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Materials & Molecular Research Division

FEB 20 1987
DOCUMENTS SECTION

Presented at the Materials Research Society
1986 Fall Meeting, Boston, MA, December 1-6, 1986;
and to be published in the Proceedings

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December 1986

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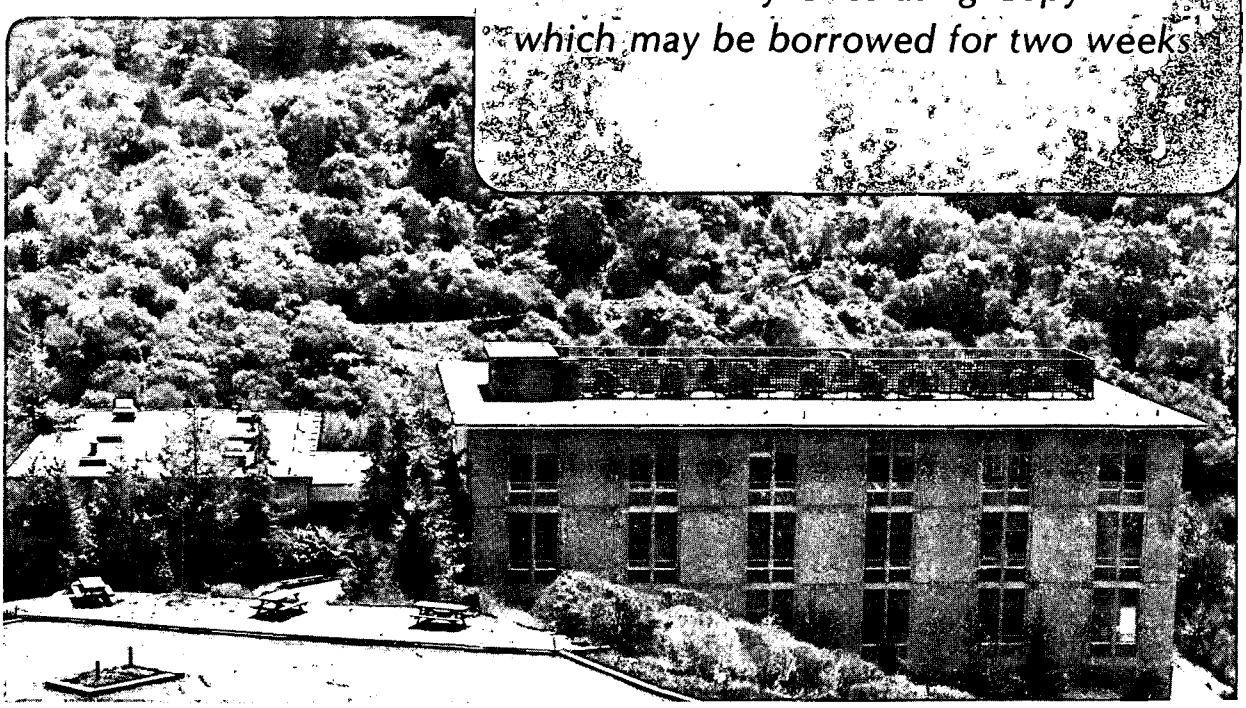

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Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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THE STRUCTURE OF Al/GaAs INTERFACES

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ABSTRACT

The structure of Al/GaAs interfaces was investigated by high resolution electron microscopy. The Al layers were deposited in a molecular beam epitaxy chamber with a vacuum base pressure of $<1\times10^{-8}$ Pa. The GaAs substrate temperature varied during Al deposition from -30°C to 400°C. Deposition of Al on cold substrates $\leq$25°C resulted in epitaxial growth of (001) Al on (001) GaAs. Droplets of Ga were observed in samples with the substrate temperature at -30°C (1x2) and 0°C (c(2x8)). Postannealing of the last sample caused formation of the AlGaAs phase. Deposition of Al on hot substrates (150°C and 400°C) resulted in the formation of the AlGaAs phase, which separated (110) oriented Al from (001)GaAs.

