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Role of inelastic effects on tunneling via localized states in metal-insulator-metal tunnel junctions

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We report a systematic study on the I-V characteristics (IVC) of tunnel junctions with barriers containing localized states. The study reveals a characteristic dependence of the IVC nonlinearity on the inelastic nature of electron transport via these localized states.

Transport via localized states in tunnel barriers is a subject of continuing importance. Issues of interest include resonant tunneling via these localized states, ^{1,2} the role of inelastic effects on the resonant tunneling, ^{3,4} and the lack of self-averaging in small, mesoscopic junctions. ^{5,6} These issues are also of interest for resonant tunneling through quantum-well structures and along one-dimensional metal-oxide-semiconductor field-effect transistor structures.⁷ At the same time, tunneling via localized states is an often implicated source of a wide range of nonidealities in the current-voltage characteristics of superconducting tunnel junctions.¹ Localized states are also believed to be a source of 1/f noise in tunnel junctions.^{8,9}

Over the past few years, tunnel junctions with thin, deposited, amorphous silicon (a-Si) barriers have been shown to be an effective model system for the study of tunneling via localized states.^{1,2} The thickness of the barrier can be varied systematically. By oxidizing or hydrogenating the a-Si barrier, the density of localized states can be reduced. Moreover, there is a great deal known about the properties of a-Si that can be used in the analysis of the data. Using such a-Si barriers, the crossover from direct to resonant tunneling, highly nonlinear and temperature-dependent I-V characteristics, and the tunneling transmission of individual localized states (in submicron junctions) have all been observed.^{1,2} A thickness-dependent suppression of transport via localized states at low bias has also been reported, and attributed possibly to Coulomb effects.²

Of particular interest currently is the role of inelastic effects on various tunneling processes. Several authors have discussed theoretically resonant tunneling via a single localized state (or a single quantum well) in the presence of electron-phonon interaction.^{4,10,11} At the same time, Glazman and Matveev¹² have emphasized that upon increasing temperature or the bias voltage, incoherent, sequential hopping across the barrier via a series of localized states—the beginning of variable range hopping —becomes favorable, despite the fact that such conduction chains are encountered infrequently. We report here a careful study of the *I-V* characteristics of *a*-Si tunnel barrier junctions and their thickness dependence that provide compelling confirmation of the predictions of Glazman and Matveev.

Building on earlier work by our group,^{1,2} we have made junctions with barriers of pure amorphous silicon in which the thickness of the barrier could be varied systematically. A new fabrication technique, related to the well-known selective niobium anodization process (SNAP),¹³ was adopted in which a sandwich structure of Nb/a-Si/Nb was made *in situ* on a sapphire substrate by electron-beam evaporation. Two silicon sources, situated symmetrically with respect to the substrate holder, were used to ensure the uniformity of the barrier. Four identical $8 \times 8 - \mu m^2$ junctions were defined photolithographically on each $\frac{1}{4} \times \frac{1}{4}$ -in.² substrate. Ion mill thinning of the top Nb layer followed by an anodization step was used to form electrically isolated junctions that were free of shorts. Sn cross-strip deposition through a stencil mask was then used to make contact to the junction. Using this approach, junctions with *a*-Si barrier thickness as small as 40 Å could be routinely made.

In Fig. 1 we show on a logarithmic scale the conductance G = I/V measured at a 5-mV bias and 4.2 K (the solid triangles) for a series of junctions as a function of the barrier thickness d. As seen in Fig. 1, the conductance decays exponentially with d, as expected for quantummechanical tunneling. The slope of this exponential dependence changes at $d \approx 100$ Å. The data for d < 100



FIG. 1. Small-bias tunneling conductance as a function of barrier thickness. The solid triangles are measured data. The open triangles represent resonant-tunneling conductance corrected for that of hopping via a pair of localized states. Values of localization length α^{-1} extracted from both direct and resonant-tunneling data are indicated. Inset shows three different tunneling processes.

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Å fall onto a straight line that we identify with direct tunneling in which $G_{dir} \propto \exp(-2\alpha d)$, where α^{-1} is the decay length of the electron wave function in the amorphous-silicon barrier [see process (a) in the inset of Fig. 1]. The data yield a value of $\alpha^{-1} = 7.0$ Å, which implies a barrier height in *a*-Si in the range 0.3–0.5 V, as discussed by Bending in Ref. 1.

The data for thicker barriers (d > 100 Å) seem to suggest that resonant tunneling via single localized state, for which $G_{\text{res}} \propto \exp(-\alpha d)$ (Refs. 1 and 2) [see process (b) in the inset of Fig. 1] is dominating the conduction. A closer examination reveals, however, that the conductance actually decreases more slowly than $\exp(-\alpha d)$, indicating that other conduction channels are present. As we shall see, these additional channels are associated with sequential hopping via localized states with certain spatial and energy distribution. The open triangles for d > 100 Å show the resonant tunneling conductance corrected for this hopping conductance as discussed in detail later in this Rapid Communication.

