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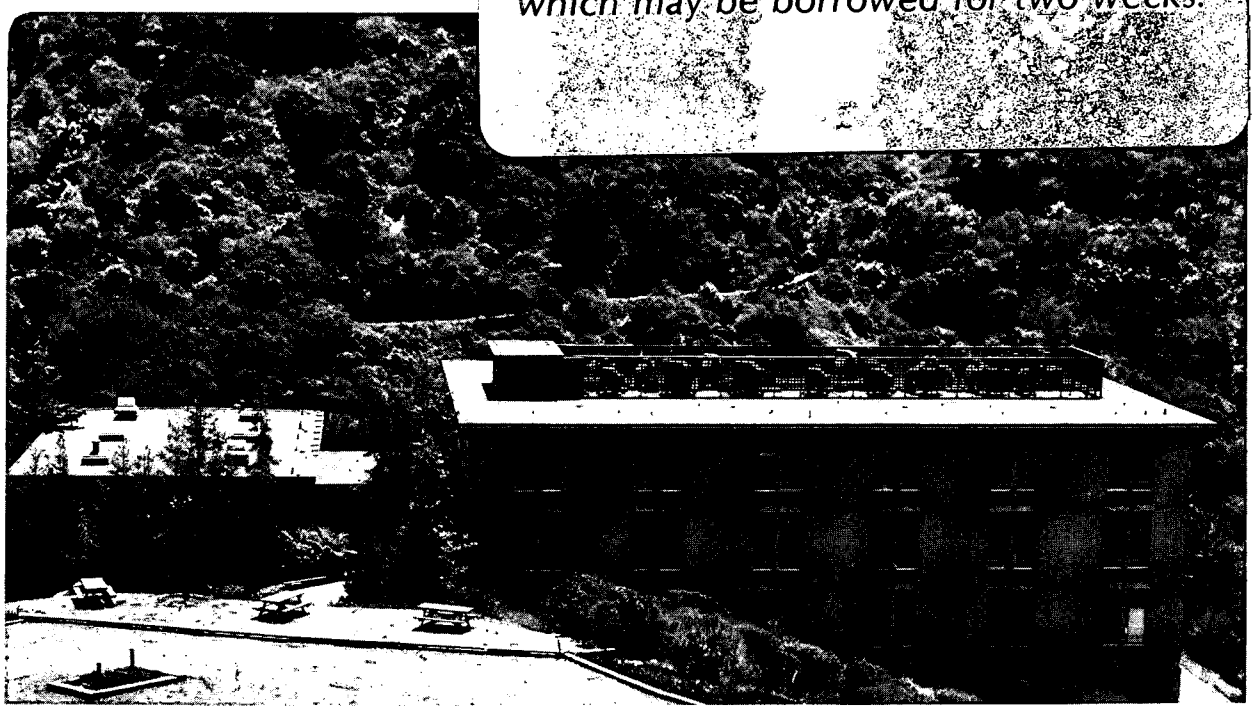

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ABSTRACT

Commonly observed faceting of (110) GaAs grown by molecular beam epitaxy has been systematically investigated. The geometry of the facets with respect to the GaAs crystal is determined and a kinetic model of facet formation is derived from experimental results. The study ultimately led to the elimination of facet formation on (110) GaAs grown by molecular beam epitaxy. Films were examined with microscopic, electrical, and optical techniques.

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INTRODUCTION

Molecular Beam Epitaxy (MBE) is a well established, ultra-high vacuum technique yielding excellent crystal quality and doping profile control.[1,2] GaAs MBE has been traditionally grown on (100) substrates as a carryover from Si technology and because of the wide range of growth conditions which result in good epitaxial layer quality. (110) GaAs epitaxial layers are also needed, however, to make full use of the anisotropic properties of the GaAs crystal. (110) GaAs has been shown to provide a more efficient ionization impact behavior for electrons, can be utilized to fabricate a p-n junction diode polarizer/modulator for use in integrated optics, and is a viable candidate for growth on (110) Si to eliminate the sheet charge layer associated with growth of the polar (100) GaAs/Si.[3-5] Until recently,[6] all published reports of (110) GaAs epitaxial layers grown by MBE have shown unsatisfactory behavior, both morphologically and electrically/optically.[7-9] The (110) GaAs surface appears replete with facets under all growth conditions of substrate temperature, arsenic overpressure and growth rate. In addition, the electronic mobilities and optical luminescence were very poor.

This paper details the examination of facet formation on (110) GaAs grown by MBE. The study has resulted in the understanding of facet alignment and geometry with respect to the GaAs crystal and a kinetic model for initial facet formation on the GaAs surface. This research has ultimately led to a method to eliminate facet formation during MBE growth.[6] The latter depends on optimal thermodynamic growth conditions combined with the exposure of stable Ga ledges in the GaAs

substrate to initiate a two-dimensional growth for the MBE process. The resulting crystals have a smooth surface morphology and excellent electrical response. Investigative methods for facet geometry determination and kinetic modeling of facet growth involved scanning and transmission electron microscopy [(SEM) and (TEM)], convergent beam electron diffraction methods (CBED), AUGER microscopy, variable temperature Hall effect and Liquid He photoluminescence (PL). This paper describes the results of the above investigations and the kinetic model for facet free (110) MBE GaAs growth.