INTRODUCTION

The mechanism of Schottky barrier formation has received theoretical and experimental attention over the past few years [1]. The interest in studying the Al/GaAs system comes from the fact that Al with an fcc structure and a lattice parameter of nearly $\sqrt{2}$ compared to that of GaAs is easy to deposit epitaxially on the (100) surface. The choice of Al also comes from its isoelectronic similarity to Ga and its ability to form semiconducting compounds with As.

The Al/GaAs system is also of special interest because of its potential use in high-speed logic integrated optics, and microwave applications. For such materials a detailed knowledge of the geometric and electronic structure of the interface is fundamental to an understanding of the electrical properties of the contact. It is well known that the properties of Schottky contacts are established within a few atomic layers of the deposited metal. Therefore surface contamination can play a significant role. A method for fabricating contamination-free interfaces is absolutely necessary for reproducible properties, and molecular-beam epitaxy (MBE) offers such advantages for in situ metal deposition under UHV conditions.

Three different epitaxial relationships have been reported between Al and the (001)GaAs substrate [2-4]. The mechanism responsible for the final orientation of the Al overlayer is still far from being understood. It was suggested that surface reconstruction and growth mechanisms can influence the resulting Schottky barrier height [4].

Therefore we started a systematic study of the structure of Al/GaAs interfaces as a function of surface reconstruction, substrate temperature, and growth rate of Al.

SAMPLE PREPARATION

The samples were prepared and subsequently analyzed in an MBE growth system equipped with several pyrolitic BN effusion cells that contained the necessary evaporants in elemental form. The following in situ instruments were available for monitoring the growth and for its analysis: reflection high energy electron diffraction (RHEED), a residual gas analyzer (mass spectrometer), an ion sputter gun, and a cylindrical mirror analyzer (CMA) with a co-axial electron gun for Auger electron and electron energy loss spectroscopies. A sample introduction chamber, interlocked with the main chamber, provided quick sample access and improved vacuum performance.

A typical operational sequence consisted of transferring a polished and etched GaAs(001) substrate onto the substrate manipulator in the main chamber. If carbon was detected, the substrate was first sputter cleaned; otherwise it was directly heated in the As beam to the deposition temperature (~550° - 600°C). The normally present oxide layer of the unsputtered substrate was removed by this heat treatment. An epitaxial GaAs film, doped n-type with Ge ($5x10^{17}$ cm^{-3} but in some samples even $3x10^{19}$ cm^{-1}) was subsequently grown to a thickness of 0.2-0.5 μm. Growth was then stopped and the desired surface reconstruction generated. The main chamber pressure was ~10^{-7} Pa. Upon closure of the As-shutter, the pressure rapidly dropped to the 10^{-8} Pa range.

After the surface preparation procedure described above, the GaAs substrate was cooled to the desired substrate temperature (T_S) and Al was evaporated. The amount of Al deposited was determined from timed depositions based on calibrated rates established from thick overgrowth. Five different types of samples were studied (Table I). Cross-section samples were prepared for study by high-resolution electron microscopy. Because of the small unit cell of Al, the JEOL 200CX electron microscope did not provide enough resolution. Therefore we used the Atomic Resolution Microscope (ARM) at Berkeley, with its 1.7 Å point to point resolution.

Table I. Description of samples used in the experiment.

No.	Substrate temp. T_S, °C	Surface[1] reconstruction	Growth rate, μm/h
114	-30	(1x2)	0.15
105	0*	c(8x2)	0.08
53	25	(4x6), (2x6)	2.00
108	150	c(2x8)	0.04
57	400	c(2x8)	0.03

[1] Ga surface density: c(8x2) > (4x6) and (2x6) > c(2x8) > c(4x4).
*Post-annealing treatment described in the text.

