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Tunneling spectroscopy in the hopping regime

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Charge transport across tunneling junctions of n-doped Ge has been investigated experimentally and theoretically. Using tunneling spectroscopy we were able to observe the density of states and the effect of the electron-electron interaction on the excitation spectrum of samples, in which hopping is the transport mechanism close to equilibrium. To analyze the data of the measurements we derive an expression for the tunneling current in the hopping regime. We use our expression for the tunneling current in order to analyze the character of the transitions. Doing so, we show that in the experiment only transitions with at most small energy transfer were relevant.

Tunneling spectroscopy is one of the methods for obtaining information on the electronic structure of solids [1]. Usually planar tunnel junctions are used to probe the density of states (DOS) of a metal or of a semiconductor. A superconducting counter-electrode with a known quasi-particle DOS serves then as reference to *verify* tunnelling. If the tunneling takes place between electrons of the same energy (elastic or resonant tunneling) the tunneling current is a convolution of the densities of states of the contact materials [2]. Thus, the density of states of one material can be extracted if the density of states of the other material is known. In the case of inelastic tunneling the electronic transitions occur with emission or absorption of phonons. In this case the tunneling current becomes also sensitive to the phonon density of states [3].

However, this method requires knowledge and skill to prepare the interfaces, especially the thin insulating layer. For about two decades the mechanical-controllable break junction technique has been used to study clean interfaces of metals over a wide range of lateral contact sizes from bulk transport to vacuum tunneling. For a break junction device it is essential to bring a considerable force to the low temperature region of the refrigerator, to break a sample into parts, and to adjust the vacuum gap between both electrodes.

Mechanical-controllable break (MCB) junctions [4–6] offer an improved alternative spectroscopic method because those junctions can be prepared in situ at ultra-high vacuum conditions to yield clean interfaces. For clean electrodes the scattering from defects in the barrier region should become less important than the reflection and transmission characteristics of the proper vacuum potential barrier, allowing one to systematically study the characteristics of the junction.

In the hopping regime tunneling spectroscopy has proven useful in investigating the impact of the electron-electron interaction on the density of states of impurity bands. In this transport regime tunnel-

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ing experiments have been performed with conventional metal-barrier-semiconductor contacts [7] and mechanically controllable break junctions [8].

Here we report tunneling spectroscopy measurements with MCB-junction on disordered semiconductors and present a theoretical investigation of the nature of break-junction tunneling current for doped semiconductors in the hopping regime [9].

In tunneling spectroscopy experiments on Ge:As using break junctions [8], the traditional formula $I(U) \propto \int N(V)\, N(V-eU)\, [f(V)\,(1-f(V-eU))]\, \mathrm{d}V$ for the tunneling current has been applied, where $N(V)$ is the density of states and $f(V)$ the Fermi function. According to this formula the tunneling current is a convolution of the density of states of the contact materials. However, since the nature of the electronic states in such system is very different from that in metals or superconductors it is not obvious that the traditional expression for the calculation of the tunneling current can also be applied to tunneling spectra in the hopping regime. The theoretical investigations published in the literature lead to controversial results [10, 11]. Therefore it is not completely clear which concrete current-voltage relationship can be expected in the hopping regime and to what extent disorder induced fluctuations manifest themselves in the tunneling current.

In the standard theory of hopping transport [12, 13] the impurities are assumed to provide localized electronic states at sites $\boldsymbol{R_m}$ with localization length α^{-1} and characteristic energies V_m. The dynamics of the charge carriers can be described by the simple rate equation with transition probabilities

$$W_{nm} = \nu(|V_{nm}|) \exp\left\{-2\alpha R_{nm} + \frac{\beta}{2}\,(V_{nm} - |V_{nm}|)\right\}. \tag{1}$$

For a hop from the site n to the site m, $\beta = 1/k_B T$, $R_{nm} = |\boldsymbol{R_n} - \boldsymbol{R_m}|$ is the distance between the sites, and $V_{nm} = V_n - V_m$ is the difference between the site energies. In a close-to-equilibrium transport problem the pre-exponential factor $\nu(|V_{nm}|)$ in Eq. (1), characterizing the ability of the phonon to induce a transition, is usually replaced by a constant, since it affects the transport coefficients only a little. In the description of a tunneling experiment, however, the structure of this quantity is essential, as also pointed out in Ref. [11], and thus has to be taken into account.

