BEEM SPECTROSCOPY OF ELECTRON TRANSPORT THROUGH AlAs/GaAs HETEROSTRUCTURES

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BEEM spectroscopy has been used to characterize hot carrier transport through AlAs/GaAs heterostructures. The dependence of electron transmission on AlAs thickness has been directly measured, and the position of the AlAs L_1 minima, which has been subject to some uncertainty in the past, has been determined. First–principles transmission calculations, based on a tight–binding formalism, are compared to the results of BEEM spectroscopy.

PACS numbers: 73.40.Kp, 61.16.Ch, 73.20.At, 68.35.–p

The characterization of semiconductor heterostructures is an extremely active area of current experimental research. This strong interest is in large part motivated by the wealth of novel device applications developed over the last decade. There is a great deal of interest in the more fundamental aspects of interface formation and band alignments, and the desire for a unified description of interfaces has spawned many theories of interface formation, each of which demonstrates agreement with a greater or lesser fraction of the accumulated experimental results. From the point of view of device performance, the determination of transport through these structures is also of great importance.

The AlAs/GaAs materials system, including the intermediate AlGaAs fractions, is the most studied family of heterostructures.[1] The capability for epitaxy in this system is highly developed, and a great deal of theoretical work has also been performed.[2,3] A precise experimental characterization, both of the AlAs/GaAs interface electronic structure and of transport characteristics in this system, is necessary for the development of a consistent theoretical description. For example, an uncertainty concerning the location of the conduction band minima within AlAs has not been resolved.[4]

Band offsets at semiconductor interfaces have conventionally been probed by using techniques such as internal photoemission and X–ray photoemission spectroscopy (XPS). Transport through heterostructures has been characterized primarily through current–voltage measurements on single– and double–barrier systems. In such two–terminal measurements, however, it is not possible to perform an energy spectroscopy of transport; in addition, the bending of the bands due to application of the voltage complicates analysis of the results. Three–terminal spectroscopy measurements have been performed[5,6] on macroscopic devices over a limited energy range.

This paper describes the microscopic characterization of the AlAs/GaAs interface

by ballistic–electron–emission microscopy[5] (BEEM). BEEM is a technique, based on scanning tunneling microscopy[6] (STM), which utilizes the STM tip to inject ballistic carriers by vacuum tunneling into a heterostructure. The resulting forward–peaked distribution of carriers may then be used to perform a spectroscopy of transport through the sample structure. By measuring the fraction of the tunnel current which enters the semiconductor collector as a function of tunnel voltage, local properties of the interface such as barrier height, electronic band structure, and interface transmission efficiency may be probed directly. Interface imaging may also be performed with nanometer spatial resolution. This technique has previously been extensively applied to the Schottky–barrier interface with great success. In the present work, a detailed BEEM spectroscopy of electron transport through the Au/AlAs/GaAs structure is presented, focusing on the development of band structure with AlAs thickness, and the corresponding effects on electron transport. The effectiveness of AlAs as a barrier to diffusion in the Au/GaAs system has already been demonstrated by BEEM characterization.[7]

A series of Au/AlAs/GaAs structures with different thicknesses of AlAs was fabricated by molecular–beam epitaxy (MBE). Substrate cleaning prior to MBE growth has been described previously.[8] The MBE procedure consisted of growth of a 1–μm–thick GaAs buffer layer ($n = 5x10^{16}$ cm^{-3}, Si doped) on the n–GaAs(100) substrate ($n = 3x10^{16}$ cm^{-3}, Si doped) under As–stabilized conditions, yielding the (2x4) surface reconstruction as observed by reflection high–energy electron diffraction (RHEED). The sample was then annealed in the As flux to promote surface smoothing. The AlAs layer was deposited under RHEED control; monitoring of the RHEED oscillations provided precise control of AlAs thickness. The sample was transferred under UHV to the Au deposition chamber for completion by evaporation of 100 Å of Au. Electron transport through these structures were characterized by BEEM spectroscopy in a nitrogen gas–purged glove–box at room temperature. BEEM spectra of collector current I_C versus

tunnel voltage V were acquired at a constant tunnel current of 1 nA. Samples with four different thicknesses of AlAs were analyzed. A qualitative energy diagram for these sample structures is shown in Fig. 1.