EXPERIMENTAL RESULTS

In sample 114 (T_S = -30°C, (1x2)) elongated domains (40-70 nm long) parallel to the interface with GaAs were observed (Fig. 1). Their thick-

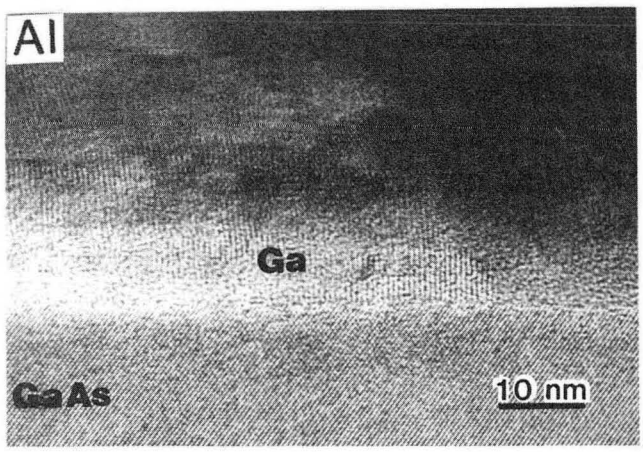

Fig. 1. Cross section of the Al/GaAs interface in the sample 114 (T_S = -30°C, 1x2). Notice the faceted domains formed within 20 nm of the interface.

ness varied from 5 to 20 nm. When the domains were thin (~5 nm), clusters of several domains with clear facets were observed within 20 nm of the interface. The measured thickness of the whole Al layer was ~70 nm. These faceted domains were not observed in the layer more than 20 nm from the interface. Between these domains Al(001)∥GaAs(001) was observed. For the cross-section samples the observed relationship between the Al layer and the matrix was Al[100]∥GaAs [110] with $[010]_{Al} \parallel [110]_{GaAs}$. The orientation of Al between domains dominated the growth, and the same oriented (001)Al grains were observed above the domains and between them. Within these domains lattice images of distance 0.41 ± 0.01 nm were observed, resulting in one row of diffraction spots on the diffraction pattern. Because of one-dimensionality such a diffraction pattern is hard to interpret. It was clear that such lattice distances do not exist in Al and Al-GaAs related compounds, including the ordered structure reported by Kuan [5]. The interface where the domains were present was rougher than the areas where the domains were not present, but even in the areas between domains the interface was not atomically flat.

In sample 105 (with T_S = 0°C, surface reconstruction c(8x2), growth rate 0.08 μm/h postannealed subsequently at 100°C, 200°C, 350°C, 450°C and 700°C), such domains, with lattice image 0.41 nm apart, were observed as well (Fig. 2a). These domains were more uniform. Their thickness was estimated at ~20 nm and their length was ~1 μm. For these areas a two-dimensional diffraction pattern was obtained (Fig. 2b) when the substrate was tilted about 26° to the (013) orientation. The indices were assigned for β Ga [6], which has 0.41 nm spacing between (020) planes. Between these domains Al(001) and GaAlAs(110) were observed. This would suggest that an exchange reaction has taken place and that this reaction does not appear to be distributed uniformly. Formation of Ga droplets seems to be characteristic of Al growth at low temperatures, and the Ga-stabilized surface seems to be helpful in the formation of these droplets. Post-annealing treatment did not remove them. Such droplets were never observed in samples with higher substrate temperatures during Al growth.

In sample 53 (T_S = 25°C, surface reconstruction (2x6), and Al growth rate 2 μm/h), most Al grains were in the (001) orientation parallel to the (001)GaAs surface, and some of the grains showed the (110) orientation with $[002]_{Al} \parallel [\bar{2}20]_{GaAs}$. Diffraction patterns from two kinds of grains are shown in Fig. 3a and 3b. The lattice image showed monoatomic steps (2-4 Å high) along the interface. No exchange reaction was discovered by dark field imaging.

