Gallium Arsenide Band Structure Calculation*†

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(Received 4 March 1964)

Energy levels, associated with some points of high symmetry, in the Brillouin zone of gallium arsenide are calculated. The variational method proposed by Brown and Krumhansl is used. The trial wave functions consist of Bloch sums constructed from nonoverlapping atomic-like functions and of plane waves. In order to calculate the crystal potential, the lattice sites are assumed to be occupied by Ga^- and As^+ ions in $4s4p^3$ configurations. The bottom of the conduction band is found to have X_1 symmetry. The indirect band gap is found to have a width of 1.63±0.8 eV. The conduction level Γ_1 is found to lie below the conduction level Γ_{15}.

THE bandstructure of gallium arsenide was calculated by a variational method developed by Brown and Krumhansl.[1] The trial wave functions consist of Bloch sums constructed from nonoverlapping atomic-like functions and of plane waves. The atomic-like functions simulate the high-frequency components of the crystal wave function near the nuclei, while the plane-wave terms are appropriate to describe the crystal wave function in the region between nuclei. Only atomic-like functions corresponding to $2s$, $4s$, $2p$, and $4p$ gallium and arsenic atomic Hartree functions were used, in order to limit the size of the resulting matrix equations.

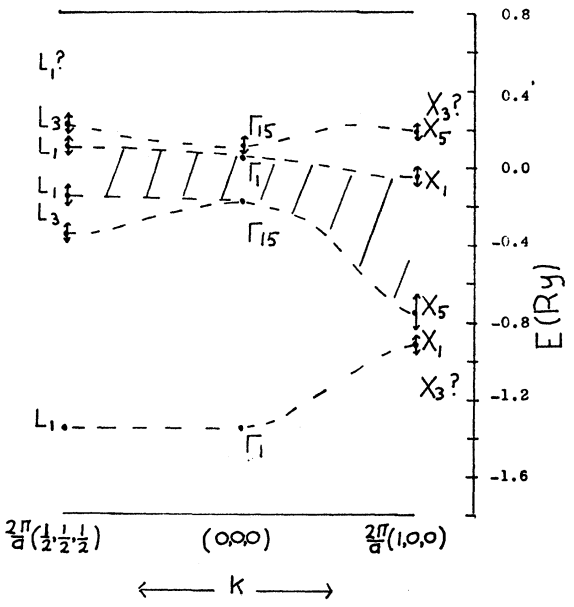

FIG. 1. Band structure for GaAs.

The trial functions were symmetrized to yield energy states of types Γ_1, Γ_{15}, X_1, X_5, L_1, and L_3.

The crystal potential was calculated from the charge distribution due to a gallium arsenide lattice consisting of Ga^- and As^+ ions, all in $4s4p^3$ configurations. Terms for exchange and correlation were not included.

Minimization of the expectation value of the energy leads to the usual matrix equation. Solutions were found for various numbers of plane waves in the trial wave function.

The calculated energy levels are marked by dots in Fig. 1; their values are listed in Table I. The arrows indicate uncertainty in their position due to poor convergence, mainly caused by the fact that $3d$-like basis functions were not included. The hatched region indicates the band gap. The bottom of the conduction band is found to be at X_1. The conduction level Γ_1 is found to lie below Γ_{15}. The indirect band gap is found to be 1.63±0.8 eV.

Our calculation yielded a band structure for gallium arsenide which seems reasonable when compared with the germanium band structure.[2] It is also in approxi-

TABLE I. Valence and conduction levels of gallium arsenide.

Symmetry	Energy (Ry)	Symmetry	Energy (Ry)	Symmetry	Energy (Ry)
L_1	···	Γ_{15}	0.12±0.04	X_5	0.20±0.04
L_1	0.10±0.04	Γ_1	0.05±0.01	X_1	−0.04±0.04
L_3	0.20±0.04	Γ_{15}	−0.16±0.02	X_3	···
L_1	−0.16±0.04	Γ_1	−1.35±0.01	X_5	−0.76±0.10
L_3	−0.35±0.04			X_1	−0.92±0.04
L_1	−0.30±0.04				

* Research supported by grant from National Science Foundation.
† Based on a thesis submitted to Rensselaer Polytechnic Institute in partial fulfillment of the requirements for the PhD degree.
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[1] E. Brown and J. A. Krumhansl, Phys. Rev. **109**, 30 (1958).
[2] F. Herman and S. Skilman, *Proceedings of the International Conference on Semiconductor Physics, 1960* (Czechoslovokian Academy of Sciences, Prague, 1961).

mate agreement with the gallium arsenide band structure calculated by Bassani and Yoshimine,[3] but yields the result that Γ_1 lies below Γ_{15}. This appears to be in better agreement with experimental evidence, such as piezoresistance and magnetoresistance measurements, which seem to indicate that the bottom of the conduction band is at Γ_1. The band gap was found to be of the same order of magnitude as that found experimentally.

