

FIG. 2. Small-angle scattering from amorphous InAs. The dashed curve shows the scattering expected from a 1-volume-% concentration of randomly distributed voids 5 Å in radii.

The above structural evidence strongly suggests that the CRN model is applicable to amorphous InAs. As mentioned, we are now confronted with evidence that bonds between like atoms exist. If the atoms retain the same charge as in the crystal, then the random distribution of wrong bonds should cause strong fluctuations in the Coulombic energy. High-energy, high-resolution photoemission experiments, however, find that the core levels remain as sharp in the amorphous as the crystalline form.¹³ To explain this result we require a spatially homogeneous Coulomb field, which would argue against the presence of such wrong bonds unless there is some mechanism which tends to keep the Coulombic field homogeneous in spite of the wrong bonds.

We must also consider the possibility that the CRN as presently constructed does not describe the structure of amorphous III-V compounds, and possibly even amorphous Ge. Although the CRN fits the RDF, it is essentially a one-dimensional curve that can be fitted by a large number of three-dimensional structures. It would be of interest to examine whether a CRN that fits experiment can be constructed with even-membered rings only. Clearly, more experiments are required to determine whether wrong bonds are present in amorphous III-V compounds.

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Angular Dependence of Photoemission from the (110) Face of GaAs

Neville V. Smith and Morton M. Traum
Bell Laboratories, Murray Hill, New Jersey 07974
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Photoelectron energy spectra have been measured as a function of angle on a (110) face of GaAs at the photon energy 10.2 eV. Marked variations are observed with both polar and azimuthal angles. We discuss implications with regard to the electronic band structure.

There has been a recent revival of interest in the angular dependence of photoelectric emission.¹⁻⁷ Experimental work so far has concentrated on the variation of the emission with polar angle^{5,7} or with different crystal faces.⁶ In this

paper, we present photoelectron energy spectra measured on a (110) face of GaAs, which display a marked dependence on both polar angle and azimuthal angle. The implications with regard to the band structure are discussed, although a full

interpretation will require detailed band calculations.

The motivation for such angular studies is readily appreciated as follows. The kinetic energy E' of a photoelectron emitted into vacuum is given by $E' = \hbar^2 K'^2 / 2m$ where \vec{K}' is its wave vector outside the material. If we measure E' and the direction of propagation of the photoelectron, we have thereby measured the three components of \vec{K}' . If we could convert these to the three components of \vec{K} , the wave vector that the electron had inside the material, we could, in principle, map out portions of the band structure directly from experiment. A specular refraction condition would require that the component of the wave vector parallel to the surface be unchanged on crossing the boundary; and in a free-electron picture, the perpendicular components would be related by $\hbar^2 K_{\perp}^2 / 2m = \hbar^2 K_{\perp}'^2 / 2m + W$, where W is the depth of the potential well. We will indicate below, however, that while angular studies promise to be most informative, the analysis of the data will not be as simple as this.

Figure 1 shows our experimental arrangement. A single crystal of *p*-type GaAs (Zn-doped with 1.4×10^{19} carriers per cm^3) was cleaved in ultra-high vacuum along a (110) face. The crystal face was then advanced to the center of a hemispherical shell whose purpose was to provide a drift region free from electric fields. Ambient magnetic fields were canceled to below 20 mG by means of three pairs of Helmholtz coils. Light was incident normally upon the cleaved surface. A slot in the hemisphere permitted photoelectrons propagating in the plane of the figure to exit from the hemisphere and pass into an analyzer whose position could be rotated so as to vary the polar angle θ continuously. The analyzer employed a channel electron multiplier and was operated on the retarding-potential principle. The azimuthal angle ϕ was varied by rotating the sample about the surface normal. The origin of ϕ is defined so that when $\phi = 0^\circ$, the analyzer rotates in the (001) plane; when $\phi = 90^\circ$, it rotates in the $(\bar{1}10)$ plane. The angular resolution was determined primarily by the size of the illuminated spot, and is estimated to be $\pm 2^\circ$ for both θ and ϕ .

Figure 2 shows a small selection of our results taken at a photon energy $\hbar\omega$ of 10.2 eV. The spectra are referred to initial-state energy taking the zero at the Fermi level E_F which, for *p*-type GaAs such as that used here,⁸ should coincide with the valence-band maximum to within 0.1 eV.