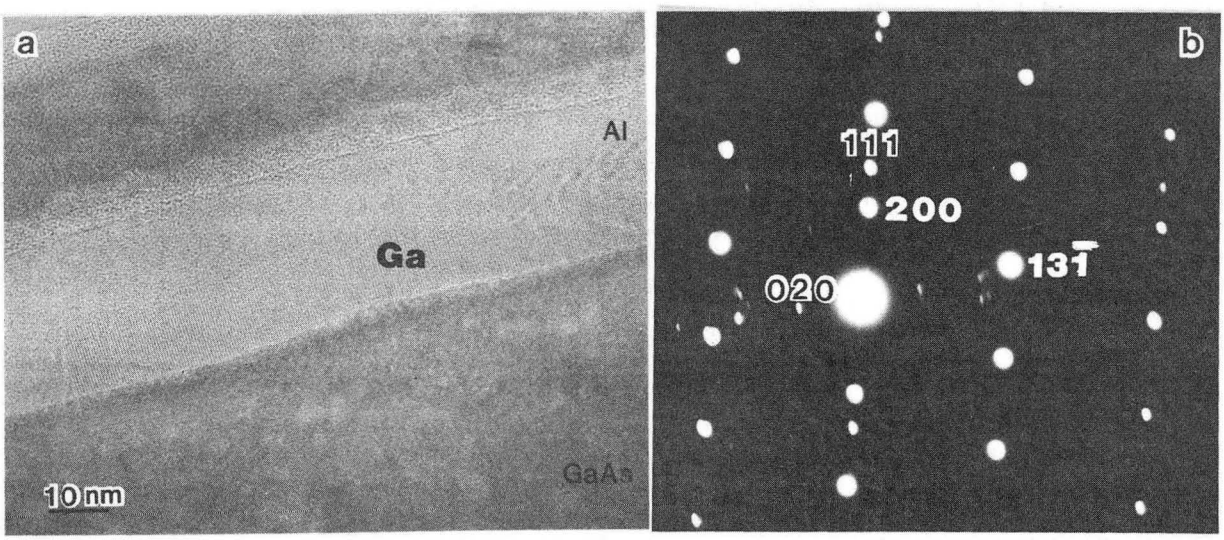

Fig. 2. a) Droplet of Ga present at the interface with GaAs in sample 105 (T_S = 0°C, c(8x2)). b) Diffraction pattern obtained in the domain shown in a) when the substrate was tilted to the [013] orientation.