The derivatives dI_c/dV of representative BEEM spectra for the four samples are plotted as a function of V in Fig. 2. Differentiation of the I_c–V data makes the multiple threshold nature of the data more apparent. The "0 ML" derivative designates a sample with no AlAs interlayer between the Au and the GaAs. Within the phase space model which has been used previously to interpret BEEM spectroscopy results, the two limiting case spectra, representing Au/GaAs and Au/AlAs, may be interpreted. BEEM of Au/GaAs has already been characterized.[7,9] The position of the first threshold represents the Schottky barrier height (SBH). In GaAs, a direct semiconductor, this is defined by the Γ point at the interface and occurs at 0.89 V. A second threshold is encountered at 1.18 V, which is produced by the onset of propagation into the L_1 minima of GaAs. A weaker third threshold, at the onset of X_1–minima transmission, also occurs at higher voltage.

The sample with the thickest (50 ML) layer of AlAs ensured that the interlayer was opaque to electrons with energies less than the AlAs conduction band minimum, and was therefore representative of transport in Au/AlAs. The Au/AlAs spectrum reflects features of the AlAs band structure. An initial threshold is observed at 1.15 V, which agrees well with previous measurements of the SBH for this system.[10] In AlAs, this is defined by conduction band minima along the Γ_1–X_1 directions. A second threshold at 1.35 V also appears in the derivative. This threshold determines the L_1–minima energy in AlAs. The location of this band has been the subject of some controversy, but appears unambiguously here. Previous measurements have relied on extrapolations of $Al_xGa_{1-x}As$ data, with experimental measurements only up to x=0.6.[4] Casey and Panish[11] provided an estimate of E_L–E_X of between 0.08 and 0.18 eV. Lee et al.[12] give

$E_L - E_X = 0.2$ eV from extrapolation of electrical measurements. Godby et al.[4] tabulate experimental values indicating a $E_L - E_X$ range from 0.25 to 0.30 eV. The value from BEEM of 0.2 eV agrees well with previous extrapolations. The Γ point should occur at approximately 2.0 V and is beyond the range of the data.

BEEM transport spectra representing intermediate thicknesses of AlAs reveal both GaAs and AlAs electronic structure and are less straightforward to interpret. The band structure of the thinnest AlAs layers is not yet bulk–like; in addition, the presence of electron tunneling and standing waves in the AlAs layer must be treated. Of primary importance is an understanding of the attenuation of GaAs substrate contributions as AlAs thickness increases. In order to provide insight into the qualitative features of electron transport in these structures, transmission probabilities were calculated using the reduced Hamiltonian method of Schulman and Chang[13]. Since the structure of the Au film deposited on the semiconductor surface is not well defined, we have chosen instead (for computational convenience) to consider structures where the Au is replaced by a material such as α–Sn that has the same structure as the underlying semiconductor and can be described straightforwardly within the method of Ref. 15. Au, on the other hand, is difficult to treat with this formalism. Since α–Sn is metallic, it may provide qualitative understanding of experimental data. In our calculations, $\mathbf{k}_{\parallel}$ is conserved; thus some thresholds (such as L_1 in GaAs) will not appear. Breakdown of $\mathbf{k}_{\parallel}$ conservation by scattering is required to detect such thresholds. The choice of metal has no effect on $\mathbf{k}_{\parallel}$ conservation, which depends only on the presence or lack of scattering. Since the details of the scattering are uncertain[21], a scattering contribution is not included in the model.

