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ASYMMETRY OF THE TUNNELING CHARACTERISTICS OF THE Pb-Al_2O_3-HgSe JUNCTION

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The tunneling characteristics of differential resistivity have been calculated for a Pb-Al_2O_3-HgSe junction. Calculations have been performed using two methods: WKB approximation and matching of wave functions. It has been shown that only the method of matching of wave functions, in which the peculiar band structure of the HgSe electrode was taken into account, allows one to explain the experimentally observed asymmetry of tunneling characteristics.

The electron tunneling in a metal-insulator-semiconductor junction in which HgSe crystals were used as semiconductor electrodes has been studied recently [1, 2]. The structures observed in the first and second derivative of tunneling characteristics have been interpreted as due to the HgSe-phonon assisted tunneling [1]. In the external magnetic field the oscillatory structures due to the Landau quantization of the HgSe conduction band have been observed [2].

The purpose of the present work is to explain the general shape of the differential resistivity characteristic of the Pb-Al_2O_3-HgSe tunnel junction. Fig. 1 (solid line) shows a typical experimental characteristic of the differential resistivity versus voltage of the tunnel junction based on HgSe crystal measured at 4.2 K. The characteristic is nearly parabolic in shape with a rather large asymmetry about $V = 0$. The fine structure near zero bias reflects the superconducting energy gap of the lead electrode. The maximum of the curve appears at the polarization corresponding to the tunneling from the metal to the conduction band of the semiconductor electrode.

Similar observations have been made by Hauser and Testardi [3] for metal-insulator--metal junctions and by Hagiwara and Tanaka [4] for metal-insulator-HgTe junctions. For metal-insulator-metal junctions the common interpretation of the observed asymmetry of tunnel characteristics relates it with the potential barrier asymmetry [5]. Hagiwara and Tanaka have explained this asymmetry as due to band bending at the surface of a HgTe electrode. They have concluded that the position of the maximum of the characteristic

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is determinated by the magnitude of the potential at the HgTe surface. Their junctions were made on pure HgTe crystals so that the value of the potential, equal to about 50 meV, was quite reasonable. Our junctions were made on HgSe crystals with electron concentrations ranging from 1×10^{17} cm^{-3} to 2.3×10^{18} cm^{-3} corresponding to Fermi energies from

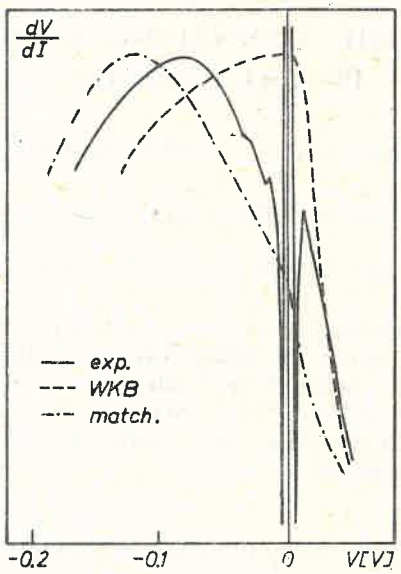

Fig. 1. Tunneling characteristics of a Pb-Al_2O_3-HgSe ($n = 1 \times 10^7$ cm^{-3}) junction calculated for the rectangular barrier model: in WKB approximation (dashed line) and by matching (dashed-dotted line). The experimental characteristic is shown by the solid line

40 to 150 meV measured from the bottom of the conduction band. According to the interpretation proposed by Hagiwara and Tanaka we should assume the surface potential to be larger than 100 meV. There are two reasons for which such an assumption seems to be unrealistic: first, electrons in the HgSe conduction band screen the surface electric field and hence cause a lowering of the surface potential barrier; and second, the tunneling characteristics measured in the external magnetic field show no structures due to the surface Landau levels.