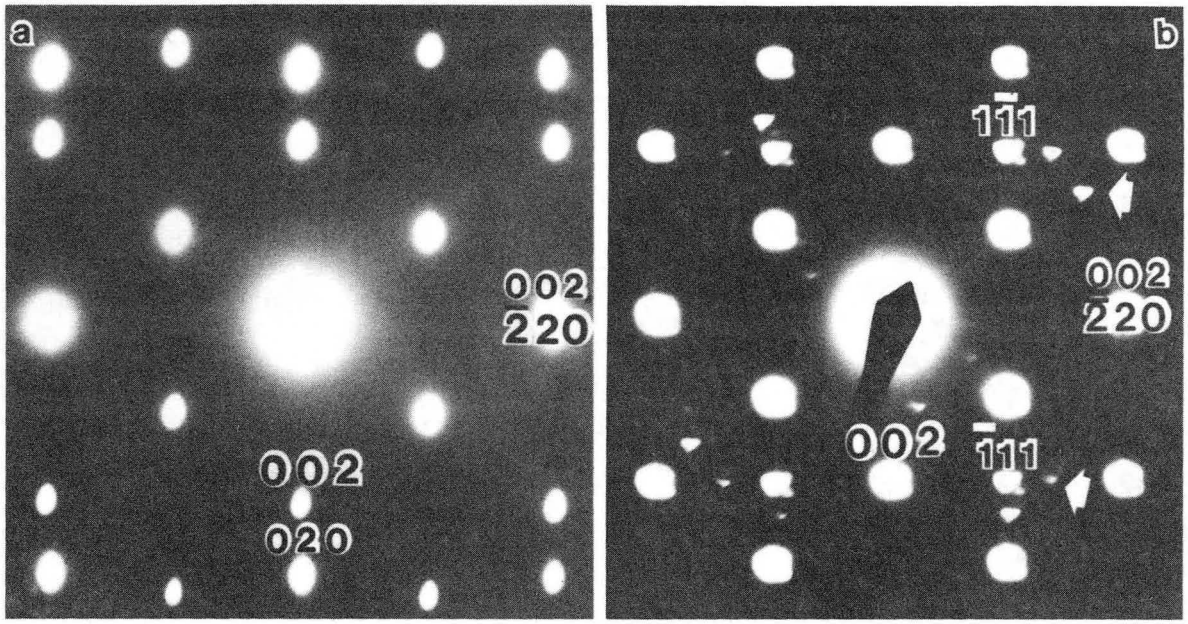

Fig. 3. Diffraction patterns from the Al/GaAs interfaces obtained for two different Al grains. Diffraction pattern a was taken from cross-section sample 53 (T_S = 25°C, 2x6), and b was taken from the sample 108 (T_S = 150°C, c(2x8)). Marked by arrows are spots from (110)R Al grains observed only for the higher deposition temperature. a) $(100)_{Al} \parallel (110)_{GaAs}$ with $[020]_{Al} \parallel [002]_{GaAs}$, which indicates the deposition plane. (b) $(110)_{Al} \parallel (110)_{GaAs}$ with $[\bar{2}20]_{Al} \parallel [002]_{GaAs}$, which indicates the deposition plane.

For the As-stabilized surface c(2x8) (sample 108), with T_S = 150°C and Al growth rate 0.04 μm/h, triangular faceted islands with (110)Al orientation were observed along the interface with GaAs, with $[002]_{Al} \parallel [\bar{2}20]_{GaAs}$ (Fig. 4). These islands were imbedded in strips of Al parallel to the interface where the $[\bar{2}20]_{Al}$ axis was inclined to the same axis in the triangular islands. A layer of AlGaAs was formed on the GaAs interface; this AlGaAs layer increased its thickness in the samples where the substrate temperature was kept at 400°C during Al growth (sample 57). The composition and orientation relationship for certain samples is shown schematically in Fig. 5. For the last two samples, with Al deposited on hot c(2x8) substrates (150°C and 400°C), additional spots on the diffraction pattern were observed. These spots (marked by arrow in Fig. 3b) were associated with Al(110)R described previously [2]. In cross-section samples it is not possible to distinguish Al(110) and Al(110)R when these two phases are present in the two separate samples. These two grains are rotated 90° towards each other, and a particular (110) axis in (001)GaAs is chosen arbitrarily during cross-section sample preparation. When such two grains are present in the same sample, this distinction is easy because diffraction patterns are arranged differently (Fig. 3b).

CONCLUSION

This study shows that during Al growth at low temperatures (≤0°C), the Al layer is epitaxially regrown on (001)GaAs, forming in most cases Al(001) grains. This is the most stable and expected Al arrangement on (001)GaAs showing fourfold symmetry for the substrate and the layer, because of a good lattice mismatch between the $GaAs_{220}$ (1.997Å) and Al_{200} (2.03Å) on two perpendicular axes. For the sample grown at low temperature, droplets of Ga were observed. The Ga droplets can be formed during formation of the Ga-stabilized surface. Post-annealing treatment made these droplets more uniform than in the case of as-grown samples at -30°C. Some exchange reaction