This method is based upon a tight–binding description of the energy bands and wave functions and is exact within that description. We specialize the method to a (100) interface and use the sp^3s^* tight–binding model of Vogl, Hjalmarson, and Dow[14]. Some

simplification results because interactions extend only to the nearest neighbors and spin–orbit coupling is neglected. Although the model has limitations, it nonetheless can provide an adequate qualitative picture of the interface. A more accurate description might be given by the method of Ando and Akera[15], who used a combination of tight binding for the boundary conditions and effective mass approximations for the bands. Stiles and Hamann[16] have also applied the method of linearized augmented plane waves to epitaxial interfaces. Such studies are, however, beyond the scope of the present work. Fortunately, many of the features of the BEEM spectra depend only on energy levels and **k** vectors, which the tight–binding model reproduces with sufficient accuracy.

This theory has been applied to a series of calculations of the total transmission probability D for α–Sn/AlAs/GaAs. Only normal incidence ($\mathbf{k}_{\parallel}=0$) is considered, and in the energy range shown only one band in α–Sn propagates, namely a band extending from Γ_{15} at $k_z=0$ to X_5 at $k_z=2\pi/a$ (Fig. 11 of Vogl et al.). All energies are referred to the GaAs valence band maximum. The AlAs valence band is offset from GaAs by 0.47 eV[17] in the tight binding calculation, so all diagonal energies of AlAs have been decreased by this amount. The α–Sn parameters are left unchanged.In Fig. 3, we show results for α–Sn/GaAs and three thicknesses of AlAs. Each plot is labelled by the number of monolayers (ML) of AlAs. Also indicated are the levels used in the tight binding calculation. The Γ_1 threshold of GaAs is at 1.55 eV, X_1 at 2.03 eV, and X_3 at 2.38 eV. In AlAs, X_1 is at 1.83 eV and X_3 at 2.21 eV. The minimum energy is along Δ, near X_1, at 1.80 eV, whereas Γ_1 is much higher at 2.57 eV and is not encountered in these calculations.

The transmission probability for the α–Sn/GaAs interface clearly shows the thresholds at Γ_1 and X_1, and to a lesser extent X_3. The L_1 threshold is at 1.69 eV but does not appear in calculations for normal incidence on a (100) interface, because transverse momentum ($\mathbf{k}_{\parallel}$) is conserved. On the other hand, both the Γ_1 conduction band and the X_1

valley in the [100] direction are final states allowed by transverse momentum conservation.

When there is an AlAs barrier, the transmission is considerably different. Below the Δ threshold at 1.80 eV, the electron must tunnel through the AlAs to reach the Γ_1 conduction band of GaAs. As a consequence, the probability D in this energy range decreases rapidly with thickness. This is reflected experimentally in the decay of the Γ threshold intensity in the data shown in Fig. 2. Over most of the range, our calculations show that the extinction constant κ is $0.16(2\pi/a)$ ($D \sim e^{-2\kappa d}$), which is close to $Im(k_z)$ for the Γ_1 band ($\approx 0.17(2\pi/a)$). A plot of $Im(k_z)$ has been given by Schulman and Chang (Fig. 1)[18], which is quite similar to our results. Tunneling via the Δ minimum (or X_1 valley) is less likely than via Γ_1 since $Im(k_z)$ for Δ is actually larger for $E < 1.69$ eV and the coupling of AlAs X_1 valley states to GaAs Γ_1 is weak over the entire energy range. For the 4 ML barrier, the calculation shows the presence of virtual standing waves in the AlAs X_1 valley below the X_1 edge in GaAs. Since the coupling to Γ_1 is weak and there is some reflection at the α–Sn interface, standing wave resonances can be set up. Ando and Akera have discussed this phenomenon in AlGaAs heterojunctions where the location of bands in the barrier have the same ordering as here. However, as discussed below, these resonances do not appear directly in the BEEM spectrum.

Although transport via the L_1 minima is not treated in the calculation, the qualitative features are similar. Since the L_1 minima in GaAs lie at lower energy than in AlAs, the presence of the AlAs layer will produce a tunnel barrier for L_1 transport. This will cause an attenuation of the intensity of the GaAs L_1 threshold in the BEEM spectra. An additional threshold will also start to appear at higher energy, at the L minima in AlAs. Electron transport in this case will not involve either Γ_1 or X_1 in either material, due to $\mathbf{k}_\parallel$ conservation.