EXPERIMENTAL

Growth of (110) and, as a standard, simultaneous (100) GaAs took place in a Varian GEN II MBE machine. The procedure for conventional GaAs MBE growth is described elsewhere.[1] Each set of MBE growths utilized the same Ga, As, and Si source material, such that no replacement of oven material would effect the experiments. For each growth run, the (110) and (100) GaAs substrates were grown for comparative studies of surface morphology and electrical and optical behavior. Si doping levels for the epitaxial layers were $\sim 5 \times 10^{15}/cm^3$.

(100) and (110) semi-insulating GaAs substrates grown by the liquid encapsulated Czochralski technique were used. The surface defect count (etch pit density) for these substrates was approximately $9 \times 10E3/cm^2$, standard for present GaAs technology. Optimal growth parameters previously determined included substrate temperature of ~570°C, arsenic overpressure of V/III~ 16/1, and growth rate (gallium flux) of 1.4μm/hr for the particular MBE machine utilized.[9] This is

not expected to vary appreciably for other Varian MBE growth chambers, provided the standard analytical equipment is utilized.

Further analysis of faceting on (110) GaAs took place in three phases: analysis of facet geometry and composition with respect to the GaAs substrate, growth and examination of initial layers on (110) GaAs, and a kinetic modeling of the initial facet formation based on experimental observation.

The observed facets on the surface of the epitaxial layers grown on (110) GaAs substrates were examined with respect to GaAs crystal geometry by scanning electron microscopy (SEM) and the orientation of their axis was determined in conjunction with Laue X-ray diffraction (Fig. 1). The directional facets were verified in their orientation by transmission electron microscopy (TEM) studies on a Phillips 400 microscope through a two beam series as well as by high resolution microscopy on a JEOL 200CX. These micrographs are shown in Figs. 2 and 3. A tilting experiment to determine the facet side angles with respect to the (110) surface was performed with a JEOL SEM. Analysis through AUGER microscopy defined the chemical character of the facets and is shown in Fig. 4. A CBED method to determine the exact nature of Ga and As planes observed in situ in the TEM was utilized to analyze the surface nature of the facets.[10]

In order to better understand the kinetics and thermodynamics of facet growth on (110) GaAs, it was necessary to examine the initial facet formation on the (110) GaAs substrates as compared with (100) GaAs epitaxial growth. Separate MBE runs of 100Å, 700Å, and 1500Å

thick epitaxy was grown on (110) and (100) GaAs substrates as shown in Fig. 5 for the former. These layers were examined by the Jeol Sem to determine the growth progression of the observed facets. A kinetic modeling of initial facet formation was derived and described. Based on the following experimental results of the facet geometry, chemical nature of the facets, and the model for initial facet formation, a successful method to eliminate facet formation was developed.[6]

Ohmic contacts for Hall effect examination of the facet free films were obtained by alloying In dots at 420°C for 20 min. in a N_2 atmosphere. Liquid He PL was performed with a 514 nm Ar laser at 25mW on the same films.

RESULTS

The typical facets observed on (110) GaAs grown by MBE are shown in the SEM image of Fig. 1. The facets are aligned along [001] as viewed from the reference stereographic projection. Tilting experiments showed that the side planes are (010) and (100) types with a back facet furface of $(11\bar{1})$, as analysis showed the sides to be roughly 40° from the (110) surface and the back to be ≅32° from the (110) surface. CBED determined the back facet surface exposed a $(11\bar{1})$Ga for all facets examined.[10] The sharp tip is regarded as the facet front.

Figure 2 shows the 000 transmitted and 100 diffracted beams with the associated bright field image of a typical facet (the complete two beam series is not shown here). The result confirms the Laue orientation of facet alignment with the GaAs crystal as

does the high resolution microscopy shown in Fig. 3. The latter shows the facet tip intersects the (110) surface along ⟨111⟩. The dots in the picture, taken with the electron beam along ⟨110⟩, represent a Ga and As pair of atoms.

Figure 4 shows the chemical content of a typical facet (point 2 of the inset) as compared with the GaAs substrate when examined by AUGER microscopy. The surrounding epitaxy and facet tip were also analyzed as indicated by points 1 and 3 of the inset and were also found to be stoichiometric. Microdiffraction with EDAX showed the same chemical makeup. No Ga balling was found.

Initial facet formation studies on (110) GaAs are shown in Fig. 5a. The SEM images show growth of 100Å, 700Å, and 1500Å of epitaxy grown on the (110) surface at both 2600X (left) and 26,000X (right). The progression of the facet formation shows defect initiation at less than or equal to 100Å of growth. The (110) surface is replete with facets by 700Å of epitaxy, and at 1500Å the facets are seen to overlap and continue to grow. The (100) standards were defect free for all growth runs.

DISCUSSION

The results of the facet geometry, composition, and initial facet formation studies suggest that faceting of the GaAs epitaxy begins with chemisorption of the first incoming atomic species as shown schematically in Fig. 6. Note that for the (110) surface, two atoms (a Ga atom and an As atom) are required to bond correctly to the substrate to begin the next layer. As shown, the bonding of the two atoms naturally exposes both types of {111}

surfaces on the (110) epitaxial layer. Kinetic studies have shown that the incoming As species is strongly attracted to the stable $(11\bar{1})$Ga configuration and will chemisorb there first.[11] In addition, the As exposed (111) tends to desorb in the ultra-high vacuum (as supported by the low sticking coefficient of As[1]) leaving behind a non-polar surface. Thus, the stable $(11\bar{1})$Ga surface exposed by the chemisorbed atoms serves as a basis for further chemisorption of the incoming molecular beams of Ga and As species. As a result, the exposed Ga rich $(11\bar{1})$, as verified with the convergent beam diffraction technique, continues to provide the stable growth surface. Facets begin to form from the fast growing $(11\bar{1})$Ga back surface, with sides of (100) and (010) filling in and thus creating the facet shape. From the thin layer growths, it is clear that the facets initiate randomly until the surface coverage is complete. The lack of change of surface morphology with change of growth rate[9] shows that the facets grow linearly with the total Ga flux. This is evidenced, as well, in Fig. 5. The {111} sides and back of the facets then begin to overlap and continue to grow.