Therefore we have tried to explain the asymmetry of the characteristic of our junction using standard methods [5] of calculating the tunneling current. The peculiar band structure of the HgSe electrode was taken into account and flat band conditions were assumed. In the first attempt we have calculated the differential resistivity using the semiclassical WKB approximation [6, 7] for a trapezoidal potential barrier. Such a model of a barrier is commonly used for explaining the asymmetry of the tunnel characteristic for metal--insulator-metal junctions [6]. Fig. 2 shows an idealized model of a tunnel junction with a trapezoidal potential barrier. The Fermi energies of the metal and semiconductor electrode are denoted by E_{FL} and E_{FR}, respectively. The trapezoidal potential barrier heights φ_1 and φ_2 correspond to the work functions of the electrodes lowered by the conduction

band edge of the insulator. The energy is measured from the bottom of the conduction band of the metal electrode.

To illustrate the results, the calculated differential resistivity as a function of voltage is presented by the dashed curve in Fig. 1 for a rectangular barrier and in Fig. 3 for a trapezoidal barrier. The potential barrier asymmetry $\Delta\varphi = \varphi_2 - \varphi_1$ assumed for the calculations

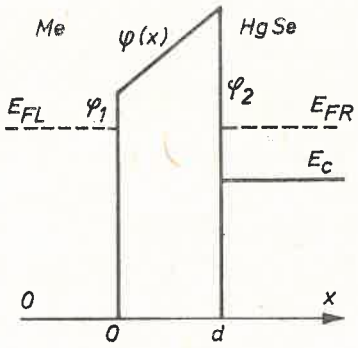

Fig. 2. Schematic energy diagram of a metal-insulator-degenerate n-type semiconductor tunnel junction

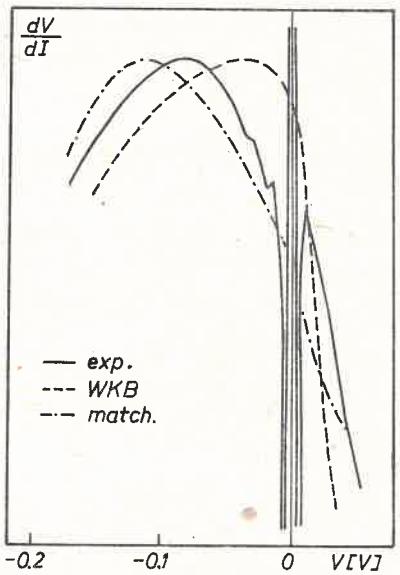

Fig. 3. Tunneling characteristics for the Pb-Al_2O_3-HgSe junction calculated for a trapezoidal barrier model: in WKB approximation (dashed line) and by matching (dashed-dotted line). For comparison the experimental characteristic (solid line) is given

was equal to 2 eV, the mean barrier height was also 2 eV and the barrier thickness was equal to $d = 25$ Å. It is noticeable that even such a large potential barrier asymmetry does not explain the extreme asymmetry of the experimental characteristic.

It is well known [7] that the semiclassical WKB approximation for wave functions of tunneling electrons can be used only in the case of a slowly varying potential barrier and for large values of wave vectors in the tunneling regions. For the Pb-Al_2O_3-HgSe tunnel junction neither assumption is fulfilled. There are large differences in values of the effective masses and Fermi energies on both sides of the potential barrier. The values of wave vectors of the tunneling electrons in the semiconductor electrode are small in comparison to those in the metal electrode. Therefore, we have used a more exact method of evaluating the tunneling current without applying the WKB approximation. In this method the exact solutions of the Schrödinger equation are matched at the classical turning points.

The expression for the tunneling current density evaluated by this method [7] has the form

$$j = \frac{em_0}{2\pi\hbar^3} \int_{E_{FL}-eV}^{E_{FL}} dE \int_0^{f(E,\Delta E_F,eV)} dE_{\parallel} D(E, E_{\parallel}, eV), \tag{1}$$

where E_{FL} is the Fermi energy of the left electrode, ΔE_F denotes the difference of the Fermi energies in both electrodes, $E_{\parallel}$ is the part of the energy related to the component of the wave vector parallel to the surface, m_0 is the free electron mass. The upper limit of the integral of $E_{\parallel}$ depends on the energy structure of the semiconductor electrode. For the calculations we have assumed the simple three band model. In this model the dispersion relation is of the form [8]

$$E(E+E_0)(E+\Delta) - \tfrac{3}{4}\frac{\hbar^2k^2}{m_{R0}} E_0(E+\tfrac{2}{3}\Delta) = 0, \tag{2}$$