Above the X_1 threshold of GaAs, the probability of transmission is large, ≈ 0.8, indicating that the electron is propagating through the AlAs via the X_1 valley, where it is strongly coupled to the X_1 states in GaAs. Observation of the onset of X_1–X_1 transmission in the data, however, will be complicated by the presence of L_1–L_1 transmission, which should also produce a strong threshold. Since L_1 in AlAs (1.35 V) lies near in energy to X_1 in GaAs (1.38 V), these two transport processes will onset at approximately the same voltage.

When the thickness of the barrier exceeds the mean free path, a different behavior is observed in the calculated transmission that does not show the thresholds of the GaAs, but only AlAs electronic structure. As shown in Fig. 3, the X_1 and X_3 thresholds of AlAs appear; again, the L_1 threshold does not appear in these one–dimensional calculations due to conservation of $\mathbf{k}_\parallel$, although it is clearly seen in the data.

In a BEEM experiment, the Γ_1, L_1 and X_1 thresholds will have the usual $(V–V_b)^2$ dependence even in the presence of the AlAs barrier. The Γ_1 current will be greatly reduced as the barrier thickness is increased, while the X_1 should remain roughly the same. The standing waves in the AlAs X_1 valley will show a slightly different threshold behavior in I_c. In the one–dimensional case, we can replace a standing wave, or closely spaced group of waves, with a threshold V_{t1} where the current is turned on and a second threshold V_{t2} slightly above V_{t1} where the negative of the current is turned on. The difference between V_{t2} and V_{t1} is an effective width of the resonance. The collector current would then be of the form

$$I_c \sim f(V–V_{t1}) – f(V–V_{t2}) \ ,$$

where $f(V–V_t)$ is the usual functional form of the BEEM collector current. However, the

large spread in $\mathbf{k}_{\parallel}$ in the three–dimensional case will broaden this threshold behavior from a step–like feature into a more gradual linear form[19], which in the derivative will in turn appear as a step. This threshold is therefore not expected to exhibit the strong resonances which appear in the calculation, but rather should resemble the standard step–like BEEM threshold in the derivative. The first threshold in the 4ML spectrum may owe some of its intensity to this resonant transport, since X_1–X_1 transport is not expected until the X_1 threshold in GaAs is reached at 1.38 V. A contribution below the AlAs X_1 also appears to be present, indicating that tunneling through the AlAs gap into Γ of GaAs is still appreciable.

In conclusion, BEEM has been used to investigate transport through AlAs/GaAs semiconductor heterostructures. The dependence of transport on AlAs thickness has been directly measured. For the case of Au on thick AlAs, the position of the L_1 minima, which has been subject to some uncertainty in the past, has been directly determined. Results of BEEM spectroscopy have been compared to first–principles transmission calculations for equivalent thicknesses of AlAs on GaAs.

The research described in this paper was performed by the Center for Space Microelectronics Technology, Jet Propulsion Laboratory, California Institute of Technology, and was jointly sponsored by the Office of Naval Research and the Ballistic Missile Defense Organization / Innovative Science and Technology Office through an agreement with the National Aeronautics and Space Administration (NASA).

