ENERGY SPACING OF GEOMETRICAL RESONANCE STRUCTURE IN VERY THICK FILMS OF SUPERCONDUCTING In

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Initial tunneling studies of geometrical resonance structure in thick In films[1] indicated that the observed oscillations were periodic in $E = V - \Delta(\mathrm{Al})$ except for the first oscillation, i.e., the one nearest $E = \Delta(\mathrm{In})$. A similar periodicity had been reported earlier for Pb,[2] although structure near $E = \Delta(\mathrm{Pb})$ had not been interpreted due to complications caused by the double energy gap exhibited by thick Pb films. New data of improved resolution will be presented for a very thick In film (33.2 μ) for which at least eight of the 12 observed oscillations are not periodic in E. Instead, all 12 are periodic in $\epsilon(E) = [E^2 - \Delta^2(\mathrm{In})]^{1/2}$. This behavior is consistent with the McMillan-Anderson theoretical result[3] which was obtained by attributing geometrical resonances to quasiparticle interference effects between scattering-coupled electron-hole states. The present data will be interpreted in terms of a primitive standing-wave model involving interference between electronlike (or holelike) states which are degenerate in energy, but which propagate with different velocities.

Details of Al-AlO_x-In diode fabrication have been outlined elsewhere.[1] Four In films were investigated (8.55, 11.8, 20.3, and 33.2 μ), the thinnest having been covered with a silver overlay (~2000 Å). The Al films employed had thicknesses in the range 300-1000 Å. Junctions had dimensions 1 mm × 1 mm and exhibited resistances in the range 2.3-14 Ω for $T = 4.2$°K. Conventional modulation techniques were employed to measure dV/dI and d^2V/dI^2.

Figure 1 presents plots of dV/dI and d^2V/dI^2 for the 33.2-μ-thick In film with some of the low-V d^2V/dI^2 data omitted for clarity. Resonances have been labeled by $\eta = 0, 1, 2, \cdots$, with $\eta = 0$ corresponding to $V = \Delta(\mathrm{In}) + \Delta(\mathrm{Al})$ or $E = \Delta(\mathrm{In})$. Although the structural feature corresponding to $\eta = 1$ is barely discernible in dV/dI, it appears quite clearly in the original d^2V/dI^2 data. Potentials corresponding to local maxima in dI/dV have been labeled V_η. For $0 \leq \eta < 8$, these potentials can be determined both from dV/dI and d^2V/dI^2, while for $\eta \geq 8$ only d^2V/dI^2 data are useful.[1]

Figure 2 presents plots of $E_\eta(\eta)$ and $\epsilon_\eta(\eta)$. With these more extensive tunneling data, it is now apparent that $E_\eta(\eta)$ is not a linear function for very thick films although it does straighten for larger η values. By contrast, $\epsilon_\eta(\eta)$ is quite linear[4] with the possible exception of the first few points. For these, however, there

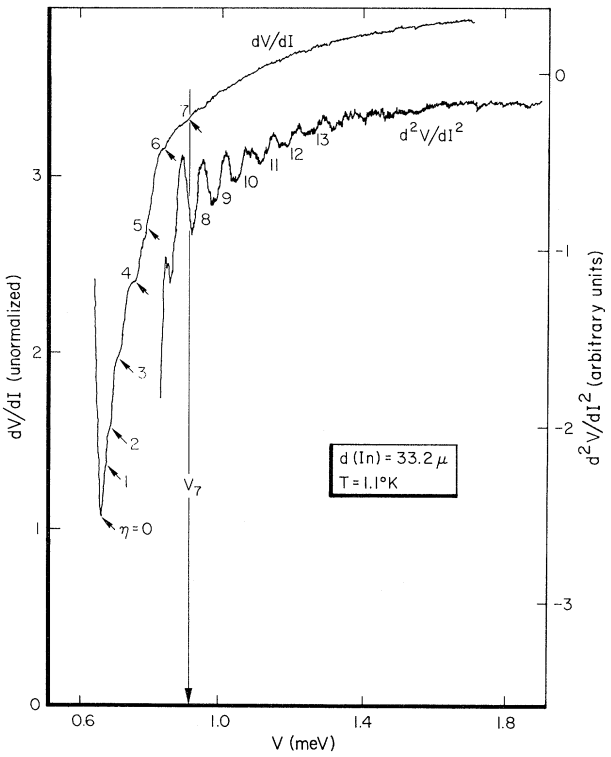

FIG. 1. Voltage dependence of dV/dI and d^2V/dI^2 for an Al-AlO_x-In tunnel diode. Modulation levels were 5-10 μV (rms) and 10-20 μV (rms), respectively. Potentials at which local maxima in dI/dV occur are denoted by V_η. Note that the structure labeled $\eta = 4$ is stronger than $\eta = 3$, and $\eta = 6$ is stronger than $\eta = 5$.