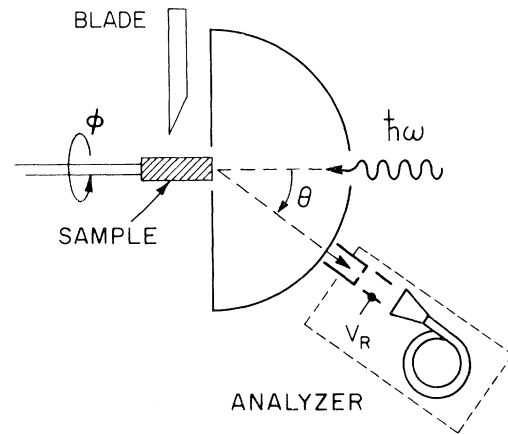


FIG. 1. Schematic diagram of the experimental apparatus showing the positions of the crystal, cleaving blade, and photoelectron energy analyzer.

Since the variation with θ has been considered by other authors,^{5,7} we concentrate here on the variations with ϕ . Qualitatively, we see that the photoelectron energy spectrum varies markedly with ϕ and that the changes are quite different for the two different values of θ shown. The most prominent feature is the dramatic growth of the peak at -1.3 eV in Fig. 2(a) as ϕ varies between 45° and 60° . As noted by Wooten, Huen, and Winsor,⁵ this peak is of some interest since it does not appear strongly in the ordinary photoemission spectra of Eden and Spicer⁹ until $\hbar\omega$ reaches about 9 eV. Only one quadrant of ϕ is shown in Fig. 2. We confirmed that the behavior in the other quadrants was consistent with the requirements of crystal symmetry.

A proper interpretation of these spectra must await detailed band calculations of the photoemission in which the anisotropies of the process are taken into account. It is not yet clear whether a volume band picture will prove to be adequate.⁶ In the meantime, however, some insight can be obtained by pursuing the simple refraction arguments given above. Let us consider electrons originating from -1.3 eV relative to E_F , corresponding to the energy of the prominent peak mentioned above. Such electrons have, after excitation, an estimated kinetic energy of 21.3 eV inside the material. We are adopting here a nearly free-electron approximation, in which it is assumed that the important plane waves in a Fourier analysis of the electronic wave functions have kinetic energies measured from the bottom of the valence bands.¹⁰ The internal wave vectors

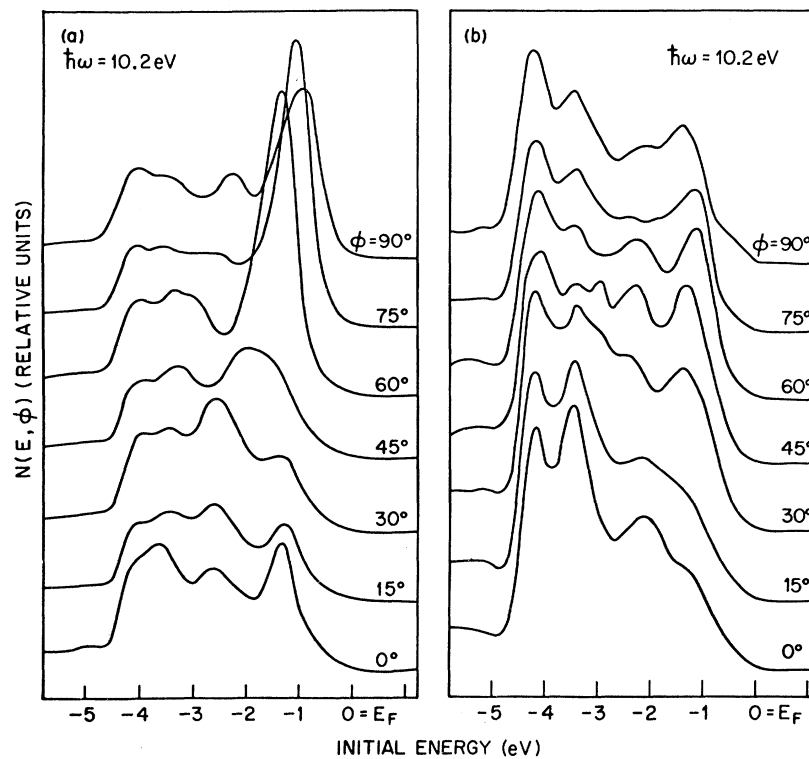


FIG. 2. Variation of the photoelectron energy spectra with azimuthal angle for (a) a fixed polar angle of 50°; (b) a fixed polar angle of 30°.