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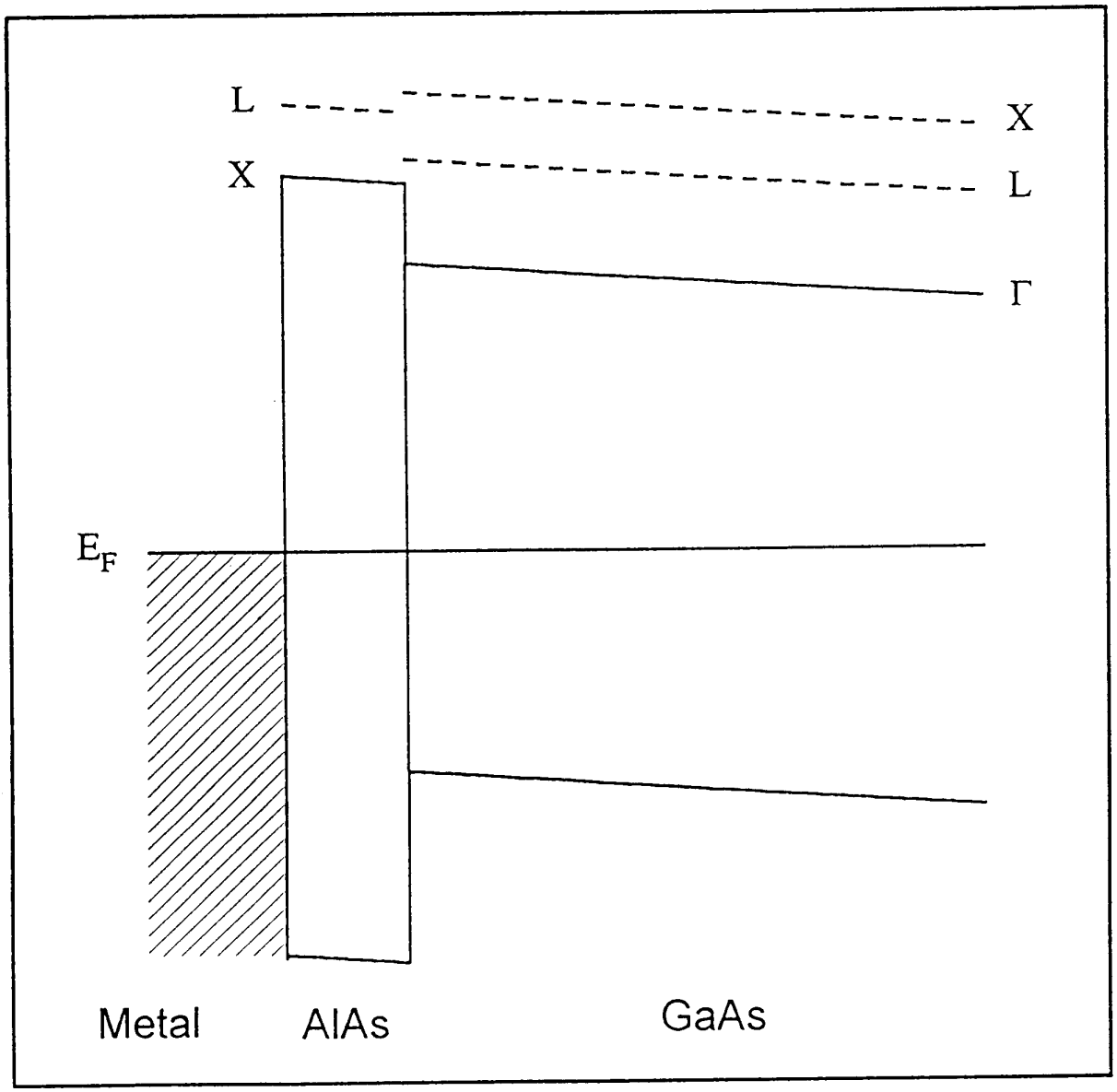
Figure Captions

Fig. 1 Schematic energy diagram for a metal/AlAs/GaAs system.

Fig. 2 Derivatives dI_c/dV for BEEM spectra of Au/AlAs/GaAs structures. Data are shown for AlAs thicknesses of 2 ML, 4 ML, and 50 ML. Also shown is a derivative spectrum for Au/GaAs (labelled "0 ML").

