Fermi-Level Pinning by Misfit Dislocations at GaAs Interfaces

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(Received 22 August 1983)

Fermi-level pinning by misfit dislocations at GaAs interfaces has been investigated. n^+-GaInAs was used to control the misfit dislocation density by varying of composition and epilayer thickness. Interfaces with zero or low dislocation densities are Ohmic to current flow, and become rectifying with increasing dislocation density. The "Schottky barrier height" increases with dislocation density in accordance with a simple physical model which assumes Fermi-level pinning at the dislocation.

PACS numbers: 73.40.-c, 73.30.+y

Recent experimental studies on the formation of Schottky barriers at III-V semiconductor surfaces and interfaces have resulted in a proliferation of theoretical models. For example, Schottky barrier formation has been described in terms of Fermi-level pinning by adatom-induced native defects,[1,2] metal-induced gap states,[3] and the electronic and chemical properties of the interface metallurgy.[4,5] Definitive testing of these models is complicated by the experimental difficulty of differentiating between metallurgical and structural (defect) effects at metal/III-V interfaces. In this paper we report the electrical properties of n-type GaAs interfaces having a controlled density of a certain type of structural defect: the misfit dislocation. We have used n^+-GaInAs as the "metal" and control the misfit dislocation density by varying composition and epilayer thickness. These interfaces are free of extraneous metallurgy since they are formed by relaxing strain at lattice-mismatched heterojunctions with slightly different compositions.

The dynamics of misfit dislocation formation is well known[6] and is shown schematically in Fig. 1. When a film with unstrained lattice constant a_f is deposited on a substrate with a different lattice constant, a_s [Fig. 1(a)], the mismatch (misfit), $(|a_f - a_s|)/a_{\text{avg}}$, will accommodate strain such that a_f is approximately equal to a_s for a film thickness less than some critical thickness, h_c [Fig. 1(b)]. This is known as a pseudomorphic film. For a film thickness greater than h_c, the misfit is accommodated by the formation of misfit dislocations, and the lattice constant of the film relaxes towards the unstrained value [Fig. 1(c)]. The strain energy necessary to form these dislocations is approximately proportional to the product of the misfit and film thickness. Thus, h_c is roughly proportional to the reciprocal of the misfit. In addition the average linear density of misfit dislocations is expected to be equal to $(|a_f - a_s|)/a_{\text{avg}}^2$. Therefore, for a given misfit, by varying of the epilayer thickness it is possible to form either a pseudomorphic interface or one with a controlled density of misfit dislocations.

Our experiment attempted to test the following hypotheses concerning the electrical behavior of GaInAs/GaAs heterojunctions: (1) for pseudomorphic interfaces, band alignment rules[7,8] determine transport properties; (2) for interfaces with misfit dislocations, Fermi-level pinning occurs at the misfit dislocation which results in carrier depletion in a region around the axis of

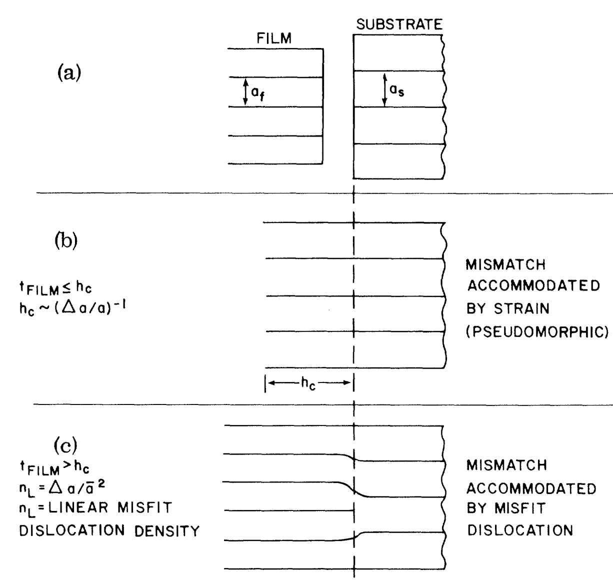

FIG. 1. A schematic representation of the formation of misfit interfaces.

the dislocation.