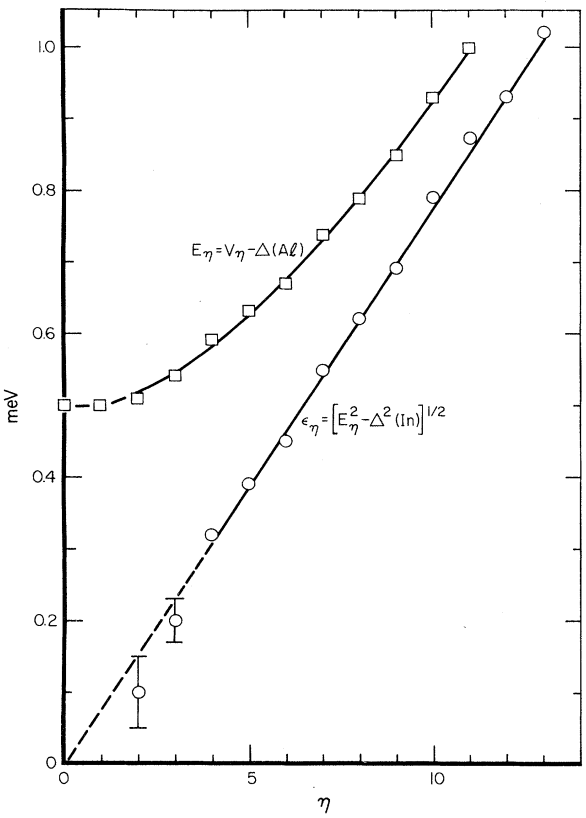

FIG. 2. Plots of $E_\eta(\eta)$ and $\epsilon_\eta(\eta)$ as obtained from the data of Fig. 1.

is considerable numerical uncertainty, reflecting the fact that ϵ is obtained as the small difference of comparatively large numbers. (In this respect, the data shown are inferior to those obtained with the other films.) Presence of an overlay does not appear important as far as the linearity of $\epsilon_\eta(\eta)$ is concerned. Results obtained with the other films are quite similar except that fewer oscillations occur in the nonlinear range of $E_\eta(\eta)$, and $E_\eta(\eta)$ definitely approaches a linear asymptote.

Another interesting feature of the data (Fig. 1) is the nonmonotonic damping of the structure near $E = \Delta(\mathrm{In})$, e.g., $\eta = 4$ is stronger than $\eta = 3$, and $\eta = 6$ is stronger than $\eta = 5$. Such behavior is not observed for the thinnest two films and is less prominent in the 20.3-μ films. This probably reflects the fact that fewer oscillations occur near $E = \Delta(\mathrm{In})$ as the film thickness decreases.

For a given excitation energy there are two energetically degenerate electronlike states (as well as two degenerate holelike states) associated with k vectors $k = k_F \pm \frac{1}{2}\Delta k$.[5] Starting from this point, and following the suggestion of McMillan and Anderson regarding interference, it is possible to construct a very simple physical model which predicts the energy (voltage) dependence of the resonances. It is postulated that like states mix (either e-e or h-h) to form a composite state which exhibits beats due to the different propagation velocities involved. The phase difference produced by crossing a film of thickness d is given by

$$\Delta\varphi \approx (2\pi/\lambda_F)(d/v_F)\Delta v \approx d\Delta k. \quad (1)$$

