Tunneling spectroscopy of quasilocal impurity states of indium in lead telluride

V. N. Vinchakov, V. I. Kaĭdanov, S. N. Lykov, and S. A. Rykov
M. I. Kalinin Polytechnic Institute, Leningrad

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A hysteresis of a tunneling conductivity of MIS structures of PbTe⟨In⟩ has been detected. This hysteresis is caused by the structural change in the crystal surroundings of the center as a result of a change in its charge.

The most typical manifestations of a quasilocalizable level[1] in PbTe⟨In⟩ are (a) the density peak of the impurity states above the bottom of the conduction band, ϵ_c, which accounts for the pinning of the Fermi energy ϵ_F and for the extremely stable concentration of the mobile electrons ($\epsilon_F - \epsilon_c \simeq 0.07$ eV, $n = 7\times 10^{18}$ cm^{-3} at $T = 4.2$ K) and (b) the length of time required to establish equilibrium between the impurity and band states ($\tau_{4.2} \sim 10^4$–10^5 s). This relaxation of long duration, which was thoroughly studied in $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Te}\langle\mathrm{In}\rangle$ in Refs. 2 and 3, has been linked[4,5] with the local deformation of the crystal surroundings of the defect upon a change in its charge and with the formation of a self-trapped barrier with a low tunneling transparency.

The objective of the experiments discussed below is to verify and improve our understanding of the resonant level by a new, independent method. The MIS structures of Pb-$\mathrm{Al_2O_3}$-PbTe⟨In⟩ were fabricated by a technique[6] involving cleavage of the (100) surface of the $\mathrm{Pb_{0.98}In_{0.02}Te}$ single crystals. The current-voltage characteristics are studied by measuring the first derivative (σ_1) and the second derivative (σ_2) of the tunnel current of the $I(V)$ curve at $T \geqslant 4.2$ K using the standard modulation technique (the modulation frequency of the bias voltage V is 497 Hz, the bias sweep rate is 230 mV/min; σ_2 is defined as the amplitude of the second harmonic of the tunnel current).

The $\sigma_1(V)$ curve, which reflects the particular features of the state density of the semiconductor, has no impurity-state peak. This is consistent with our expectation if the long relaxation period is taken into account. At the same time, this curve exhibits a hysteresis (Fig. 1), which is absent in PbTe-based MIS structures without an In impurity. The behavior of the $\sigma_2(V)$ curve is also unusual: Tracing the faint features of σ_1 outside the hysteresis loop and the minimum at $V = 0$ due to the superconductivity of the Pb contact, we see that σ_2 "ignores" the horizontal part of the hysteresis loop. Let us analyze these features in terms of the self-trapped-barrier phenomenology.

Suppose that ϵ_0 is the energy of the resonant level on a single-electron scale, q is a coordinate which characterizes the local deformation, k is the effective rigidity, and Q is the deformation potential of the electronic term ϵ_0. The energy of the system "electron + In + surroundings"

$$E_1(q) = \epsilon_0 + \frac{kq^2}{2} - Qq$$

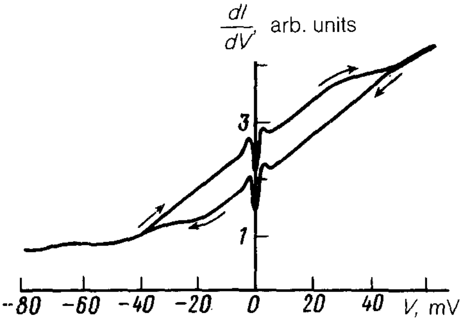

FIG. 1. Hysteresis of the differential conductivity of the MIS tunnel structures of PbTe⟨In⟩ ($T = 4.2$ K).

has a minimum which is separated from the delocalized state by the self-trapped barrier, $\epsilon_A = (\epsilon_0 - \epsilon_F)/4$ (Fig. 2c). At equilibrium, the pinning occurs at the level $\epsilon_F = \epsilon_0 - Q^2/2k$.

We assume that σ_1 reflects the structure of the band state density in the contact layer of the semiconductor of thickness λ, which is on the order of the mean free path of the tunneling electrons. With increasing bias voltage V, some of the electrons are trapped by the empty impurity centers when their energy reaches ϵ_0. This causes a growth of the deformation which corresponds to the minimum $E_1(q)$. This state of the system is metastable during the experiment. The charge of the self-trapped centers in the λ layer raises all electron terms (the hatched part in Fig. 2a) to a value determined by the quasineutrality condition. A further increase in V causes the charge of the impurities to increase, the bands begin to bend following a change in eV, and the density of the finite (band) states of the electrons that tunnel from the Fermi level of