Three samples of GaInAs/GaAs heterojunctions were prepared by molecular-beam epitaxy (MBE), inspected by transmission electron microscopy, and tested electrically. The MBE depositions were as follows: a 1000-nm film of GaAs doped with 2×10^{18} Si atoms cm^{-3} was epitaxially deposited on a (100) GaAs n-type substrate doped with Si at the same concentration. This was followed by a 500-nm layer of GaAs doped with 2×10^{16} Si atoms cm^{-3} and then terminated by a layer of GaInAs doped to 5×10^{18} Si atoms cm^{-3}. Prior to electrical measurement Ohmic contacts were formed to the entire bottom side of the substrate and in circular patterns on the GaInAs surface. Samples 1 and 2 were identical except for the thickness of the GaInAs layer. Samples 2 and 3 were identical except for the composition of the GaInAs layer. The GaInAs composition for samples 1 and 2 was $Ga_{0.93}In_{0.07}As$ with a corresponding misfit of 0.5%. The thickness of the GaInAs layer for sample 1 was 100 nm and chosen to be less than h_c and hence the layer was designed to be pseudomorphic. The thickness of the GaInAs layer of sample 2 was 1000 nm, and chosen on the basis that the GaInAs/GaAs interface should contain misfit dislocations with an average spacing of 120 nm. The composition of the GaInAs layer of sample 3 was $Ga_{0.80}In_{0.80}As$ which has misfit of 1.5%, and was chosen to produce interface dislocations with an average spacing of about 40 nm.

The transmission electron microscopy studies were performed with a beam energy of 200 keV. For this energy the extinction distance of electrons in GaAs is approximately 300 nm (greater than the thickness of the sample 1 epilayer and less than the epilayer thickness of samples 2 and 3). Sample 1 proved to be crystalline and free from dislocations [Fig. 2(a)]. In this sample the electrons should have easily penetrated past the interfacial region. Sample 2 also appeared crystalline and dislocation free throughout the top region (300 nm from the surface) after backside thinning. However, when a specimen of sample 2 was ion milled so that the interface was contained within the extinction depth, a distinct dislocation network was revealed [Fig. 2(b)]. Dark-field studies showed that they were oriented as expected along [110] directions. The separation between dislocations ranged from 90 to 200 nm, with the average being about 140 nm. From the transmission electron microscopy studies on sample 3 (not shown in Fig. 2) it was found that

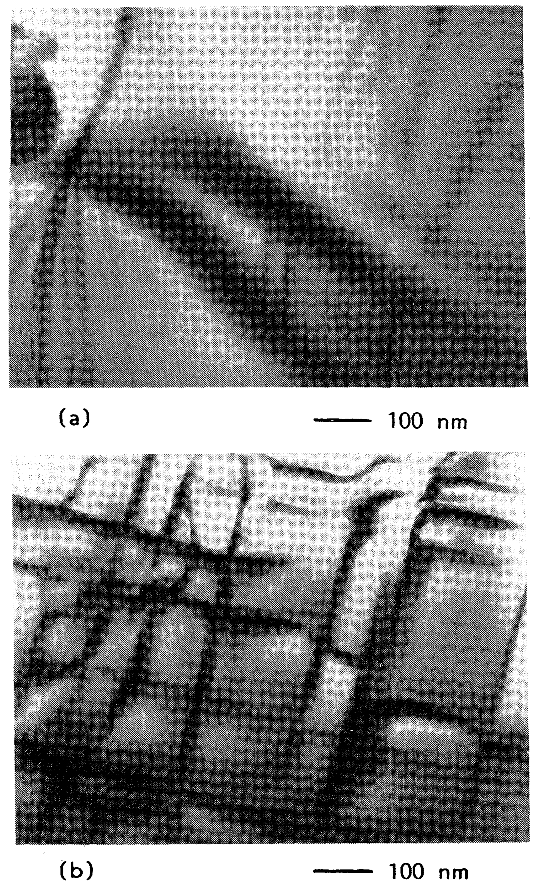

FIG. 2. Transmission-electron photomicrographs of the pseudomorphic interface of sample 1 [Fig. 2(a)], and the interface of sample 2 containing misfit dislocations [Fig. 2(b)].

the spacing ranged from 20 to 120 nm, with the average being about 50 nm.

A linear plot of current agains voltage is shown in Fig. 3(a) for the three samples. Note that for the pseudomorphic sample 1, the interface shows Ohmic behavior, whereas for samples 2 and 3 which have misfit dislocations the interface shows rectifying behavior. The nonlinear behavior of samples 2 and 3 is further quantified in Fig. 3(b), and leads to the extraction of a "barrier height," as determined by J at $V=0$ (see, e.g., Sze[9]). The values for sample 2 are 0.11 V at 77 K and 0.36 V at room temperature, and for sample 3, where the dislocation density is about three times that for sample 2, the values are 0.17 and 0.49 V at 77 K and room temperature, respectively.