Once the correct Ga-rich ledge introduction on the (110) GaAs surface was provided by angling the substrate 6° towards the $(11\bar{1})$Ga as described in Ref. 6, two dimensional or layer by layer growth was accomplished. The exposure of Ga-rich ledges, like the starting point of the facets from the back $(11\bar{1})$Ga surfaces of the chemisorbed Ga-As pair, was the decisive factor in obtaining facet free (110) GaAs grown by MBE. As shown in Fig. 7, angling the (110) substrate 6° toward

the (111)As yields As rich ledges and angling 6° toward either of (010) or (100) yields non-polar ledges. Epitaxial films grown on angled (110) substrates exposing non-polar ledges or polar ledges of As exposure did not improve the faceting of the GaAs films.

In order to be certain that substrates are angled correctly before (110) growth, a simple etching of a (100) surface on the GaAs boule is required which will differentiate the $(11\bar{1})$Ga and (111)As on the (100) face by the rectangular etch pits.[12] Once the $(11\bar{1})$Ga is determined from the GaAs boule, the (110) substrates can be sliced, making sure they are angled 6° toward the Ga-rich $(11\bar{1})$.

The facet free films shown in Fig. 8 were examined by variable temperature Hall effect, liquid He PL, and other electrical and optical methods which showed predictable doping levels (N_{Si}~$4x10^{15}/cm^3$) with excellent room temperature mobility of ~5800 cm^2/V-sec and strong exciton (1.514 eV) luminescence.[6] When compared to the (100) standards, the excellent electrical and optical quality of the correctly angled (110) GaAs films indicated that the planar growth process and correct site chemisorption of the Ga and As species had been ensured, supporting the above model of facet initiation.

CONCLUSION

This systematic study of commonly observed faceting on (110) GaAs grown by MBE showed that the facets were aligned along [001] with exposed sides of {100} and a back Ga-rich $(11\bar{1})$ surface. Kinetic modeling of initial facet formation suggested facet formation initiated from the stable $(11\bar{1})$Ga back surface. Introducing Ga rich ledges to

the substrate surface provided a preferred chemisorption site for the incoming As species. A method to obtain substrates of Ga-rich ledge exposure is outlined. As a result of this investigation, excellent (110) MBE GaAs crystal quality was then consistently obtained as exhibited by smooth surface morphology, high room temperature electron mobilities, and excellent PL results.

ACKNOWLEDGEMENTS

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FIGURE CAPTIONS

FIG. 1. Scanning electron microscope image of faceted (110) surface (6000X). Superimposed facet edge outlines are drawn. These outlines are transferred to the stereographic projection shown to indicate facet geometry with respect to the zinc blende crystal.

FIG. 2. Transmission electron microscopy 100 two-beam image of a thinned facet in plan-view. The facet orientation is seen to lie along [001] with reference to the (110) stereographic projection of Figure 1.

FIG. 3. High resolution transmission electron micrograph of thinned epitaxial facet. The facet planes at the tip are seen to intersect the (110) surface along <111>. The facet tip appears amorphous, or it may, alternately, be thicker than the surrounding area.

FIG. 4. AUGER microanalysis of a typical facet as compared with (100) GaAs bulk. Inset is the AUGER image (SEM) of a facet where points 1, 2 (shown), and 3 were analyzed, all with the same chemical content. The lower As signal is due to a difference in sputter rate, and the As/Ga ratio corresponds to the value observed in the bulk GaAs sample.

FIG. 5. (110) GaAs epitaxial layers of 100Å (top), 700Å (middle), and 1500Å (bottom) shown at 2600X (left pictures) and 26,000X (right pictures). Faceting is seen to occur at $\leq$100Å.

FIG. 6. Idealized (110) surface of GaAs showing top layer configuration of atoms. (Black circles = Ga, white circles = As). Chemisorption of Ga and As pair are shown in the drawing. The chemisorption exposes both types of {111} faces, angled 35 degrees form the (110) surface. These {111} faces are indicated by the area outlined by the dotted lines.

FIG. 7. Schematic of (110) GaAs surface showing ledge configuration when angling the substrate. Angling 6° towards (111)Ga reveals ledges of all Ga exposure, angling 6° towards the opposite (111)As exposes ledges of all As atoms, and angling toward either (010) or (100) yields ledges of non-polar nature as indicated by the side view of alternating Ga and As atoms on edge.

FIG. 8. Scanning electron micrograph of facet free (110) GaAs at both 2600X and 26,000X.