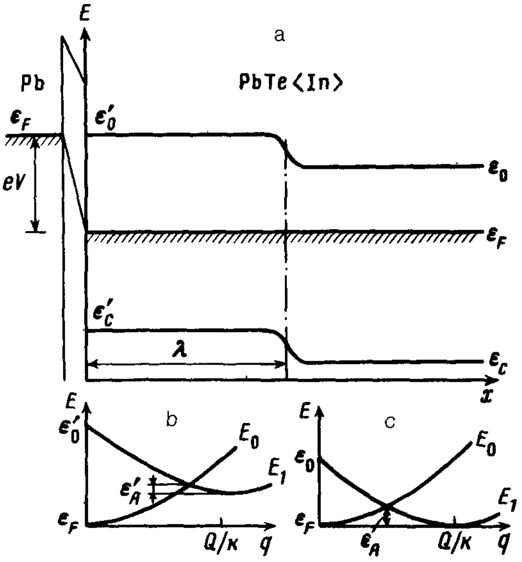

FIG. 2. (a) Energy level diagram of MIS tunnel junction for charged In impurity centers. (b) Configuration diagram which corresponds to the surface layer of PbTe⟨In⟩. (c) Diagram showing the unperturbed volume of the semiconductor.

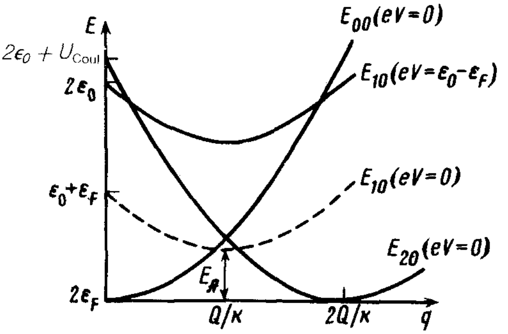

FIG. 3. Configuration diagram showing the pinning of the Fermi energy by two-electron centers.

the metal remains the same. This behavior is seen in the saturation of $\sigma_1(V)$ and in the nonlinearity of the I–V characteristic, i.e., σ_2. An increase in the charge of the layer λ is limited by the inverse transitions of electrons from the impurities to the delocalized state, whose rate increases with decreasing ϵ'_A due to the bending of the bands (Fig. 2b). When the charge rate is equal to the discharge rate, an increase in V no longer contributes to the bending of the bands and $\sigma_1(V)$ and $\sigma_2(V)$ again begin to change.

The bending of the bands, which is metastable to the extent that the transparency of the self-traped barrier is small, continues in the reverse sweep of V. The band state density of the tunneling electrons in the layer λ in this case remains at a lower level compared with that of the volume. Correspondingly, the values of the inverse σ_1 dependence also turn out to be lower. In other words, a hysteresis occurs. A rapid discharge of the self-trapped centers begins at $V<0$. At this point the threshold at which the nonequilibrium holes are captured by the impurity is reached. These holes remain at the site where the conduction electrons tunnel into the metal. The terms in the layer λ bend downward and the left edge of the hysteresis loop forms in an analogous manner. At $T>35$ K the hysteresis of σ_1 and the anomalies in σ_2 vanish, in agreement with the previously observed decrease in the long relaxation times by several orders of magnitude.[2]

This scheme does not account for the absence of the paramagnetic effects.[1] Furthermore, it seems to have serious flaws when quantum fluctuations of the self-trapped barrier are taken into account. A model which is consistent with a double charge of the impurities is preferable.[7] In addition to the cancellation of the magnetic moment of the localized spins, this model may also turn out to have a higher self-trapped barrier (and correspondingly smaller fluctuations), $E_A \simeq (\epsilon_0-\epsilon_F)/2 - U_{\rm Coul}/4$, if the Coulomb repulsion energy $U_{\rm Coul}$ is low. In such a model the energy of the system "2 electrons + 2 In centers + surroundings" is

$$E_{nm} = (1+\delta_{n1}\delta_{m1})\frac{kq^2}{2} + (n+m)(\epsilon_0 - Qq) + (\delta_{n2}+\delta_{m2})U_{\text{кул}} + (2-n-m)(eV+\epsilon_F),$$

if the deformation of the two occupied centers is the same, where $n, m = 0, 1, 2$ are the occupation numbers of the centers ($n+m \leqslant 2$), and δ_{kl} is the Kronecker symbol. The thresholds ($q=0$) of different charge channels of the self-trapped centers, which correspond to the possible finite configurations of $E_{nm}(q)$, can be determined from an analysis of a pair of tunneling electrons.

If $E_{20}<E_{10}$ in the ground state ($V=0$, $q>0$), the pinning level ϵ_F is determined by the energy minimum of the E_{20} configuration. As V is increased, the threshold of E_{10} is reached first (Fig. 3), but the barrier between E_{10} and E_{20} is missing. A double charge of the In centers therefore occurs through the intermediate E_{10} state. The qualitative interpretation of Fig. 1 is the same as before.

From the experiment we estimate the following parameters of the model: $\epsilon_0-\epsilon_F \gtrsim 0.025$ eV and $E_A \sim E_{10}^{\min} - E_{20}^{\min} \sim 0.01$ eV. The low height of the self-trapped barrier accounts for the resonant scattering in PbTe⟨In⟩ at $T \geqslant 100$ K (Ref. 1).

The results reported above are direct experimental evidence of the validity of the self-trapped-barrier hypothesis for PbTe⟨In⟩. They also show that tunnel spectroscopy can be used for systems of this sort.

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