We are able to explain qualitatively our results by a simple model shown schematically in Fig. 4. The top part of Fig. 4(a) depicts the physical con-

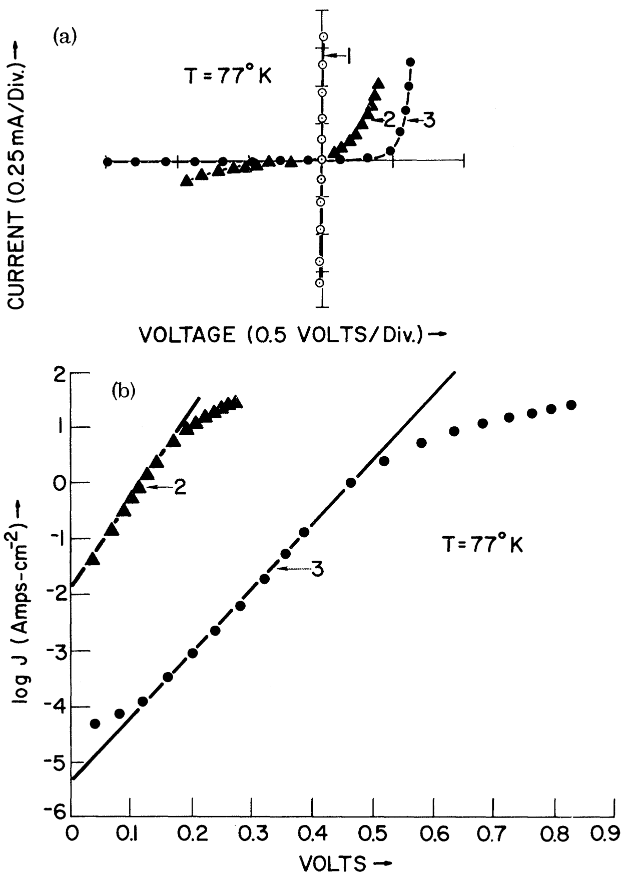

FIG. 3. Current-voltage measurements of three different GaInAs/GaAs interfaces (1, 2, and 3), with cross section 1.2×10^{-4} cm^{-2}. (See text for detailed description.) In (b), the GaInAs is biased positive with respect to the GaAs.

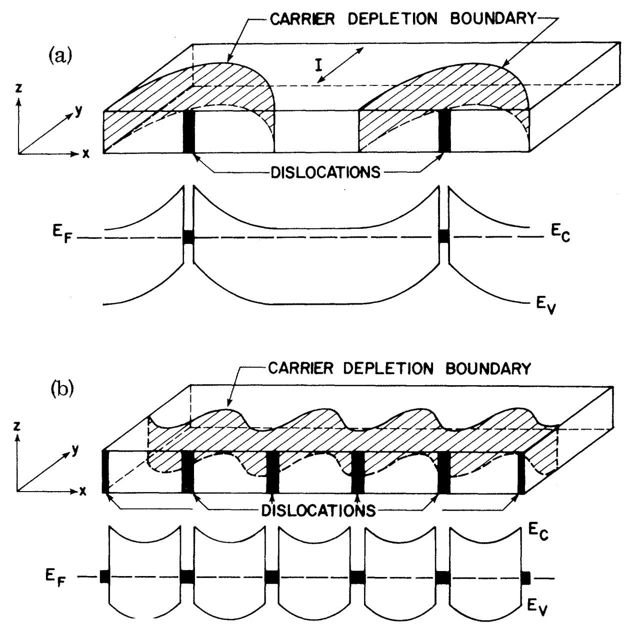

FIG. 4. A schematic represention of the expected electronic behavior of misfit dislocations. (See text for detailed description.)