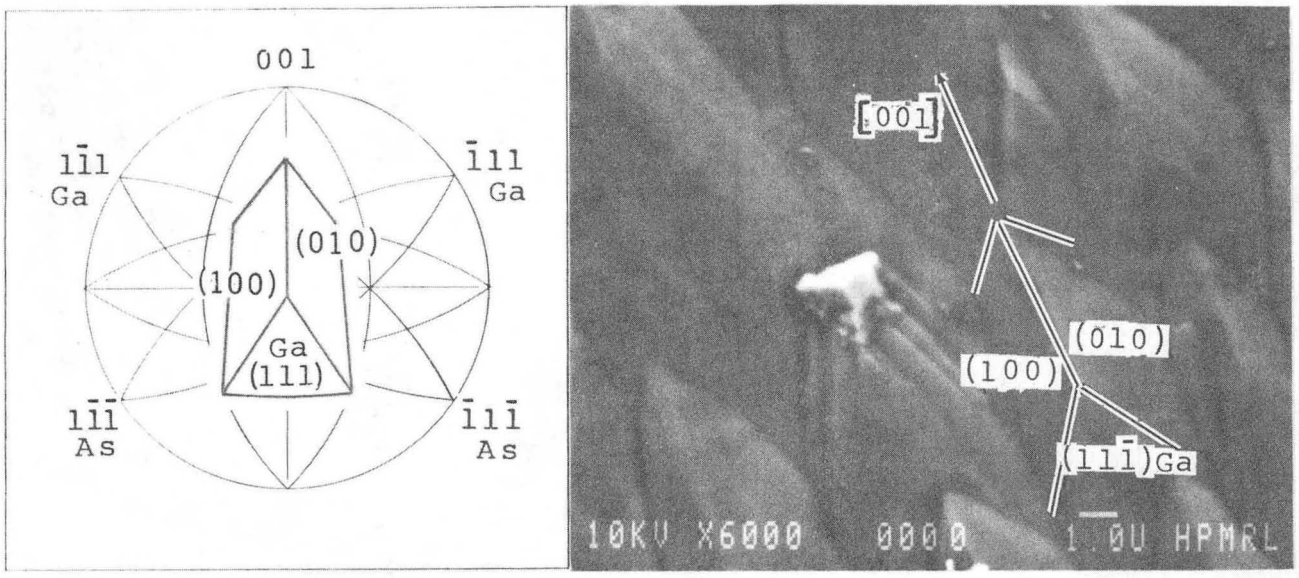

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Figure 1.

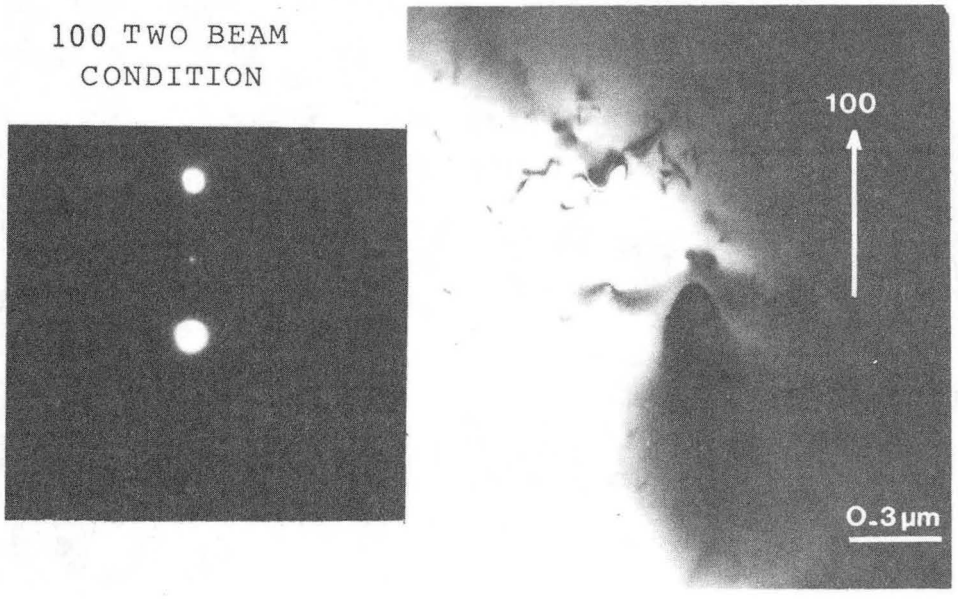

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Figure 2.