I wish to express my gratitude to Professor E. Brown for his guidance and encouragement throughout the completion of this work. I further wish to acknowledge that most of the computations were performed at the Rensselaer Polytechnic Institute Computer Laboratory.

[3] F. Bassani and M. Yoshimine, Phys. Rev. **130**, 20 (1963).

PHYSICAL REVIEW VOLUME 135, NUMBER 2A 20 JULY 1964

Spectral Shape and Attenuation Length for Hot Electrons in the Presence of Finite Absorption

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(Received 2 March 1964)

The space and energy distribution of electrons released into a field-free semiconductor provides a means of studying the interaction of the electrons with the material, as experiments by Bartelink, Moll, and Meyer have shown. In the presence of finite absorption, or large energy losses per collision, the conventional methods of solving the Boltzmann equation governing the distribution function fail to give reliable results. We have found that a considerable amount of information may be obtained from the Boltzmann equation itself without a spherical harmonic expansion by studying its Laplace transform with respect to energy. In particular, we obtain an analytic expression for the exponential attenuation length which reduces to the BMM expression in the limit of small absorption and small energy loss. We obtain expressions for the average energy loss and average spread of the distribution, both of which increase linearly with distance, and for the total intensity of the distribution, which decreases exponentially with the distance through which the electrons must diffuse. This form of variation is independent of the energy distribution of the source of hot electrons. Therefore, if the energy distribution of electrons is measured at two different distances from the same source, the rate at which the average energy, for example, decreases with distance may be determined. This rate, being independent of the source distribution, is a characteristic of the medium, as is the BMM attenuation length. These two quantities together provide sufficient information to determine the mean free path for optical phonon emission and the mean free path for impact ionization. Measuring the energy distribution of the electrons in the medium can be done by measuring the distribution of electrons emitted into the vacuum provided that the angular distribution of the particles is known. This angular distribution may be approximated from knowledge of the Laplace transform. The effect of this analysis on the interpretation of the BMM experiments is to suggest that the mean free path for impact ionization in silicon may be closer to 300 Å than to 200 Å.

I. INTRODUCTION

THE space and energy distribution of particles released into a field-free medium by a high-energy localized source provides a means of studying the interaction of the particles with the medium. A recent example of this technique is to be found in a paper by Bartelink, Moll, and Meyer dealing with the emission of hot electrons from shallow $p-n$ junctions in silicon.[1] In the experiments reported in the BMM paper, electrons in the silicon are accelerated by an electric field and are then allowed to diffuse through a field-free region in which they may either lose energy or—in effect—be absorbed. Other examples may be found among the problems faced by the designers and users of nuclear reactors.[2] Here, the particles of interest are neutrons, and not surprisingly, a substantial part of neutron transport theory is concerned with the calculation of just this space- and energy-dependent distribution function.[3]

The similarities between the hot electron problem of the BMM experiment and the neutron diffusion problem are so great that it was virtually inevitable that BMM should have employed one of the most useful of the approximations developed by the neutron transport workers—the Fermi age theory[2–4]—in the analysis of their experiments. The hot electron problem is, however, sufficiently simpler than the neutron diffusion problem that it is possible to obtain much exact information about the distribution without making the age theory approximation. This is important because, although the age theory is known to be valid in the limit of infinitesimal absorption and infinitesimal energy loss per collision, its validity for the finite absorptions and finite

[1] D. J. Bartelink, J. L. Moll, and N. I. Meyer, Phys. Rev. **130**, 972 (1963). The authors and this reference will be denoted BMM.
[2] R. L. Murray, *Nuclear Reactor Physics* (Prentice Hall, Inc., Englewood Cliffs, New Jersey, 1957).
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