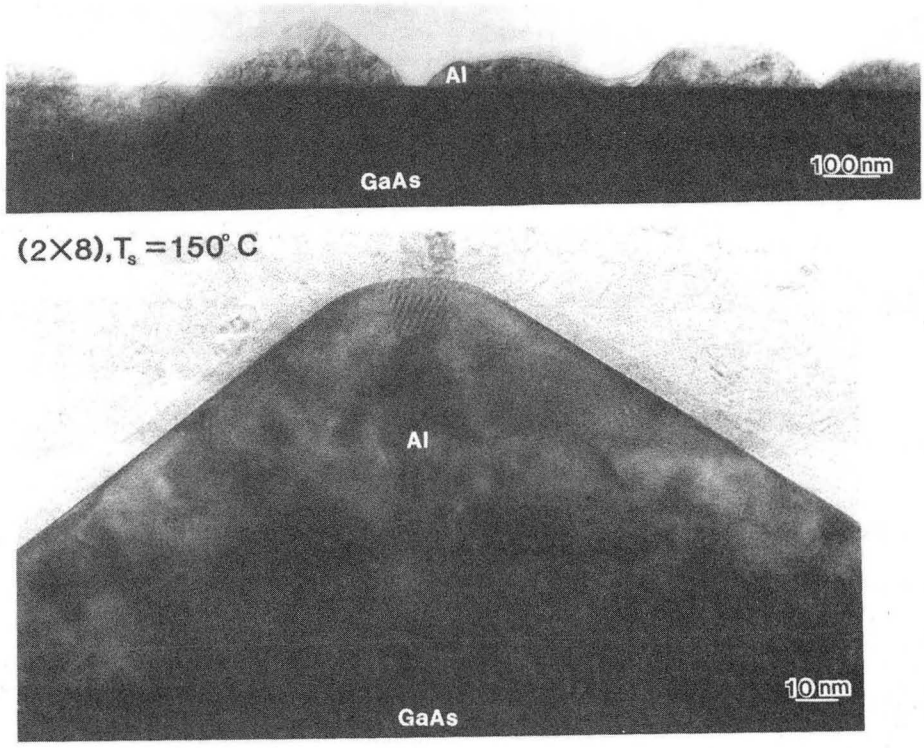

Fig. 4. Al(110) triangular islands formed on the interface with GaAs in sample 108 (T_S = 150°C, c(2x8)). The thin layer of GaAlAs was observed by dark field imaging.

took place, and formation of GaAlAs as well as (001)Al was observed in several areas of the samples, but their composition varied from place to place (from 5% of Al to 25%). This exchange reaction was not observed on As-stabilized surfaces at room temperature, in agreement with previous observations [2,4].

For higher temperatures for c(2x8) As-stabilized surfaces, formation of the AlGaAs phase was observed. The thickness of the AlGaAs layer increased for the sample with T_S = 400°C. The Al layer adjacent to the AlGaAs in most cases had a (110) orientation parallel to the (001)GaAs. Formation of triangular islands was characteristic of higher growth temperatures. Some of the grains were randomly oriented in all investigated samples. The Al (110)R and (110) orientations reported earlier [2] were found in the samples deposited at high substrate temperature (150°C and 400°C). This can be related to the GaAs surface reconstruction c(2x8), which shows only twofold symmetry. In such cases the Al epitaxial regrowth occurs only on one axis, and (110) or (110)R grains with twofold symmetry are present.

No dependence of the Al orientation on the growth rate was observed during this study.

ACKNOWLEDGEMENTS

This work was supported by the Materials Science Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The electron microscopy was performed at the National Center for Electron Microscopy in Berkeley. The authors would like to thank Drs. E.R. Weber, P. Petroff and M. O'Keefe for fruitful discussions, and G. Landgren for his contributions in the MBE growth.

