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ABSTRACT

Gold contacts deposited on ultrahigh-vacuum cleaved (110) GaAs show Schottky barrier-type behavior which becomes "ohmic" upon annealing due to leakage currents at the periphery of the contact. In this study, electron microscopy is used to investigate the structure and composition of both rectifying and low-barrier "ohmic" contacts. The results show that Au can form both types of contacts on GaAs, depending on the deposition conditions and the defects formed near the interface.

The basic mechanism of formation of ohmic and barrier-type ("Schottky") contacts on GaAs is still a subject of controversy, despite intense investigations in this field [1]. Models of Schottky-barrier formation on GaAs currently being studied include the perfect metal-semiconductor interface (the "metal-induced gap states" model) [2,3,4], the formation of anion-microclusters (the "effective work-function model") [5], and the creation of deep level defects near the metal-semiconductor interface (the "unified defect model") [6,7]. None of the models have yet been directly confirmed by experiment.

Room-temperature deposition of several monclayers of Au onto clean cleaved GaAs (110) surfaces results in the transition from a system in which the Fermi-level is unpinned to a system in which the Schottky- barrier height is fully established. Barrier heights on unannealed thick-metal film diodes (≈100nm) determined by electrical measurements are found to be essentially identical to those reported at the initial stages (several monolayers) of Schottky-barrier formation. However, annealing of thick metal film Au/n-GaAs devices above the Au-Ga eutectic temperature (≈360°C) leads to "ohmic" behavior, while annealing of sub-monolayer to several-monolayer coverages of Au on n-GaAs results in a significant barrier. Because Au has a high work function and is not known to form a shallow donor level in GaAs, the physical mechanism responsible for this observed "ohmic" behavior remains unclear. A recent study of Au contacts formed on clean cleaved

GaAs (110) surfaces showed that "ohmic" behavior is caused by leakage currents at the periphery of the contacts, while a rectifying barrier is found under the central part of the device [8,9]. These structures are of particular interest because they exhibit both barrier type and "ohmic" behavior within the same Au/GaAs contact. In this letter, results are presented of the first study that directly compares the electrical characteristics of "ohmic" and Schottky contacts with their microstructures. Conclusions are drawn about the physical mechanisms responsible for the formation of both Schottky and "ohmic" contacts in the Au/GaAs system.

Both analytical and high-resolution transmission electron microscopy were applied to samples that had been characterized by electrical measurements. Photoemission- spectroscopy studies were also performed, using the same sample-preparation method employed during the initial stages of Schottky barrier formation. Gold diodes of ≈500μm diameter were formed by *in-situ* metal deposition on a clean cleaved GaAs (110) surface in an UHV chamber (base pressure ≈2 x 10^{-10} torr). As-deposited diodes showed a reproducible barrier height of ≈0.9 eV (see Table 1). Annealing of 10 min. each was performed in a N_2 environment. Measurements of I-V characteristics were performed in atmospheric conditions at room temperature and are shown in Figure 1. The same trends were reported earlier [8]. A large current increase was found at low forward voltages for devices which were annealed above the Au-Ga eutectic temperature (≈350°C).

To remove the current path at the periphery region ($\approx$1-3μm) of small barrier height, a mesa etch was performed. Three types of samples were prepared: as-deposited, annealed at 405°C, and annealed at 405°C with subsequent mesa-etching. Plan-view thin foils, transparent to electrons, were prepared from these samples. The periphery of the as-deposited sample repeated the shape of the mask through which the Au was evaporated (Fig. 2a). A similar peripheral shape was observed after mesa-etching (Fig. 2b). Only in some cases, where the etching time was too short, was the leakage current reduced significantly but not completely eliminated. The periphery of such contacts was not as smooth as the periphery of as-deposited contacts.