Figure 2 shows the conductance as a function of applied voltage for the same series of junctions as in Fig. 1. The influence of the superconducting energy gap is evident at bias voltages below 4 mV for the thinner barriers. However the gap structure smears out progressively with increasing thickness and disappears for $d \ge 90$ Å. Examining the data of Fig. 2, we note that there is a relatively flat, voltage independent region (up to 20 mV) in the curve for d = 60 Å, indicating a linear *I-V* characteristic. However, nonlinearity is clearly evident at high bias, and increases as bias is increased. Moreover, as *d* increases, the voltage at which nonlinearity sets in decreases. This behavior is manifestly inconsistent with simple direct or resonant tunneling which are essentially voltage independent. It is also inconsistent with the well-known $G \propto V^2$



FIG. 2. Voltage dependence of the conductance of barriers with increasing thickness.

behavior expected from the reduction of a barrier height due to the applied voltage.

The role of inelastic effects on tunneling via localized states was noted on the basis of experimental data.¹ Several theoretical studies have been devoted to the subject.^{3,4,10,11} In Refs. 3 and 4, the relative importance of variable range hopping and resonant tunneling was discussed in the context of quasi-one-dimensional systems. In particular, Stone and Lee⁴ found using a phenomeno-logical model that inelastic effects broaden the resonant tunneling transmission, but the integrated transmission remains unchanged. Experimental evidence for this prediction was seen by Bending and Beasley.¹

More recently, two groups independently developed a microscopic theory of tunneling via a single localized state coupled to the phonons in the barrier.^{10,11} Both found that the resonant transmission is broadened and that side bands at the phonon frequencies appear in the transmission function. Both groups also rigorously showed that the integrated transmission was constant, as suggested by Stone and Lee. More importantly for the experiments described in this paper, Glazman and Matveev¹² found that as either voltage or temperature is increased, localized states which are well separated in energy and therefore not resonant become accessible to tunneling electrons via coupling to phonons. Consequently the contribution from hopping through a sequence of localized states [see the process (c) in the inset of Fig. 1] increases in importance relative to resonant tunneling. In particular, they found that as the bias voltage increases the dominant contribution comes from channels with an increasing number of hops. This in turn leads to an unusual and characteristic voltage dependence of the conductance G = I/V. Quantitatively, they obtained the following expression of the self-averaged hopping conductance due to a channel involving *n* localized states:

$$\langle G_n \rangle \propto \frac{S}{a^{-1}d} (ga^{-2}deVn^2)^n \\ \times \left[\left(\frac{E_0}{eV} \right) (\lambda)^{(n-1)/2} \exp(-ad) \right]^{2/(n+1)}, \quad (1)$$

where S is the junction area, g is the density of localized states in the barrier, V is the applied voltage, E_0 is the depth of localized states in the barrier, and λ is a dimensionless electron-phonon coupling parameter. To keep the notation consistent we clarify that $\langle G_1 \rangle$ is equivalent to $G_{\rm res}$ for resonant tunneling via single localized state and that $\langle G_0 \rangle$ is the same as $G_{\rm dir}$.

Equation (1) can be understood as follows. Since the transport is by incoherent hopping, any conduction chain containing n localized states is effectively a series of n+1 resistors. When these localized states are equally spaced and situated within an energy band of width eV near the Fermi energy, the chain has an optimal conductance that depends on V. In addition, the total conductance of the n-state channel will be proportional to the number of such chains within the entire area of the junction.

Returning now to Eq. (1), we can make the following identifications. The factor $S/\alpha^{-1}d$ is the total number of statistically independent conduction chains contained in a

barrier of area S. The factor $(ga^{-2}deVn^2)^n$ gives the probability of forming an effective chain (i.e., with its *n* states having appropriate spatial and energy distribution). And the factor

$$[(E_0/eV)(\lambda)^{(n-1)/2}\exp(-\alpha d)]^{2/(n+1)}$$

is the characteristic conductance associated with the optimal chain. The voltage dependence of this factor follows from the energy dependence of the individual inelastic hopping events.

From Eq. (1) we see that $\langle G_n \rangle$ has a power-law dependence on V, $\langle G_n \rangle \propto V^{n-[2/(n+1)]}$. Thus as V increases the total conductance $\langle G \rangle$ is dominated by channels with successively higher n. It follows that at low bias the leading correction to a constant $\langle G \rangle$ should go as $V^{4/3}$, corresponding to hopping via two localized states (i.e., n=2). To test this prediction, in the inset of Fig. 3 we show $(\langle G \rangle - \langle G_0 \rangle)/\langle G_1 \rangle$ versus bias voltage for the d=70 Å junction. The curve has a slope of 1.35, close to the theoretically predicted exponent $\frac{4}{3} = 1.33$. When G vs V is plotted in the same fashion for thicker barriers, we obtain larger values of this slope at higher bias, and they are also close to those predicted by the theory.

