Location of the L_1 and X_3 Minima in GaAs as Determined by Photoemission Studies*

L. W. JAMES, R. C. EDEN, J. L. MOLL, AND W. E. SPICER
Stanford University, Stanford, California 94305

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Direct experimental evidence for the location of the L_1 conduction-band minima in GaAs at 0.09 ± 0.02 eV above the X_1 minima has been obtained using newly developed second-derivative methods for measuring electron energy distribution of photoemitted electrons with high resolution. The X_3 conduction-band minima have also been located at 0.58 ± 0.04 eV above the X_1 conduction-band minima, in close agreement with recent orthogonalized-plane-wave band-structure calculations.

THEORETICAL calculations of the band structure of GaAs have difficulty in accurately placing the location of the L_1 conduction-band minima. In fact, accurate experimental location of this point can provide a critical parameter for the empirical adjustment of band calculations. Such location is also very important for detailed high-field transport calculations such as those relevant to the Gunn effect. Indirect estimates from earlier experimental data have placed the L_1 minima at approximately 0.09–0.2 eV above the X_1 minima.[1]

Earlier measurements of photoemitted electron-energy-distribution curves from GaAs were able to separate the electrons thermalized in the Γ_1 and X_1 minima, but did not have sufficient resolution to resolve the L_1 minima.[2]

In a material such as GaAs, where the photon-absorption length is long compared with the electron-scattering length at low photon energies, most of the photoexcited electrons will scatter into one of the conduction-band minima before being emitted. However, those excited near the surface will be emitted without suffering any significant energy loss. Thus peaks which occur in emitted electron-energy distribution curves for GaAs at low photon energies correspond either to conduction-band minima into which electrons have been scattered or to final energy states of an optical transition. Peaks corresponding to final energy states tend to move in energy as the photon energy is changed, whereas peaks corresponding to conduction-band minima stay at a constant energy.

In the case where two peaks are very close together in energy, the weaker peak will appear as a shoulder on the side of the stronger one. Because of the difficulty in locating these shoulders during analysis of the energy distribution curves, new techniques were developed so that the derivative of the energy distribution curve can also be recorded.

The experimental equipment used to obtain these curves is shown in Fig. 1. The p^+ GaAs single crystal is cleaved in a vacuum of 10^{-11} Torr and covered with alternate layers of cesium and oxygen to lower the work

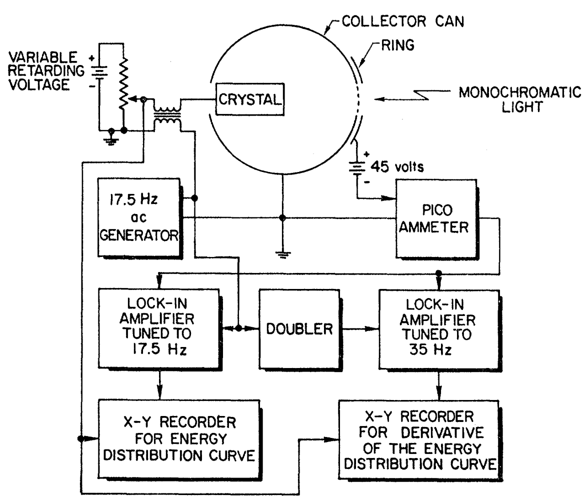

FIG. 1. Experimental apparatus.

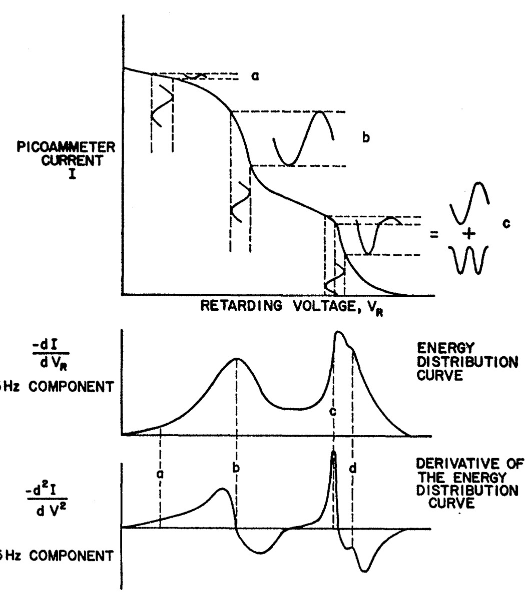

FIG. 2. Measurement technique for electron energy distributions and their derivatives.

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[2] R. C. Eden, J. L. Moll, and W. E. Spicer, Phys. Rev. Letters **18**, 15 (1967).