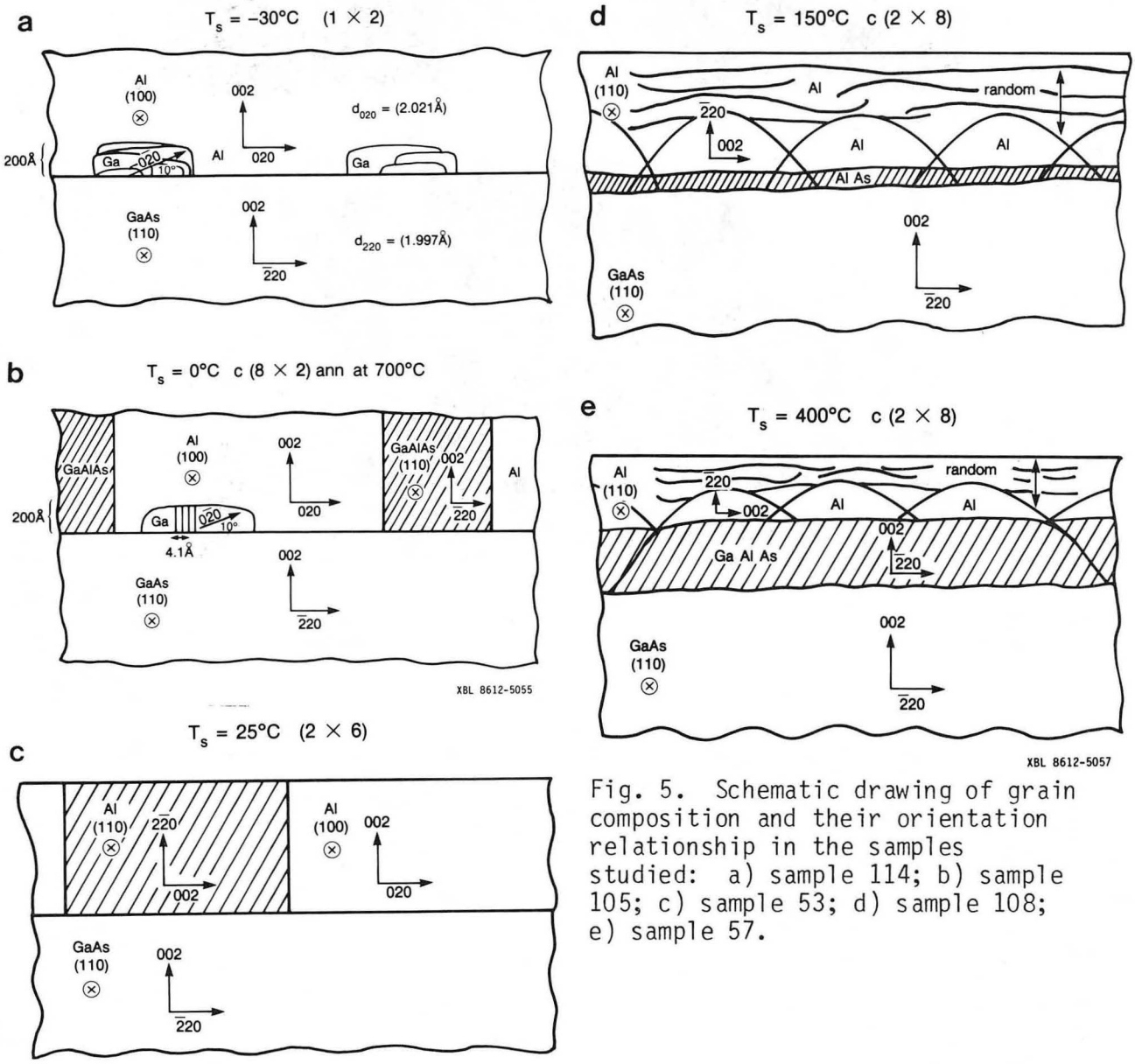

Fig. 5. Schematic drawing of grain composition and their orientation relationship in the samples studied: a) sample 114; b) sample 105; c) sample 53; d) sample 108; e) sample 57.

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This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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