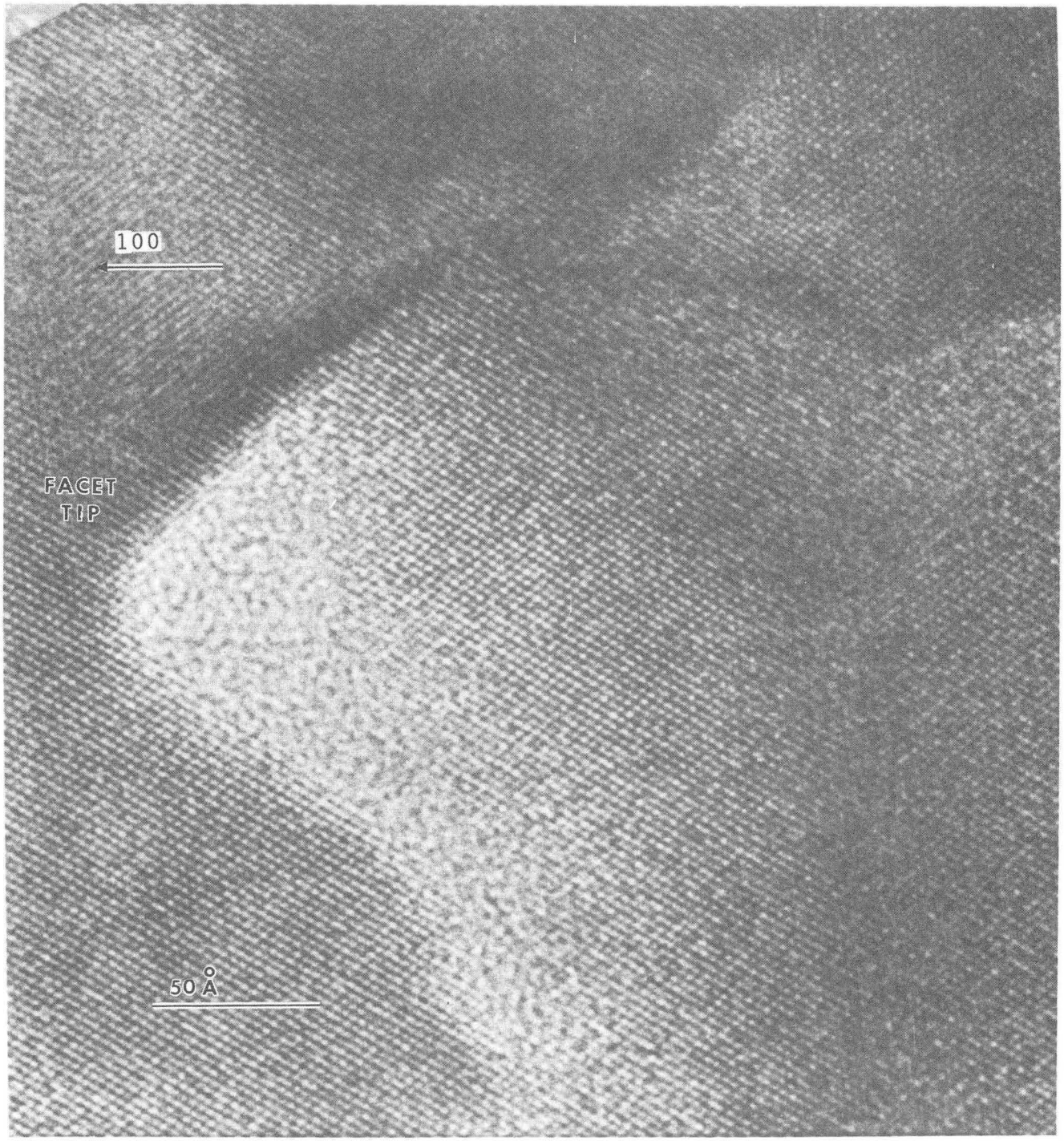

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Figure 3.

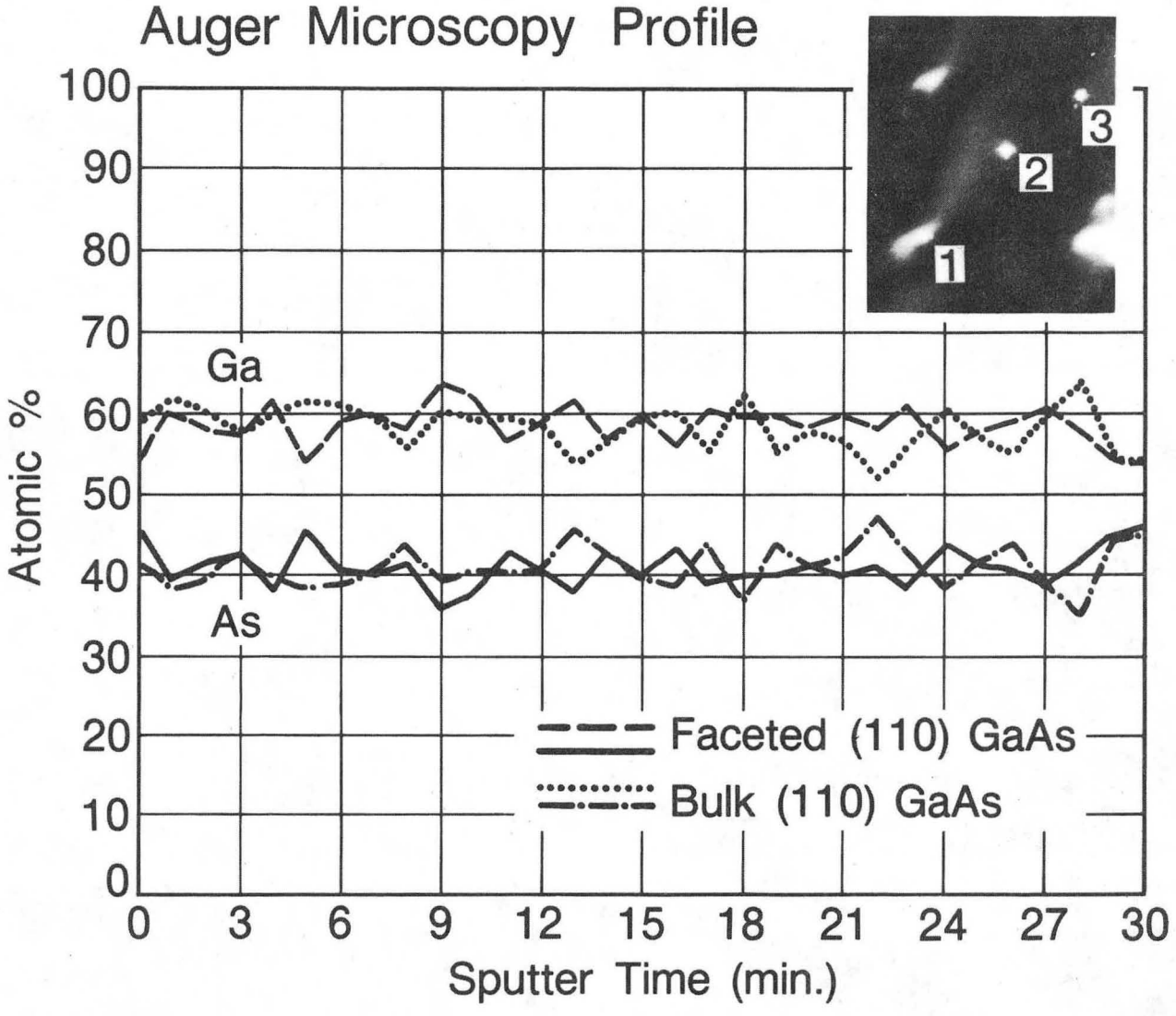

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Figure 4.