The excitation energy[6] $E = [\Delta^2 + \epsilon^2]^{1/2}$ is uniquely determined by Δk, as is ϵ. Elementary arguments are employed to evaluate $E(k)$:

$$\zeta \pm \epsilon \approx (\hbar^2/2m)(k_F \pm \tfrac{1}{2}\Delta k)^2, \quad (2)$$

$$\Delta k \approx 2\epsilon/\hbar v_F \approx \Delta\varphi/d, \quad (3)$$

$$E \approx \{\Delta^2 + [(\hbar v_F/2d)\Delta\varphi]^2\}^{1/2}. \quad (4)$$

If one stipulates that the appropriate boundary condition is that an integral number of beats be contained in the film ($\Delta\varphi = 2\pi\eta$), the McMillan-Anderson results are obtained:

$$E \approx \{\Delta^2 + [(\pi/d)\hbar v_F \eta]^2\}^{1/2}, \quad (5)$$

$$\epsilon(\eta) \approx (\pi/d)\hbar v_F \eta = \tfrac{1}{2}\Delta p(\eta) v_F. \quad (6)$$

Equation (6) fits the data of Fig. 2 quite well with $v_F = 1.23 \times 10^8$ cm/sec, in satisfactory accord with the anomalous skin-effect value 1.28×10^8 cm/sec.[7]

The physical picture underlying the above equations may be described as follows: In an infinite medium, running waves associated with $k = k_F \pm \frac{1}{2}\Delta k$ are combined to form a beat-modulated running wave. In order to satisfy the time-independent boundary conditions imposed by bounding surfaces, this wave is combined with its time-reversed form to produce a beat-modulated standing wave. Placing beat nodes at the boundaries insures that the wave function vanishes there, and requires that an integer number of beats be contained in the film.[8] Amplitudes of the standing-wave states will be determined by the degree of coherent reflection at the boundaries, i.e., by boundary conditions. Overlay enhancement effects[1] are presumably the result of decreased surface damping produced by altering the boundary condition at x

$= d$. In this respect, it might be interesting to see if Al-AlO_x-Ag/In/Ag diodes (with relatively thin silver films) produce significantly sharper structure in analogy to multiple-beam interferometers, i.e., two silver mirrors rather than one. The present model proposes e-e (or h-h) composite states into which electrons (or holes) tunnel preferentially because such states satisfy a macroscopic quantum condition of the "beat" or envelope" momentum $\Delta p = (2\pi/d)\eta\hbar$. This point of view seems to differ significantly from the physical picture underlying the McMillan-Anderson calculation, although both yield the same energy spectrum. There appears to be some reason to believe that simultaneous solutions of the three-dimensional Gor'kov equations (lamina of thickness d) may lead to a régime qualitatively similar to the one discussed.[9]

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BAND STRUCTURE AND OPTICAL PROPERTIES OF DIAMOND*

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Recently several authors[1-4] have discussed new measurements of the optical properties of diamond, and they have raised many questions about the measurements and about the theoretical interpretation of the data. To answer a few of these questions, we present in this Letter a calculation of the electronic band structure of diamond. The band structure was calculated by means of the empirical pseudopotential method (EPM)[5,6] which has been used[5-8] successfully to interpret the optical properties of a large number of semiconductors and insulators. The analysis of the resulting diamond band structure yields some new interpretation of the structure in the optical reflectivity. Within the scope of this interpretation, the calculated band gaps agree with experiment to within ~0.01 Ry near the fundamental band gap and to within ~0.05 Ry over a range of 1.0 Ry.

The EPM involves choosing pseudopotential form factors which give band structures consistent with the experimental measurements. These form factors are first constrained to give a few of the principal band gaps in agreement with experiment and then used to determine the electronic band structure at many points in the Brillouin zone. The pseudopotential form factors V_K used for diamond are (in Rydbergs) $V_{111} = -0.811$, $V_{220} = 0.337$, $V_{311} = 0.132$, and $V_{222} = 0.041$. The V_{222} form factor, which is identically zero for a linear superposition of spherical atomic potentials, is included here to account for the distribution of valence charge[9,10] arising from tetrahedral bonding. This tetrahedral distribution of charge accounts for the presence of the otherwise forbidden (222) reflection in x-ray data.[11,12]

The band structure of diamond appears in Fig. 1. The calculation of the energy bands is convergent to ~0.003 Ry. The lattice constant was taken to be 3.57 Å.[13] In Table I we list the principal energy gaps of this band structure and the corresponding experimental values. The location of the conduction-band minimum is also included in Table I. The error in the experimental energies at which the peaks occur in the optical constants is large both because of the inherent broadness of the