For a break junction we consider two samples separated by a distance l. We denote the labels of the left sites with lower case letters m, n and those of the right sites with upper case ones M, N. Both samples have the same densities of states in the absence of the electric field, that is $N_L(V)|_{\boldsymbol{E}=0} = N_R(V)|_{\boldsymbol{E}=0}$. If both samples are separated very far from each other, there are no transitions between left sites and right sites and both samples are in equilibrium. If we now decrease the sample separation, tunneling transitions between the left and the right sample become possible with transition probabilities

$$W_{mM} = \nu(|V_{mM}|) \exp\left\{-2\kappa l_{mM} + \frac{\beta}{2}\,(V_{mM} - |V_{mM}|)\right\} \tag{2}$$

The tunnel transitions between the left and the right sample do *not* contain the localization length α and the site separation R_{mM}, but the *vacuum tunneling parameter* κ between the two bulk samples and an effective tunneling length $l_{mM} = l + \delta l_{mM}$. The quantity δl_{mM} is a small correction to the tunneling distance between the two samples taking into account the different wave function amplitudes for a given pair (m, M) of localized states. κ^{-1} is of the order of a few Ångstroms, whereas α^{-1} typically takes values around 10 nm. The current j cross the junction can be calculated by averaging the quantity

$$\boldsymbol{j} = -\frac{e}{\Omega}\left[\sum_m \boldsymbol{R}_m\, \frac{\mathrm{d}\rho_m}{\mathrm{d}t}\, \sum_M \boldsymbol{R}_M\, \frac{\mathrm{d}\rho_M}{\mathrm{d}t}\right]. \tag{3}$$

Here ρ is the occupation probability of the site m and M. Ω is the total volume which contains the sites in the summation in Eq. (3). We now use the fact that the tunneling rates (2) are orders of magnitudes smaller than the hopping rates (1) so that separate equilibriums are established in the samples. ρ_m and ρ_M are therefore Fermi functions $f_{L/R}(V)$ with chemical potential $\mu_{L/R}$. Applying the principle of detailed balance and performing the configuration average using of the densities of states,

we obtain the expression

$$\langle j_x \rangle = e\tilde{W} \int_0^{eU} \mathrm{d}V' \int_0^{V'} \mathrm{d}V \, N_L(V) \, N_L(V' - eU) \, \nu(V' - V) \, . \tag{4}$$

Here $\tilde{W} \propto \exp(-2\kappa l)$ is given by an integral over the transition probabilities. Furthermore, $N_L(V)$ is the density of states in the left sample and μ_L has been chosen as the zero point of the energy axis.

In investigating the expression (4) we focus on a density of states of the type

$$N_L(V) = N_0 + N_\gamma |V|^\gamma \, , \tag{5}$$

where $\gamma \approx 2$ for three-dimensional systems at zero temperature and N_0 vanishes at zero temperature [13, 14]. The results for tunneling experiments on systems with such a density of states are depicted in Fig. 1. The experimental data in Fig. 1 show a dip in the density of states for small V. These data indicate that the derivative of the tunneling current in the vicinity of $V \approx 0$ is not zero. However, our Eq. (4) shows that in the hopping regime the derivative of the tunneling current with respect to the voltage at $V = 0$ is always zero, if the transitions are inelastic. If, e.g, we use the deformation potential approximation of Ref. [13], which yields

$$\nu(V) = \nu_0 \frac{|V|}{\left(1 + \left(\frac{V}{2\hbar s \alpha}\right)^2\right)^4} \tag{6}$$

(s is the velocity of sound and ν_0 a constant), we find that

$$\langle j_x \rangle \propto V^{3+\zeta} \, , \tag{7}$$

for small V. Here $\zeta = 2\gamma$ if $N_0 = 0$ and $\zeta = 0$ otherwise. This implies $d\langle j_x \rangle / \mathrm{d}V|_{V=0} = 0$, which is contradiction to the experiments (see Fig. 1).