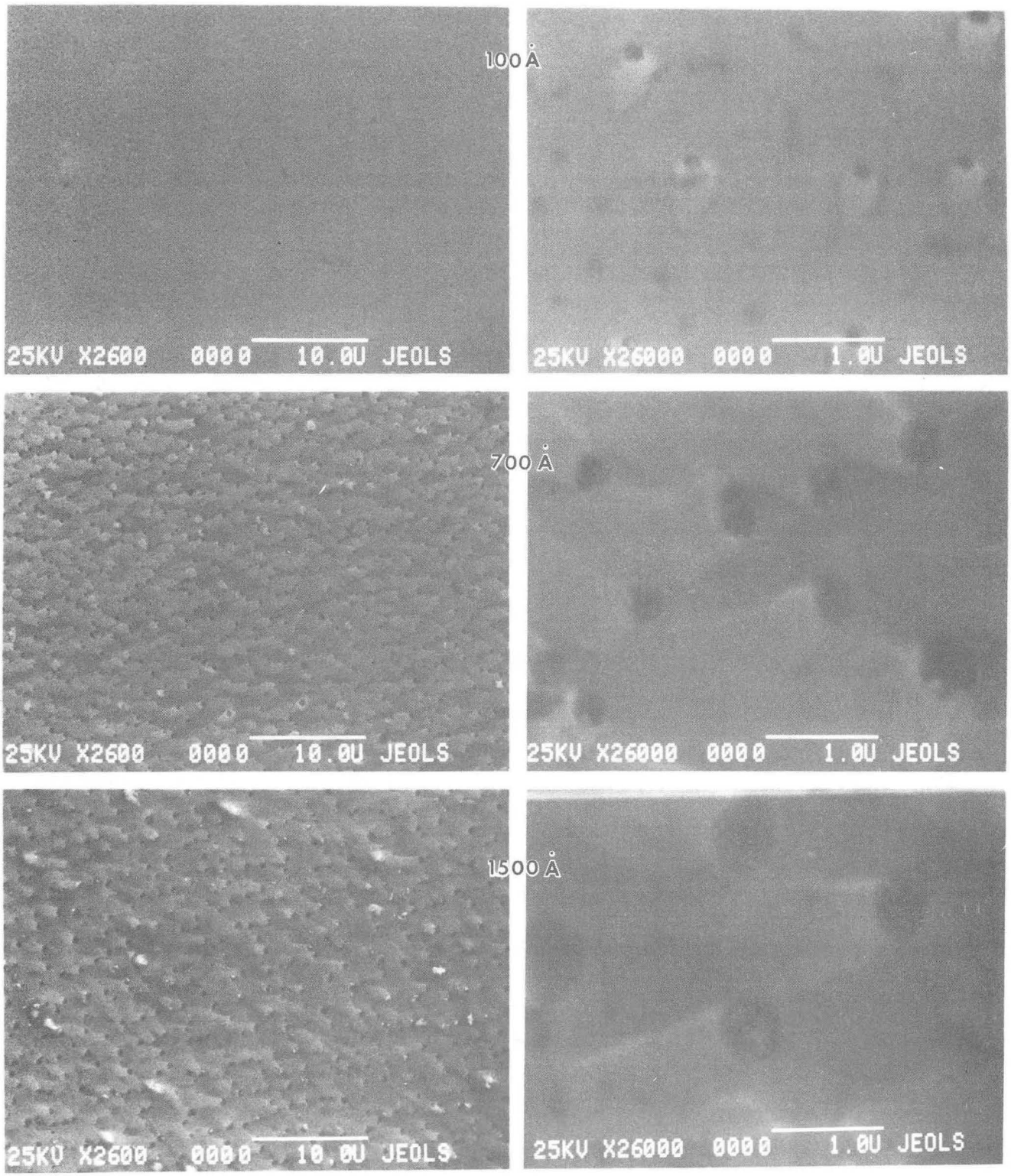

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Figure 5.