TEM micrographs from the periphery of annealed samples showed elongated Au crystallites on the GaAs surface (Fig. 2c). These crystallites can be seen easily in high resolution images, where Moire fringes characteristic of a thin Au film are present (Fig. 2d). These elongated crystallites extend for 1-3 μm outside the original periphery of the as-deposited diodes. It can easily be seen that the Au flowed from the original contact dots. The question arises as to how this predominantly Au overlayer melted at such low temperatures, and a possible explanation comes from energy dispersive x-ray spectroscopy (EDXS). Spectra of these crystallites taken in plan view with a beam diameter $\approx$ 4 nm show that the crystallites are Ga-rich. The measured (Ga K_{α}) / (As K_{α}) ratio of the crystallites is about 5-10% higher than the same ratio obtained from the areas between the crystallites and from areas on the substrate far from the Au dots. In addition, spectra were taken from different areas of the cross-section samples, starting in the substrate far from the interface and approaching the interface in ≈10 nm steps until the electron beam reached the top of the Au layer (Fig. 3). The (As K_α) / (Ga K_α) ratio remained constant in the substrate far from the interface. The ratio increased ≈ 10 nm from the Au interface, suggesting an accumulation of As near the interface. Similar results were obtained for both unannealed and annealed samples, although the annealed samples showed a larger accumulation of As at the interface. The intensity ratio showed an increase of ≈1.5-2% for unannealed samples and ≈ 5-6% for annealed samples, compared with the same ratio measured in the substrate far from the interface. In the Au layer the diffusion of both Ga and As was observed, with clear Ga domination at the Au surface. However, no new Au-containing phase was formed in the samples. Although the Ga concentration in the Au layer was not enough to form a new crystallographic phase, it was probably enough to decrease the melting temperature of the Au overlayer. This would allow a thin Ga-rich gold film to flow from the original dots at the periphery during annealing at 405°C.

An interesting observation made during this study was the instability of the As concentration near the Au/GaAs interface under electron beam illumination. The spectra taken of the substrate far from the Au layer showed a constant (As K_α) / (Ga K_α) ratio for different exposure times.

Near the interface the ratio was found to change with time and the As concentration approached the bulk value for long illumination times. In order to achieve satisfactory statistics, it was necessary to use long (300-500 sec) exposure times. This problem was solved by moving the beam position after short illumination times, keeping the distance from the interface constant for the desired total measurement time. The instability of excess As near the interface suggests that these atoms are quite mobile e.g. a significant fraction exists as interstitials.

In addition to the analytical observations, TEM micrographs from annealed cross-section samples show clusters of a new phase in the GaAs ≈ 10 nm from the interface (Figure 4). Large precipitates were often observed, and the selected-area-diffraction pattern of these structures shows spots characteristic of hexagonal As [10].

These findings show that the As distribution is different beneath the Au layer and beneath the free GaAs surface. Obviously, As outdiffusion is suppressed by the presence of the Au layer but occurs freely from the area surrounding the Au contact. This indicates that the local stoichiometry of the crystal may be the key to understanding the observed variation in contact properties (Schottky vs. ohmic) of the Au/GaAs system. The elongated Ga-rich Au crystallites on the periphery of Au contacts are strongly correlated with the change to ohmic behavior of those contacts. Arsenic accumulated near the interface in the Au/GaAs system correlates with the observed Schottky barrier formation, because this strong rectifying behavior was observed for both unannealed and annealed samples once the peripheral leakage current was removed.

In conclusion, it is possible to form either "ohmic" or Schottky- barrier contacts with Au on clean GaAs, depending on the method of deposition. Deposition from the vapor phase apparently releases enough energy to form defects rich in anions that can cause Fermi-level pinning near the midgap. Conversely, gentle Au deposition by the flow of Ga-rich Au out of the Au layer leads to low defect densities and "ohmic" interfaces. These results clearly show for the first time, that a near-perfect Au/GaAs interface does not necessarily show Fermi level pinning. However, two models for Schottky contact formation, the "effective work-function model" ascribing the barrier to anion microclusters and the "unified defect model", are both consistent with the results of this study. In the latter case, the defects responsible for Fermi level pinning are believed to be anion-rich. For example, anion antisite defects, which have bulk energy levels similar to the Fermi level pinning positions [11] may be responsible for Schottky barrier formation.

