_0=21$ nm, respectively.

thickness formed at the InAs/GaP interface due to Fermi level pinning associated with MD intersections.[1] This model was applied to different InAs films with various constant background carrier densities, assuming N_s, N_0, and x_0 as variable parameters. Three ECV carrier profiles for InAs films that were 0.25-, 0.5-, and 1.0-μm-thick and grown on GaP substrates are shown in Fig. 4. The average background carrier density, N_0, for the 0.25-, 0.5-, and 1.0-μm-thick films are 4×10^{17}, 6×10^{17}, and 2×10^{16} cm^{-3}, respectively. The calculated carrier profiles for these three films show good agreement with the measured carrier profiles. Also for these three films, N_s and x_0 are $N_s=7.4\times10^{12}$ cm^{-2}, $x_0=12$ nm, $N_s=6.2\times10^{12}$ cm^{-2}, and $x_0=15$ nm, $N_s=6.3\times10^{12}$ cm^{-2}, and $x_0=21$ nm, respectively for increasing film thickness. It is interesting to note that the three N_s values calculated were very close to the misfit dislocation intersections or dreidl density of 6.4×10^{12} cm^{-2}.[1,2] The close agreement between calculated and measured N_s values and $N(x)$ profile provides good support four model.

In conclusion we have investigated the correlation between defect profiles with carrier profiles of InAs epilayers on GaP substrates. The equation for defect density and carrier density was deduced from threading dislocation annihilation model and showed good agreements with experimental data.

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