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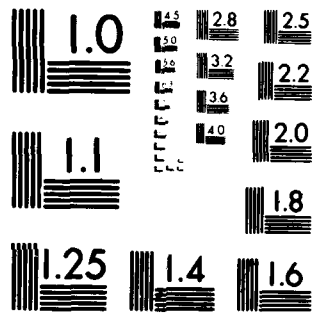
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TECHNICAL REPORT #3

SITE-SPECIFIC DENSITIES OF STATES FOR CLEAVED AND  
SPUTTERED GaAs (110) FROM AUGER LINE SHAPES

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SITE-SPECIFIC DENSITIES OF STATES  
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FROM AUGER LINE SHAPES\*,\*\*

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The nature and extent of interfacial chemical reactions are major factors affecting the electronic properties of semiconductor-metal or semiconductor-semiconductor interfaces. These reactions and the resulting chemical phases may depend strongly on the surface structure and the extent and nature of structural defects. A first step to understanding defect-related chemical phase formation and interfaces is to correlate local chemical properties with structural defects. We have made an initial attempt to do this for GaAs (110) by comparing the results of several techniques. We have examined the cleaved and sputtered GaAs (110) surface with x-ray photoemission spectroscopy (XPS), Auger electron spectroscopy (AES) line shape analysis, low-energy electron diffraction (LEED), and scanning electron microscopy (SEM).

In the Auger process, because the initial core hole is localized around one atom, the probability of exciting a valence electron in a core-core-valence transition falls off quite rapidly away from the core. (1) Consequently, the charge distribution that is probed by such transitions is site-specific and may differ if the initial core hole is made on the anion or the cation. (2)

This is in contrast to a photoemission measurement, where sites widely separated in R may contribute to the photoelectron intensity at a particular value of energy. ↖

Auger and XPS measurements are made with standard instrumentation. In order to extract true intensity distributions, both the Auger and XPS measurements are deconvoluted with an instrument/loss function to correct for (1) the

analyzer broadening; and (2) the inelastic scattering of the electrons as they traverse the solid.<sup>(3)</sup> Additionally, a Lorentzian or a sum of Lorentzians is included in the deconvolution to correct for the broadening and satellite lines in the XPS data resulting from the achromaticity of the x-ray source<sup>(4)</sup>, and for the broadening in the Auger data resulting from the lifetime of the core levels involved in the transition.<sup>(4)</sup>

LEED and SEM measurements were made on the cleaved and sputtered GaAs (110) surface. LEED data were recorded with an on-line vidicon camera.<sup>(5)</sup> SEM measurements were made in a standard SEM with a field emission source.

Changes in both the Auger line shapes and in the XPS valence band spectrum are evident with sputtering. On the basis of the Auger results and the scanning electron micrographs, these changes can be explained by a surface enrichment in Ga due to preferential sputtering of As. The composition range over which GaAs can exist as a single phase is quite narrow, ranging from 49.9%Ga to 50.01%Ga.<sup>(6)</sup> Any Ga in excess of this will form a second phase. The scanning electron micrographs of the sputtered surface show Ga-rich bubbles of diameter about 1 $\mu$ m or less covering about 10-20% of the surface. Annealing of the GaAs caused these bubbles to align preferentially along [100] directions, probably along steps. The LEED results show a large density of steps and also additional damage that may be a combination of finite-size and misorientation effects.<sup>(7)</sup>

Auger KLL spectra and XPS 3d core level spectra show an As depletion of from 15-20%, corresponding to a near-surface composition that is ~60%Ga and 40%As.

The Auger line shapes verify the two-phase nature of the surface. The Auger  $M_1 M_{45V}$  lines of Ga and As were measured and the line shapes extracted for the cleaved and sputtered surfaces. These transitions involve the same core levels for both ion cores and thus should reflect a local valence-band density of states around each site in the same way. A sum of the As and Ga lines shows good agreement in peak positions with the valence band density of states measured by XPS.<sup>(8)</sup> The Ga and As lines are quite different from each other, however.

When the surface is sputtered, the line shapes change. The As line shows only a general decrease in intensity without much change in its features. The reduction in area of the line is approximately 20%. The Ga line, shown in Figure 1, shows marked changes as the surface is sputtered. The changes can be explained by considering the Ga line as the superposition of a spectrum from Ga in GaAs and from pure Ga. An Auger electron from a Ga atom in a Ga environment and one from a Ga atom in a GaAs environment cannot be distinguished on the basis of energy, and so the observed line should be the superposition of intensities from the two phases. Because As can exist in this situation only as As in GaAs (and not likely as pure As or any other As compound) the observed decrease in the As Auger line reflects simply the decrease in As at the surface.



The XPS valence band measurements show changes upon sputtering of the surface that are consistent with the formation of a two-phase region on the surface, although this conclusion could not have been arrived at solely on the basis of the XPS results. In the valence band spectrum, peaks preferentially associated with the As atoms, such as the p-like states at the top of the band and the s-like As states at  $\sim 10\text{eV}$ , decrease in magnitude, while those features related to Ga atoms increase in magnitude.

LEED results on these surfaces<sup>(6)</sup> are also consistent with this description of the structure of the sputtered surface, although it is not yet possible to distinguish incoherent two-phase mixtures from finite-size or misorientation effects in a single phase.

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### Figure Caption

1. Ga  $M_1$   $M_{45}$ V site-specific density of states. Solid curve-cleaved surface; dashed curve-sputtered surface.