where m_{R0} is the effective mass at the bottom of the conduction band, E_0 is the $\Gamma_6-\Gamma_8$ energy gap, Δ is the spin-orbit splitting. For this type of dispersion relation the function of energy appearing in upper limit of integral (1) has the form

$$f(E, \Delta E_F, eV) = \tfrac{2}{3}\frac{m_{R0}}{m_0} \frac{(E-\Delta E_F+|eV|)(E-\Delta E_F+|eV|+E_0)(E-\Delta E_F+|eV|+\Delta)}{E_0(E-\Delta E_F+|eV|+\tfrac{2}{3}\Delta)}. \tag{3}$$

The barrier transmission coefficient D is given by

$$D = \frac{k_R}{k_L}\frac{m_0}{m_{R0}} \frac{16\exp(-2\gamma)}{\frac{b}{a} + \frac{ab}{k_L^2} + \left(\frac{m_0}{m_R(E)}\right)^2 \frac{k_R^2}{ab} + \left(\frac{m_0}{m_R(E)}\right)^2 \frac{a}{b}\left(\frac{k_R}{k_L}\right)^2}, \tag{4}$$

where $m_R(E)$ is the energy dependent effective mass of the electrons in the conduction band of the HgSe electrode [8], k_R and k_L are the one dimensional wave vectors of tunneling electrons in the semiconductor and metal electrode, respectively

$$k_R = \sqrt{\frac{2m_0}{\hbar^2}(f(E, \Delta E_F, eV) - E_{\parallel})}, \qquad k_F = \sqrt{\frac{2m_0}{\hbar^2}(E-E_{\parallel})},$$

where $f(E, \Delta E_F, eV)$ is given by Eq. (3). The exponential term γ is given by

$$\gamma = \frac{1}{\hbar} \int_0^d \kappa(x) dx$$

with the barrier wave vector $\kappa(x)$ of the form

$$\kappa(x) = \sqrt{\frac{2m_0}{\hbar^2} (\varphi(x) - E + E_{\parallel})}$$

$a = \kappa(0)$, $b = \kappa(d)$. The potential barrier $\varphi(x)$ used in the expression for $\kappa(x)$ has a trapezoidal form (see Fig. 2):

$$\varphi(x) = \varphi_1 + E_{FL} + (\varphi_2 - \varphi_1 - |eV|) \frac{x}{d}.$$

Using the described expressions for tunneling current and taking their derivatives with respect to the voltage we obtain the theoretical tunneling conductivity of the junction.

The numerical calculations of the inverse conductivity integrals were performed for the symmetrical and asymmetrical potential barriers. The theoretical characteristics are nearly parabolic in shape with a large asymmetry about zero voltage even for a rectangular potential barrier. It is worth noticing the large difference between the characteristic calculated in WKB approximation and that calculated by the matching of wave functions. For comparison both characteristics for the rectangular barrier are shown in Fig. 1. Neither theory takes into account the effects connected with the superconducting state of the metal electrode. Hence, the calculated curves do not show the fine structure near zero-bias which is seen on the experimental curve. The assumption of the trapezoidal barrier causes a light shift in position of the maximum. The numerical results of the derivative resistivity (tunneling characteristics) for the trapezoidal potential barrier are shown in Fig. 3 (the dashed-dotted line). The values of parameters used for the calculations are: $E_{FL} = 5.0$ eV, $E_{FR} = 0.04$ eV + 5.0 eV, $\varphi_1 = 2.5 + 5.0$ eV, $\varphi_2 = 1.5 + 5.0$ eV, $d = 30$ Å, $m_{R0}/m_0 = 0.03$, $E_0 = 0.22$ eV, $\Delta = 0.45$ eV.

The results of our calculations show that the general shape of the tunneling characteristics of Pb-Al_2O_3-HgSe junctions depends mainly on the band structure of the HgSe electrode. The potential barrier parameters determine the magnitude of the tunneling resistivity, but the experimentally observed large asymmetry of tunneling characteristics can be explained only by taking into account the extreme difference of the wave vectors of tunneling electrons in both electrodes.

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