Table 1: Barrier heights and ideality factors of as-deposited and annealed Au diodes on UHV cleaved n-GaAs (110).

	doping $5\mathrm{x}10^{16}$ $[\mathrm{cm}^{-3}]$a)			doping $2\mathrm{x}10^{17}$ $[\mathrm{cm}^{-3}]$b)		
annealing temp.	Φ_b(I-V) (±.02eV) [eV]	n (±.02)	Φ_b(C-V) (±.05eV) [eV]	Φ_b(I-V) (±.02eV) [eV]	n (±.02)	Φ_b(C-V) (±.05eV) [eV]
room temp.	0.92	1.05	1.00	0.87	1.10	0.95
150°C	0.91	1.06	0.99	-	-	-
220°C	0.85	1.07	0.92	-	-	-
290°C	0.80	1.06	0.89	-	-	-
405°C c)	-	-	-	0.72	1.12	0.83
430°C c)	0.80	1.06	0.88	-	-	-
495°C c)	0.80	1.05	-	-	-	-

a) doping determined by the C-V technique, the manufacturer specified $1\mathrm{x}10^{17}$ $[\mathrm{cm}^{-3}]$.

b) doping determined by the C-V technique, the manufacturer specified $7\mathrm{x}10^{17}$ $[\mathrm{cm}^{-3}]$. It should be noted that these diodes formed on the more heavily doped substrates exhibit slightly lower I-V barrier heights due to barrier height lowering mechanisms such as the image force and tunneling.

c) after mesa-etching

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Figure Captions:

Figure 1: I-V characteristics of thick (≈100nm) Au diodes on n-GaAs. The lower curve represents the forward and reverse I-V characteristic of the unannealed diode (Φ_b=0.87eV). After annealing at 405°C for 10 min., the I-V characteristics are found to be almost completely dominated by non-rectifying peripheral leakage current, see upper trace (the results for forward bias greater than ≈0.25V indicate a small rectifying barrier). The middle curve shows the strong rectifying diode characteristics (Φ_b=0.72eV) after elimination of the peripheral leakage current by mesa-etching.

Figure 2: Periphery of Au contacts:

a) as-deposited sample,

b) annealed (405°C, 10 min.) and mesa-etched sample,

c) annealed (405°C, 10 min.) sample (black areas show holes in GaAs after chemical thinning),

d) high-resolution image of the extended Au crystallites marked in (c).

Figure 3: EDX-spectra of as-deposited Au:GaAs diodes (cross-section sample)

a) GaAs substrate far from the interface

b) GaAs ≈10nm from the interface

c) Au layer ≈4nm from the substrate

Figure 4: Au:GaAs interface in the annealed sample (405°C, 10 min.). Clusters of a different phase are seen in the GaAs ≈10nm below the interface.