dition of a slab of GaAs arbitrarily containing two dislocation lines. The GaInAs/GaAs heterojunction lies in the x-z plane, and dislocations are parallel to the z axis. The GaInAs film intersects the $-y$ axis, and GaAs substrate intersects the $+y$ axis. The dislocations are assumed to form a line of deep levels which deplete free charge in the GaAs radially from the dislocation to the depletion boundary. We can estimate the radius of the depletion boundary by solving Poisson's equation in cylindrical coordinates, which yields the expression

$$\varphi = qNr_s^2/2\epsilon[\ln(r_s/r_0) - 0.5] \simeq 0.8 \text{ V},$$

where φ is the pinning position of the dislocation, N is doping concentration in the GaAs, r_s is the radius of the depletion boundary in the GaAs, and r_0 is the effective radius of the dislocation. The pinning position is assumed to be 0.8 V from the conduction-band edge (the average value for n-type Schottky barrier heights in Ref. 9). The exact choice is not critical to the qualitative conclusions of our model. Figure 4(a) depicts the case for a lightly doped n-type GaAs in which $2r_s$ is less than the average dislocation spacing, L, and hence the depletion boundaries do not overlap. The electronic consequence of this is shown schematically by the energy-band diagram along the x axis. For the region between the two depletion boundaries, electrons flowing across the heterojunction will experience no potential barrier except for that due to offset in conduction-band alignment. For the GaInAs compositions and doping used in this study Ohmic behavior is expected at both room temperature and 77 K.[7] Since Ohmic behavior is expected for the case of Fig. 4(a), it is also expected for pseudomorphic samples (i.e., sample 1). However, as the misfit dislocation density is increased or doping level on the GaAs side of the heterojunction is decreased, the depletion regions will eventually overlap. This overlap will cause a barrier to current flow resulting in a nonlinear current-voltage dependence. This situation is shown schematically in Fig. 4(b). The exact variation in the band edges with position has not been calculated; hence a quantitative comparison of data with the model is not yet possible. However, the band edge is expected to decrease with distance along the x axis from the dislocation for distances between 0 and $L/2$ where L is the average spacing between dislocations. The important point is that for a given GaAs doping, as $L/2$ decreases from r_s to 0, the "barrier height" halfway between the dislocations is expected to increase from 0 toward the pinning value. The results of Fig. 3 support this interpretation. We attribute the apparent temperature dependence of the barrier heights to the statistical fluctuations in dislocation spacings and it is expected to decrease for smaller average spacings or smaller spacing fluctuations. We believe therefore that misfit dislocations at n^+-GaInAs/n-GaAs interfaces act as linear arrays of deep levels with an energy which appears to be about the same as the Fermi-pinning position observed for GaAs surfaces and GaAs interfaces. Further n- and p-type doping and misfit-density experiments plus a quantitative interdislocation band-bending model are needed to determine the uniqueness of this interpretation.

The authors wish to acknowledge valuable discussions with S. Pantelides, W. Dumke, N. Braslau, M. Brodsky, J. Freeouf, and S. Keller. K. Kavanagh acknowledges support by a Bell-Northern Research Fellowship; this work was supported in part by the Defense Advanced Research Projects Agency.

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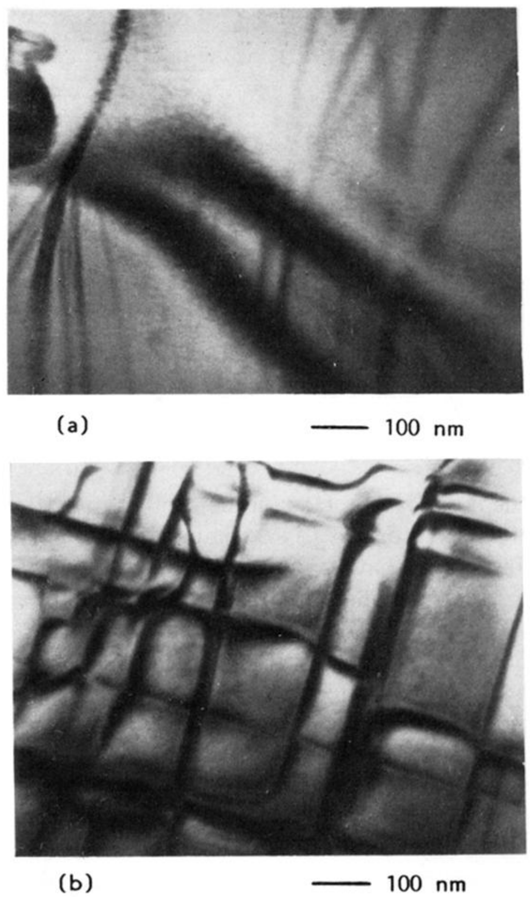

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