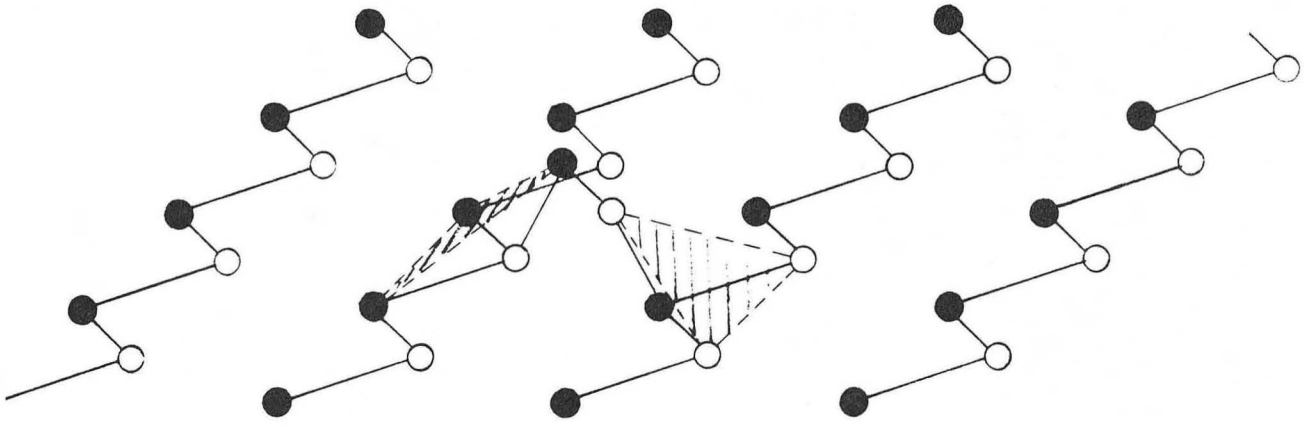

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FIGURE 6 Idealized (110) surface of GaAs showing top layer configuration of atoms. (Black circles = Ga, white circles = As). Chemisorption of Ga and As pair are shown in the drawing. The chemisorption exposes both types of {111} faces, angled 35 degrees form the (110) surface. These {111} faces are indicated by the dotted lines.

Figure 6.