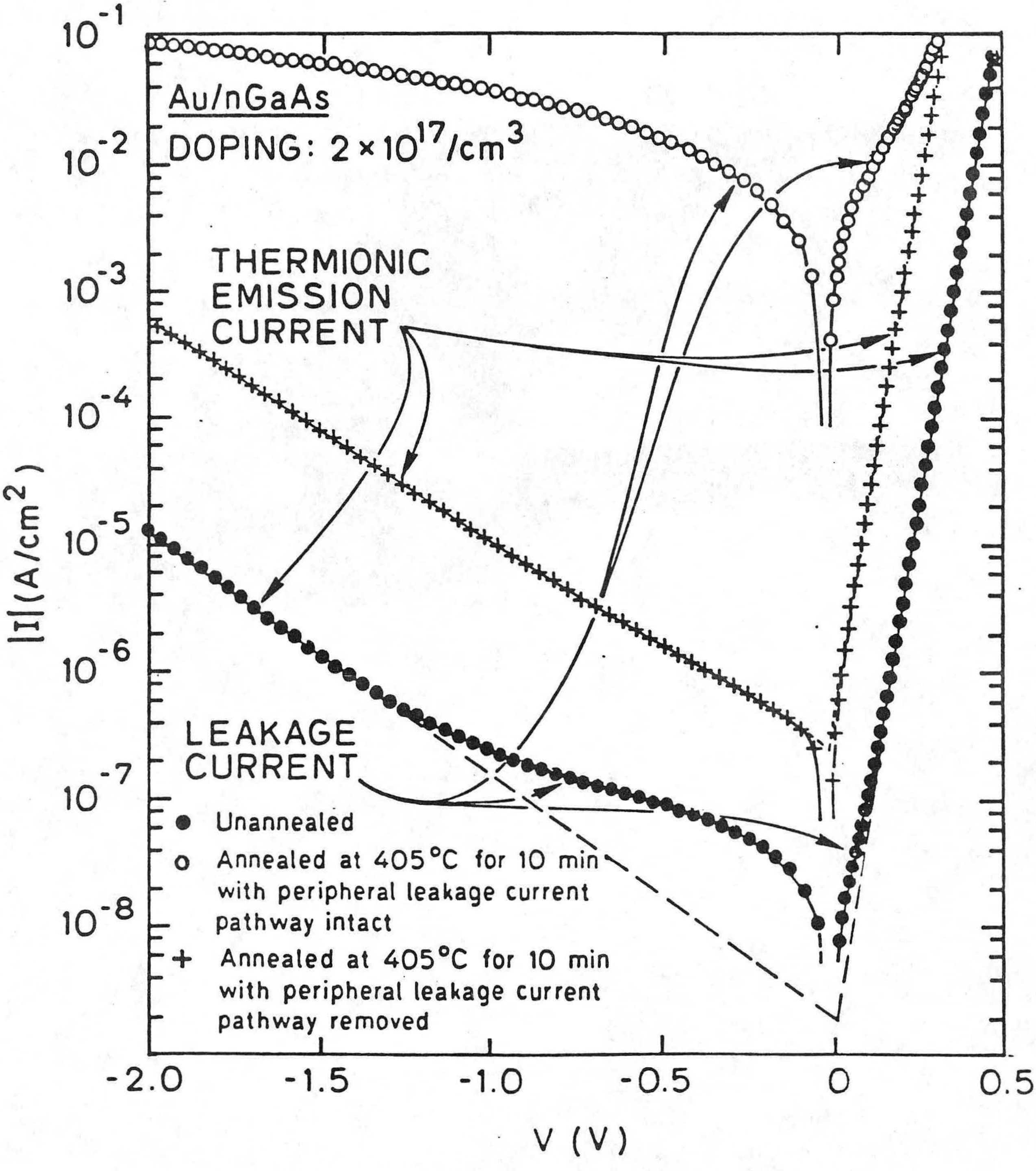

Fig. 1

XBL 8512-4870

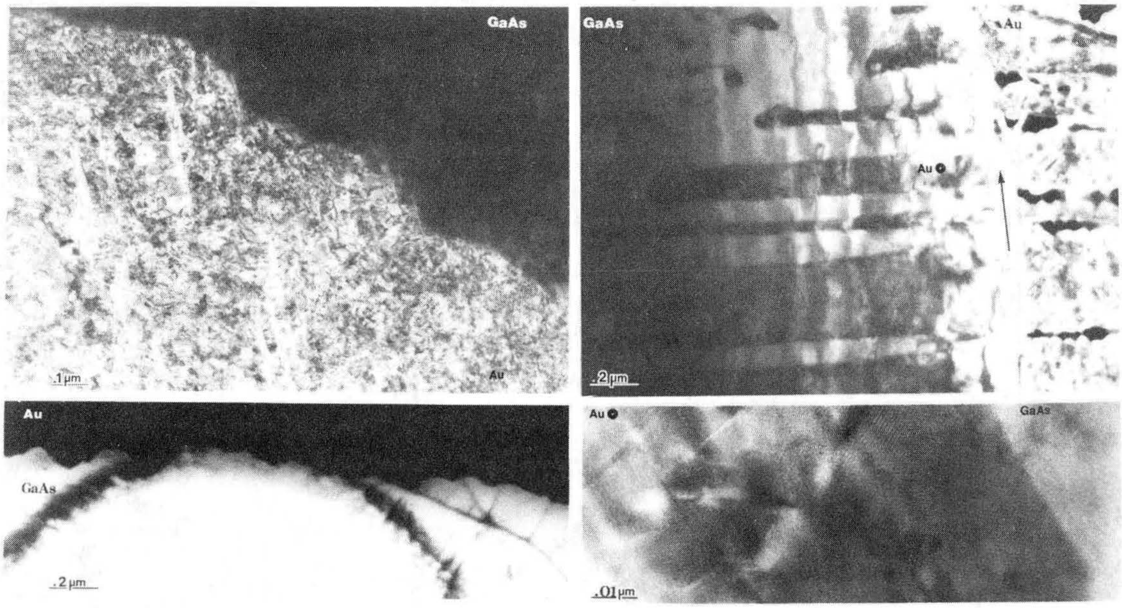