From the data in the inset and using Eq. (1), we can estimate for d = 70 Å the dimensionless electron-phonon coupling constant λ . Also from the expression for λ in Ref. 12, we infer a value $\Lambda = 3.5$ eV for the deformation potential in our *a*-Si barrier. Finally, given this λ and an estimate of *g*, we can calculate $\langle G \rangle / \langle G_1 \rangle$ from Eq. (1) as a



FIG. 3. Comparison between the experiment and the theory. The inset shows the normalized conductance as a function of bias voltage for d = 70 Å barrier. The slope of the curve is the power exponent for hopping channels with two localized states.

function of V for all values of d including contributions from all orders of n (we have taken $g = 5 \times 10^{18}$ for our barrier¹⁴). The result is shown in Fig. 3 where we show the calculated $\ln(\langle G \rangle / \langle G_1 \rangle)$ vs $\ln(V^*/V)$, where V^* is a voltage scale defined through $ga^{-2}deV^* = 1$, together with the corresponding experimental results. Given that there is only one material-related parameter in the fit, the overall agreement is striking.

This plot allows one to observe from yet another perspective the nature of the nonlinearity in the I-V characteristics. To the right-hand side of the plot (small bias) the curves go asymptotically to a voltage-independent conductance reflecting the sum of the direct tunneling (n=0) and the resonant tunneling (n=1) channels alone. Moving to the left (large bias) the conductance becomes more nonlinear as channels with larger n begin to contribute. This trend is shown explicitly for the 120-Å curve, where the calculated threshold voltages V_n at which the nth channel opens up are indicated for reference.

Let us now return to Fig. 1. As we noted earlier the conductance data for d > 100 Å contain contributions from these hopping channels as well as resonant tunneling. The amount of this hopping conductance can be determined as follows: We know that

$$\langle G(V \approx 0) \rangle = \langle G_0 \rangle + \langle G_1 \rangle \approx \langle G_1 \rangle$$

since it is voltage independent, and $\langle G_0 \rangle / \langle G_1 \rangle \ll 1$ in this thickness range. Approximating

$$\langle G(5 \text{ mV}) \rangle = \langle G_0 \rangle + \langle G_1 \rangle + \langle G_2 \rangle \approx \langle G_1 \rangle + \langle G_2 \rangle,$$

then

$$\ln\langle G(V \approx 0) \rangle \approx \ln\langle G_1 \rangle$$

$$\approx \ln\langle G(5 \text{ mV}) \rangle - \ln(1 + \langle G_2 \rangle / \langle G_1 \rangle).$$

From this one can actually calculate the correction to $\ln\langle G(5 \text{ mV}) \rangle$ to obtain $\ln\langle G(V \approx 0) \rangle$, i.e., the true zerobias conductance. The open triangles in Fig. 1 represent the resonant tunneling conductance with this correction. These corrected data yield a slope closer to that expected for resonant tunneling. Note that a value of $\alpha^{-1} = 6.8$ Å inferred from this slope is close to $\alpha^{-1} = 7.0$ Å obtained from the slope for direct tunneling. This confirms more quantitatively the interpretation of the data as a crossover (at bias ≤ 5 mV) from direct to resonant tunneling as d increases.

We note in Fig. 3 that the measured conductance data always lie below the calculated value for low bias. This may be related to the charging effects in the barrier.^{2,15} As also can be seen from Fig. 3, the rise of the slopes of the measured conductance curves does not quite follow that of the calculated curves at large bias ($V \ge 0.4$ V), indicating that on going to higher-order hopping channels there is a limit beyond which, for a finite-size junction, one may run out of localized states to support the hopping.

In conclusion, we have elucidated the role of inelastic effects on electron tunneling via localized states in thin amorphous barriers. These effects result in sequential hopping through localized states. It is shown that the increasing nonlinearities in the I-V characteristics are associated with the opening up of hopping channels with an in-

creasing number of hops. It is also shown that the voltage and thickness dependences of these effects are in good quantitative agreement with the theory. We believe these results should provide insight into the physics of electron tunneling in a broader range of systems in which inelastic effects are important. Also, the effects of inelastic pro-

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cesses on superconductive tunneling, such as the Josephson current and the gap structure, are of equal importance and interest, and deserve a thorough investigation in their own right. Research in that direction is emerging.¹⁶

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