On the other hand, if we assume that the transitions are elastic, so that $\nu(|V - V'|) \propto \delta(V - V')$ then the expression (4) reduces to the result by Bardeen, according to which the derivative of the tunneling current with respect to the voltage is non-zero if $N_0 \neq 0$. A similar result can, however, also be obtained from quasi-elastic approximation, in which

$$\nu(V) = \nu_0 \theta(\omega - |V|) \, . \tag{8}$$

Here ν_0 is a constant frequency and ω is the maximum amount of energy transferred in one hop. In this approximation the formula for the tunneling current takes also the simple form

$$\langle j_x \rangle = e\nu_0 \tilde{W} \omega \int_{\mu_L}^{\mu_L + eU} \mathrm{d}V \, N_L(V) \, N_L(V - eU) \, , \tag{9}$$

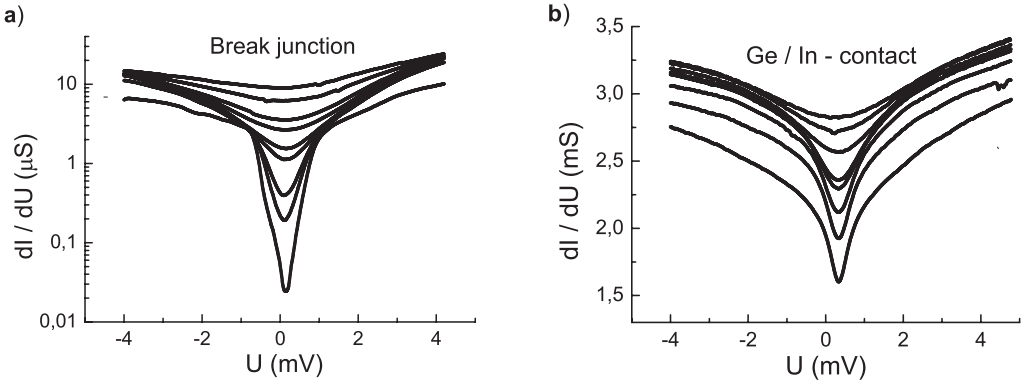

Fig. 1 a) Differential conductance $\mathrm{d}I/\mathrm{d}V$ of Ge:As for several temperatures, measured by the break-junction device. b) The same, measured by conventional tunnel spectroscopy using an indium contact.

if $\omega \ll eU$. Evaluating the current explicitly to the density of states (5) we obtain

$$\langle j_x \rangle = e\nu_0 \tilde{W} \omega eU \left[N_0^2 + \frac{2}{\gamma+1} N_0 N_\gamma |eU|^\gamma + \frac{(\Gamma(1+\gamma))^2}{\Gamma(2+2\gamma)} N_\gamma^2 |eU|^{2\gamma} \right].$$

Thus the results for the elastic approximation agree with those of the quasi-elastic approximation if the experimental resolution is smaller than the quasi-elastic energy, as it is expected. Accordingly, our results show that the transitions in the experiment of Ref. [8] are either elastic, or quasi-elastic transition with very small energy transfer.

In order to be sure that the break-junction measurements can be interpreted in a similar way as that of a conventional metal-barrier-semiconductor tunnel junction we have performed tunnel spectroscopy of Ge:As in the hopping regime for various temperatures using both techniques. The results are shown in Fig. 1. It is clear that in both cases the Coulomb gap is filled by thermal excitations as the temperature is increased [8]. Although the overall trends in both data sets are the same, there are some differences to be noticed. These difference can be attributed to the fact that in the case of the break-junction the differential conductance is proportional to the convolution of two shifted impurity band spectra whereas in the case of the conventional junction it is proportional to that of the DOS of the semiconductor and the metal.

In conclusion we have shown that break-junction spectroscopy can be used for samples with hopping transport in a similar fashion as it is done for metals.

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