Fig. 2 XBB 857-5105A

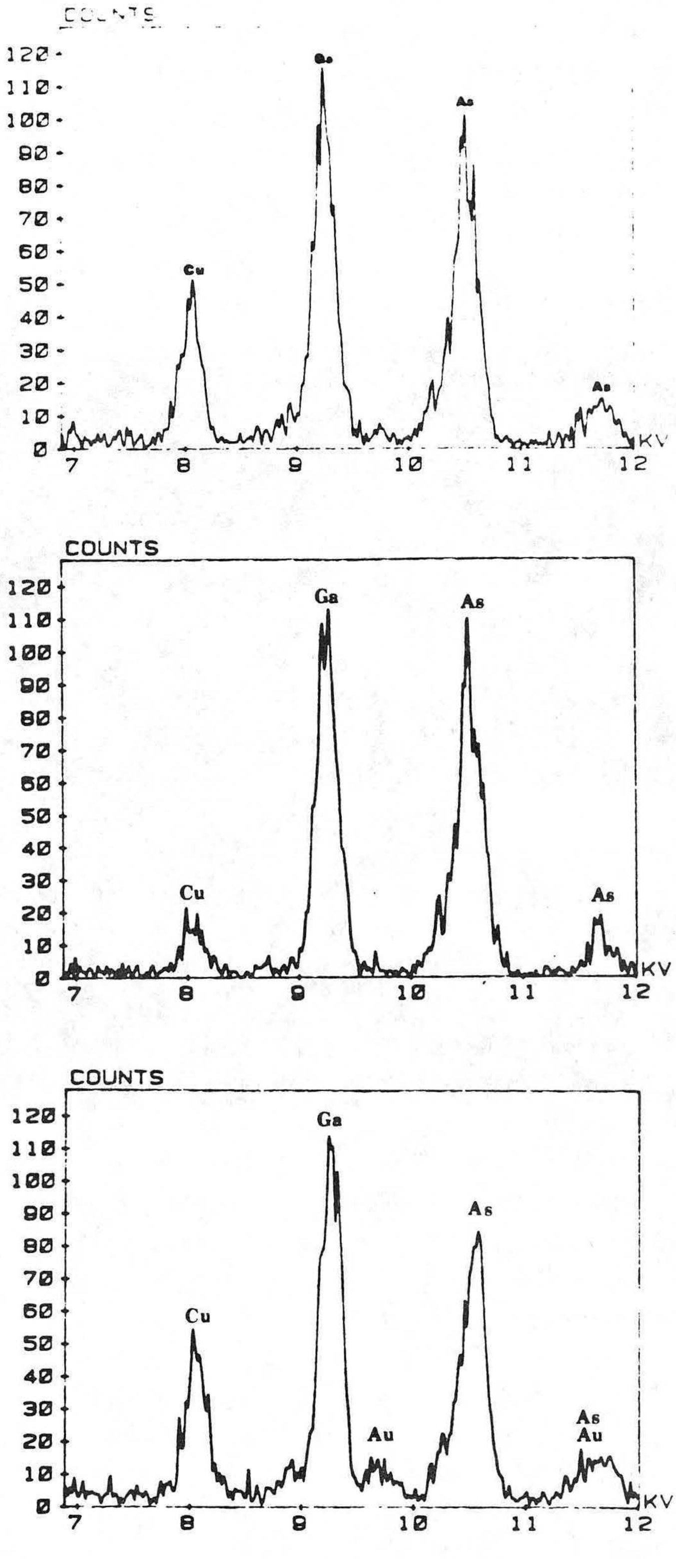