Fig. 3 One–dimensional transmission calculated for α–Sn/GaAs, α–Sn/AlAs/GaAs for AlAs thicknesses of 2 and 4 ML, and α–Sn/AlAs. Also indicated are the tight binding values for conduction band minima Γ_1 and X_1 in GaAs and X_1 in AlAs.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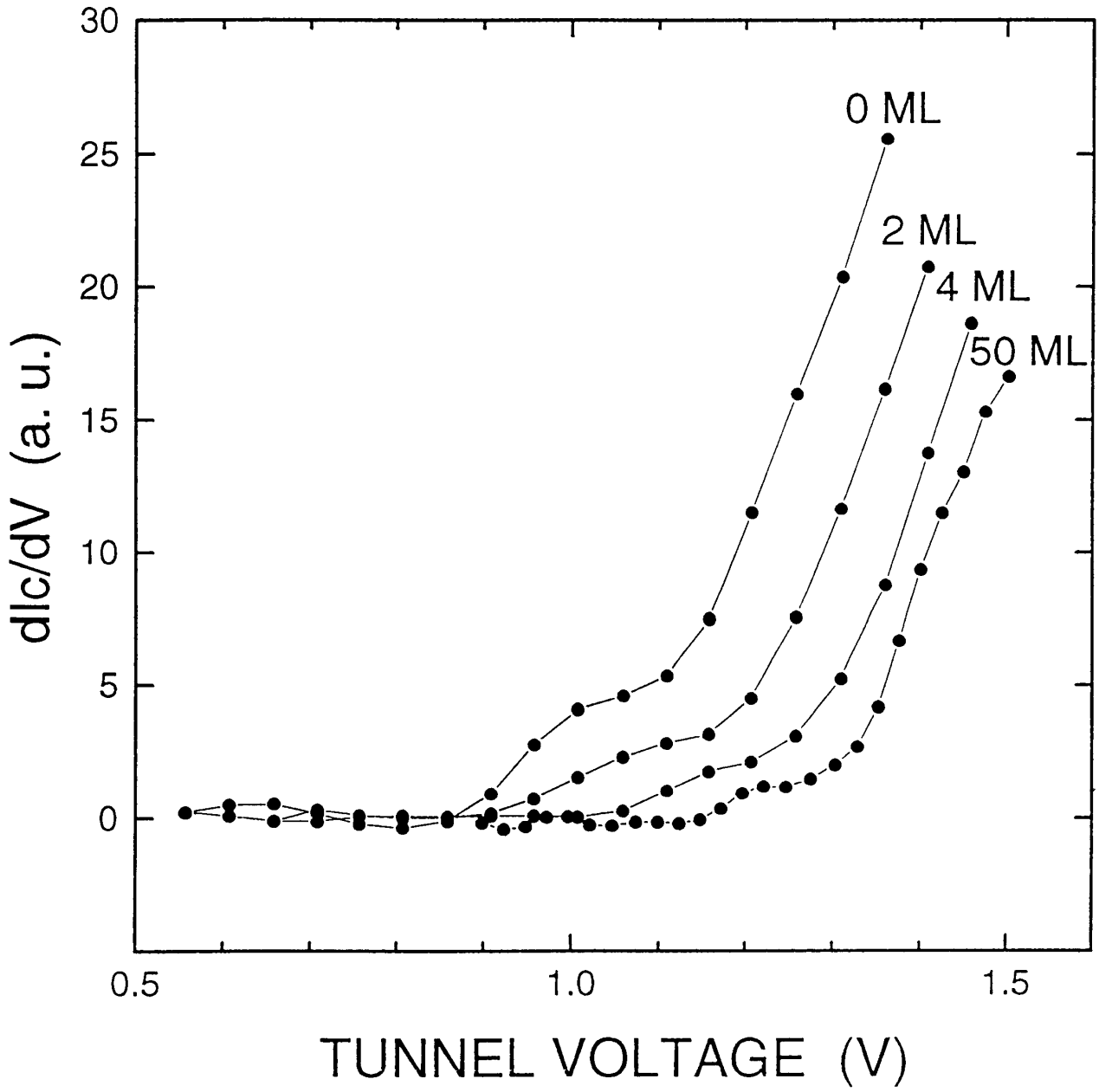
30
25
20
15
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dIc/dV (a. u.)
0 ML
2 ML
4 ML
50 ML
0.5
1.0
1.5
TUNNEL VOLTAGE (V)