\vec{K} of electrons of this energy lie on a sphere of radius 2.12 (expressed in units of $2\pi/a$, where a is the lattice parameter) which is so large as to lie well outside the boundaries of the reduced Brillouin zone. As it turns out, the wave vectors \vec{K} of electrons capable of escaping can be translated into reduced wave vectors \vec{k} by subtracting one of only five reciprocal-lattice vectors: \vec{G}_{220} , \vec{G}_{111} , $\vec{G}_{11\bar{1}}$, \vec{G}_{200} , or \vec{G}_{020} . The various values of θ and ϕ on the sphere may therefore be partitioned into five regions according to which \vec{G} is required. The full lines in Fig. 3(b) separate these regions and are simply the curves of intersection between the sphere and various boundaries in a repeated-zone scheme. The region labeled 220, for example represents that part of the sphere surface falling inside the repeated zone centered on the vector \vec{G}_{220} . We will refer to these regions as the “220 zone,” and so on.

The dotted circles in Fig. 3(b) represent wave vectors of constant polar angle. The labels 30°, 50°, and 90° refer to the external measured polar angle. Using the simple refraction model, these correspond respectively to 11.5°, 17.7°, and 23.4° inside the material. At $\theta=30^\circ$, correspond-

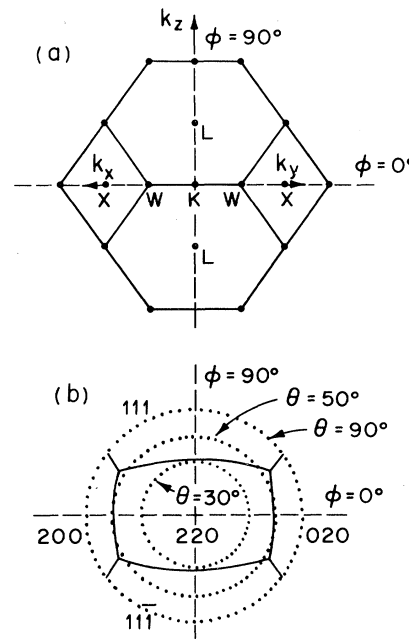


FIG. 3. (a) The reduced Brillouin zone of GaAs as seen along a surface normal ($\langle 110 \rangle$ direction). (b) The five regions (or zones) into which the θ, ϕ values can be partitioned for free electrons whose kinetic energy is 21.3 eV inside the material; in the region labeled 111, for example, the internal wave vector \vec{K} and its reduced wave vector are related by $\vec{K} = \vec{k} + \vec{G}_{111}$.

ing to the spectra of Fig. 2(b), we remain always in the 220 zone as φ is varied. At $\theta=50^\circ$, however, corresponding to the spectra of Fig. 2(a), we actually sample all five zones. Interestingly, the dramatic growth of the -1.3 -eV peak occurs within the 111 zone. This, of course, does not explain *why* the dramatic growth occurs at these particular angles. We do note, however, that there are three contributing factors which should be considered. The first possibility is that the joint density of states for direct transitions at $\hbar\omega=10.2$ eV from states -1.3 eV below E_F may be exceptionally large in this particular region of k space. Or, secondly, it may be that the momentum matrix elements for the transitions are exceptionally large. The third possibility is more subtle and concerns the matching conditions on the wave functions at the surface. In the terminology of Mahan's nearly free-electron approach,³ this strong peak could arise from a "primary cone" due to optical transitions in which the final-state wave function has the plane wave $\exp[i(\vec{k}+\vec{G}_{111})\cdot\vec{r}]$ as its major component. There could also be contributions from various "secondary cones" due to final states in which this plane wave is a subsidiary component. The important point for our purposes is that there is likely to be an angular dependence due solely to a selective matching to various Fourier components in the final-state wave function. In the 111 zone we couple only to the $\exp[i(\vec{k}+\vec{G}_{111})\cdot\vec{r}]$ component and so on. In this regard, we note in Fig. 2(a) that a new peak emerges at -1.3 eV for values of φ close to zero. This could be not just because we are sampling states in a different region of k space, but might also indicate an appreciable $\exp[i(\vec{k}+\vec{G}_{020})\cdot\vec{r}]$ content in the final-state wave functions, which is detectable only when we pass into the 020 zone. This is, of course, only a speculation and needs to be tested by band calculations. We note that Mahan's approach could be extended to GaAs by using the eigenvalues and wave functions of, say, Cohen and Bergstresser's empirical pseudopotential band structure.¹¹

In summary, we have shown experimentally that the photoemission from GaAs is quite aniso-

tropic. The wealth of information obtainable is more fully appreciated when one realizes that the spectra of Fig. 2 represent only a small sampling of the angles and photon energies investigated. The ultimate explanation of the results promises to offer detailed information on both the energies and wave functions of the electronic states.

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