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Fig. 3

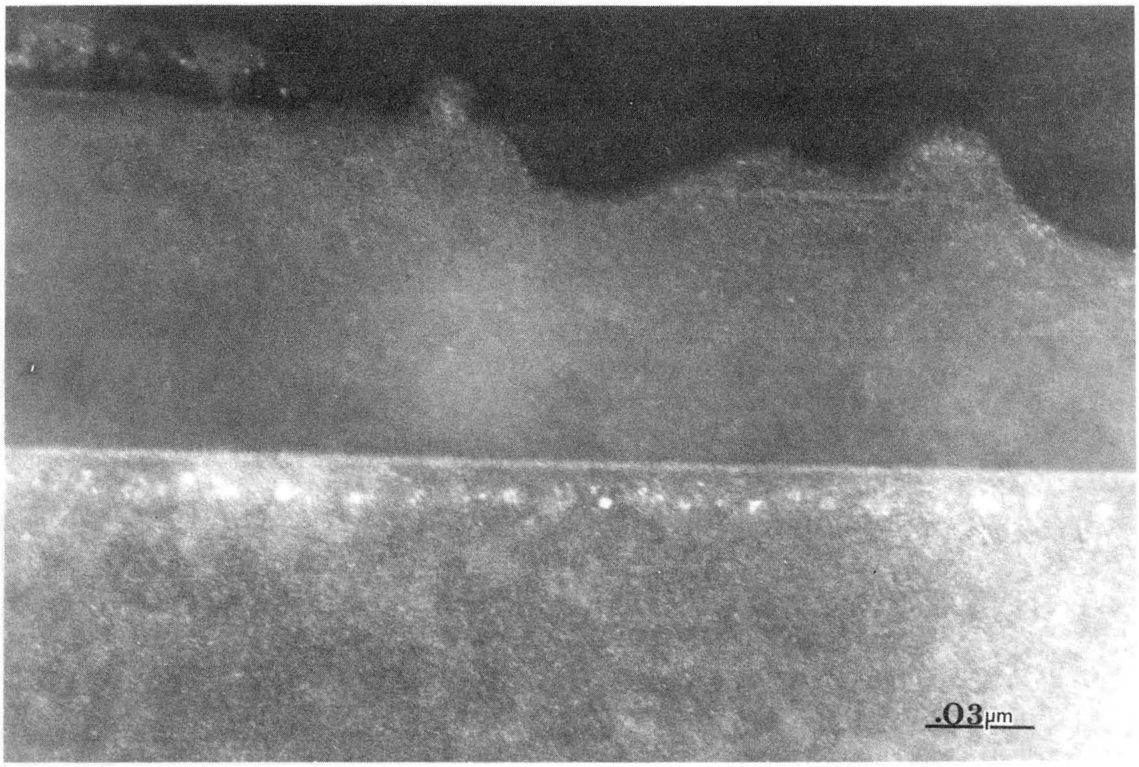

Fig. 4

XBB 857-5115