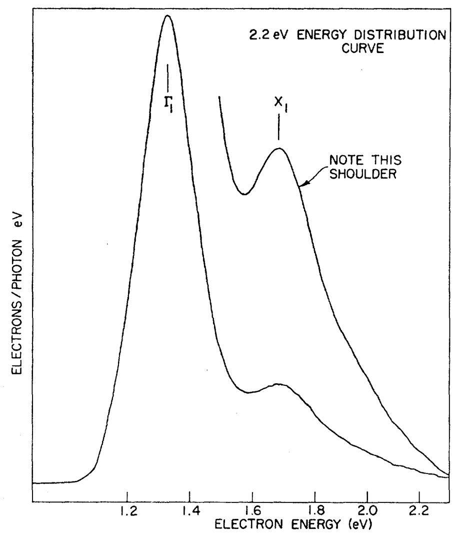

FIG. 3. p^+ GaAs photoemitted electron energy distribution curve for a photon energy of 2.2 eV.

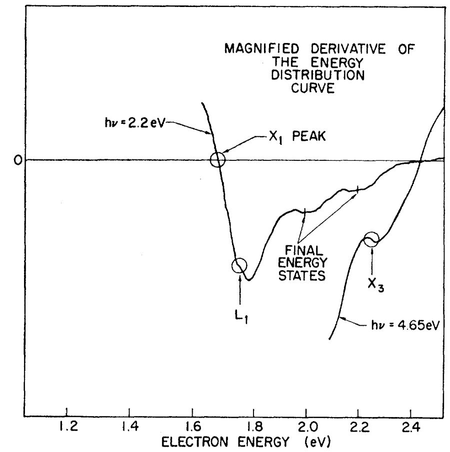

FIG. 4. Derivative of energy distribution curves. A curve (corresponding to point c and higher in Fig. 2) is given for $h\nu=2.2$ eV showing the position of the dominant X_1 peak as well as the L_1 shoulder and shoulders due to the unscattered electrons in the original optical excitation spectra (labeled "Final Energy States"). Although the L_1 structure is weak, it was completely reproducible and occurred at the same energy for a large range of $h\nu$. In contrast, the final-energy shoulders moved with $h\nu$. Also included in this figure are data for $h\nu=4.65$ eV showing only that portion corresponding to the X_3 conduction-band minima. This structure did not move with $h\nu$.

function. A small 17.5 Hz ac voltage is applied to the crystal in series with a variable retarding voltage. When the retarding voltage is increased, the collector-can current decreases as the lower-energy electrons are repelled from the collector can. The small 17.5-Hz component of the collector-can current is proportional to the derivative of the collector-can current with respect to retarding voltage, as shown in points a and b of Fig. 2. This is just the electron current in an incremental energy range, or the electron energy distribution curve. The second harmonic (35 Hz) component of the collector-can current is proportional to the second derivative of collector-can current with respect to retarding voltage, or the derivative of the energy distribution curve, as shown in point c of Fig. 2. Notice particularly at point d the manner in which a shoulder on the energy distribution curve shows up on the derivative of the energy distribution curve.

In order to obtain the required high resolution, many steps were taken to reduce all electric fields in the experimental apparatus except for an accurate spherical retarding potential. Instead of measuring the entire collector-can current, only that portion going through a screened hole in the collector can at a point on a line perpendicular to the crystal face is measured (see Fig. 1). It has been experimentally determined that this current is an accurate and higher resolution sample of the total collector-can current over the photon energy range of interest.

Figure 3 shows an energy distribution curve for p^+ GaAs with a Zn doping of $1\times10^{19}/\text{cm}^3$ taken at a photon energy of 2.2 eV. The peaks corresponding to the Γ_1 and X_1 minima are clearly visible. The shoulder corresponding to the L_1 minima is present, but barely discernable. Figure 4 shows the corresponding derivative of the energy-distribution curve. Here the kink in the derivative curve corresponding to the L_1 shoulder is more evident, and its location can be accurately determined with respect to the X_1 peak. This structure is present at the same final energy in all curves taken over a photon energy range of 2.0–4.25 eV, leading to its positive identification as a conduction-band minimum. Comparisons with calculated band structures show that this minimum must be the L_1 minimum.

By a similar analysis the X_3 conduction-band minima have been located at 0.58 ± 0.04 eV above the X_1 minima. One of the derivative curves indicating the X_3 minima is also shown in Fig. 3. A recent GaAs band calculation by Herman *et al.*,[3] making use of certain of experimental values for Γ_1, L_1, and X_1, predicts an X_3-X_1 value of 0.6 eV, giving excellent agreement.

Many more detailed features of the GaAs band structure are evident in the high-resolution curves, and an analysis of them will be presented at a later date.

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[3] F. Herman, R. L. Kortum, C. D. Kuglin, J. P. VanDyke, and S. Skillman, in *Methods of Computational Physics*, edited by B. Adler, S. Fernbach, and M. Rotenberg (Academic Press Inc., New York, 1968), Vol. 8.