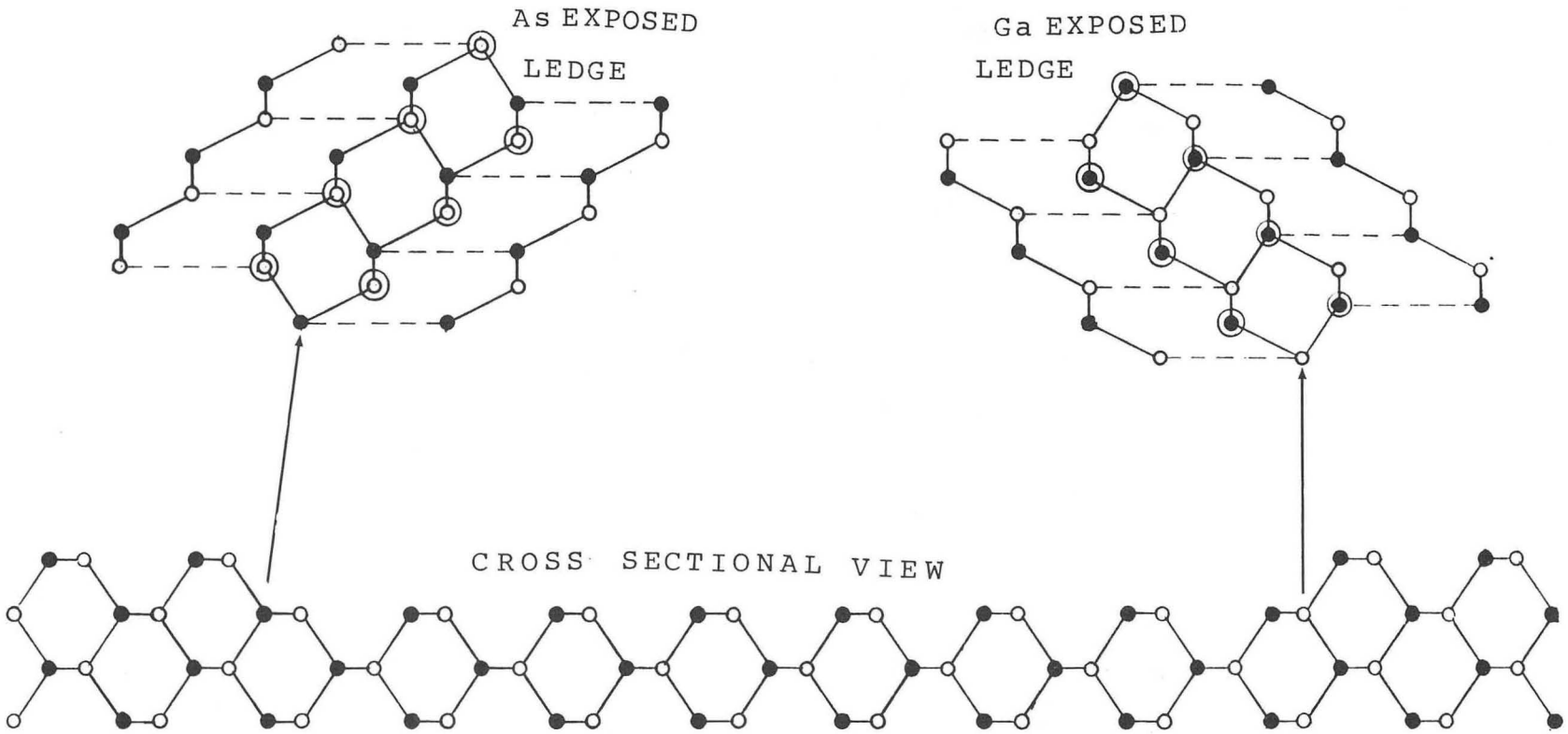

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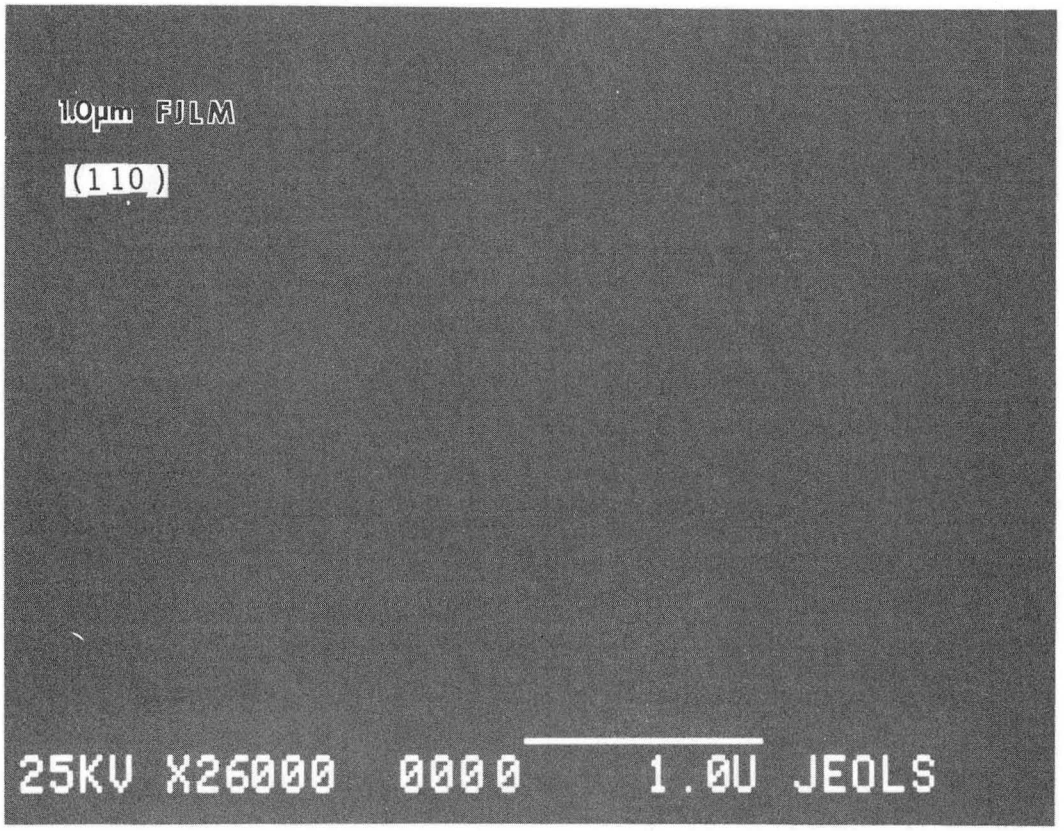
Figure 7.



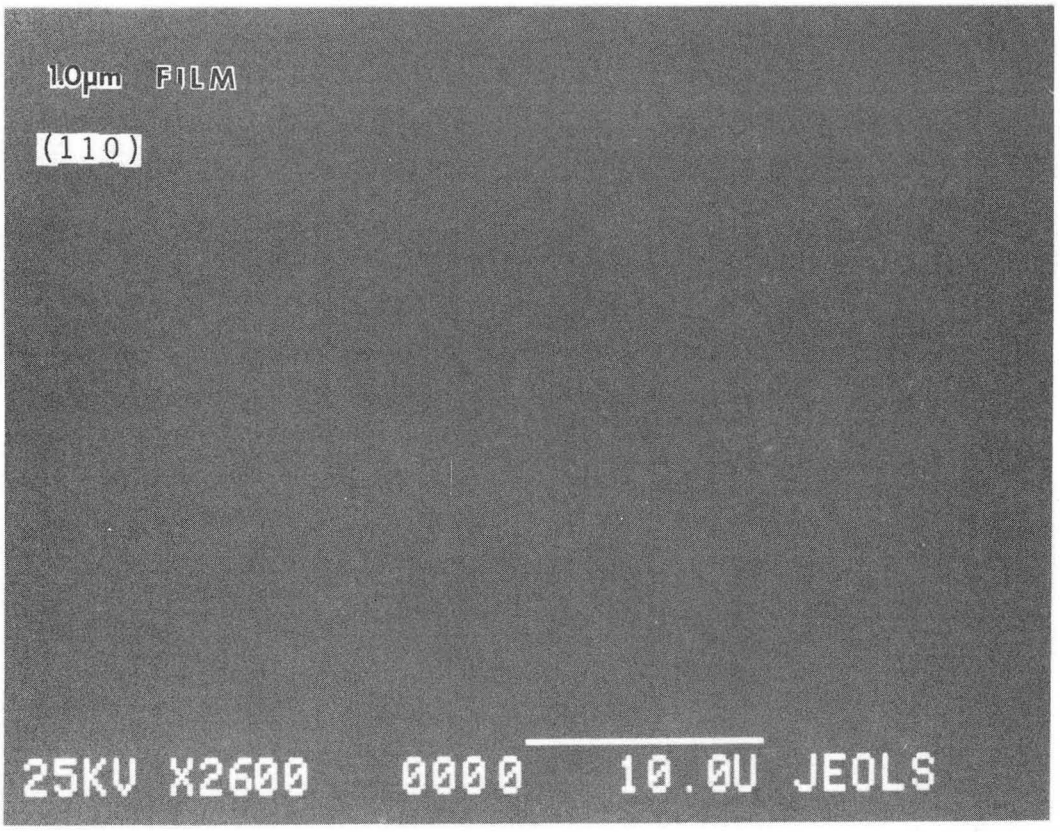


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Figure 8.

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