

Transport limitations in tunneling spectroscopy of Ge(111)c(2×8) surfaces

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Scanning tunneling spectroscopy is used to study *p*-type Ge(111)c(2×8) surfaces at temperatures between 7 and 61 K and over a wide range of tunnel currents. The spectral feature arising from Ge rest-atoms is found to shift in voltage with increasing tunnel current. Comparison of the current dependence of the results with electrostatic computations of tip-induced band bending yields poor agreement. A model is discussed in which the observed shift in the rest-atom state arises from an accumulation of nonequilibrium carriers at the surface.

PACS numbers: 73.20.Hb, 71.20.Nr, 61.16.Ch

In scanning tunneling spectroscopy (STS) studies of semiconductors, transport of carriers within the semiconductor is a subject which is not well understood. In most cases it is assumed that this transport plays no role, since the resistance of the tunnel junction itself is typically 1 GΩ. However, with the advent of low-temperature scanning tunneling microscopes over the past five years, results from a number of studies have indicated nonequilibrium carrier dynamics in the experiments. In particular recent work from both Takayanagi and co-workers^{1,2} and Dujardin *et al.*³ report remarkable temperature dependence of their results, for Si(001)2×1 and H-covered Ge(111)c(2×8) surfaces respectively, leading to the suggestion that the transport of carriers in the semiconductor may in some way be affecting the results.¹⁻⁴ Earlier work at room temperature for SiC(0001)-√3×√3-R30° surfaces also demonstrated the existence of transport limitations in the semiconductor during STS experiments.⁵

In this work we study tunneling spectra acquired from *p*-type Ge(111)c(2×8) surfaces, over the temperature range 7 to 61 K. In an effort to probe possible limitations in the semiconductor transport on the results, we perform experiments over a wide range of tunnel currents, with setpoint currents (*i.e.* corresponding the current near one of the endpoints of the spectra) ranging from 2 pA to 7 nA. Features arising from the surface adatoms and rest-atoms are identified in the spectra. The position of the rest-atom peak is found to shift as a function of the tunnel current magnitude. We find that these shifts are much larger than those expected on the basis of electrostatic tip-induced band bending

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(*i.e.* in the limit of zero current). Additional voltage shifts are needed, and we attribute those to a nonequilibrium accumulation of tunneling carriers at the surface.

Pieces of $\{111\}$ -oriented Ge wafers, p -type with room-temperature resistivity of $0.2 \Omega\text{cm}$, were cleaved in ultra-high-vacuum (pressure of about 1×10^{-10} Torr), exposing a $\{111\}$ crystal face. Cleavage was performed at room temperature, and immediately afterwards the samples were resistively heated to a temperature of about 500°C for a few minutes. This procedure is known to produce large, well-ordered areas of $c(2 \times 8)$ reconstruction.⁶ Within a few minutes after heating, the samples were cooled to about 50 K and were introduced into a liquid-He cryostat containing the home-built STM.⁷ Probe-tips were formed prior to sample cleavage by making a controlled mechanical contact of a tungsten tip to a clean copper surface, thereby transferring copper atoms to the end of the tip. Metallic tips are reliably formed in this manner.⁸ Tunneling spectra were acquired using a voltage modulation of 10-20 mV and employing a lock-in amplifier to obtain the conductance. As previously described,⁹ we use the technique of continuously varying sample-tip separation to ensure a large dynamic range in the measurements. Normalization of the spectra is done by first scaling the conductance dI/dV to *constant* sample-tip separation using *measured* values of the inverse decay constant κ (with current proportional to $\exp(-2\kappa s)$ for tip-sample separation s) which are in all cases within $\pm 0.1 \text{ \AA}^{-1}$ of the value $1.0 \text{ \AA}^{-1}$. We then compute the normalized conductance $(dI/dV)/(\overline{I/V})$ using parameters of $a' = 2 \text{ V}^{-1}$ and $\Delta V = 1 \text{ V}$ as defined in Ref. [9].

In Fig. 1 we display spectra acquired from the $\text{Ge}(111)c(2 \times 8)$ surface at temperatures of 7, 15 and 61 K, and for a tunnel current setpoint of 0.3 nA. A number of features can be readily identified in the spectra. A band gap is visible extending from -0.1 to 0.5 V . The surface Fermi-level (0 V in the spectra) is located near the bottom of this gap, as expected for p -type material. A large spectral peak is seen centered at about 0.7 V and it can be attributed to the empty states associated with the surface adatoms,^{6,10} in agreement with inverse photoemission results.¹¹ This peak displays a splitting, arising from the two inequivalent types of adatoms in the $c(2 \times 8)$ structure.¹⁰ In the filled states, at about -1.4 V , a spectral feature derived from the surface rest-atoms is visible. As shown below, the location of this peak shows a continuous variation as a function of current, but the low-current position of -0.9 eV relative to the valence band (VB) maximum is in reasonable agreement with the location seen in photoemission of -0.7 eV .¹² Above the rest-atom band, for voltages extending up to -0.1 V , the observed tunnel current derives from VB states. Finally, above the adatom band, at voltages above $+1.0 \text{ V}$, the current derives either from conduction band (CB) states or possibly from higher-lying surface bands.

Figure 2 displays the dependence of our results on the current setpoint. As the current increases the rest-atom peak is observed to shift, with relatively little change seen elsewhere in the spectra. Figure 3 summarizes our results for the location of the rest-atom peak, as a function of the tunnel current. The currents there correspond to the *actual* currents (not the setpoints) measured in each case for the rest-atom peak. For

convenience we can *approximately* convert this current scale into a scale of sample-tip separation, as shown at the top of Fig. 3. This conversion is not exact since we are discussing spectral feature at different voltages, but over the voltage range of interest this separation scale is accurate for relative separations to within $\pm 0.2 \text{ \AA}$. The zero in this separation scale is not precisely known, and we have assumed a separation of $7 \text{ \AA}$ for a current of 1 nA (tunneling resistance of about $1.5 \text{ G}\Omega$). Prior experiments have determined separations, for particular tunneling resistances, of $7.4 \text{ \AA}$ and $8.1 \text{ \AA}$ for $0.1 \text{ G}\Omega$,^{13,14} and $8.0 \text{ \AA}$ and $9.3 \text{ \AA}$ for $2 \text{ G}\Omega$.^{15,16} Based on those results we can be quite confident that the actual zero of separation for the data in Fig. 3 is not *less* than that indicated on the graph, and it might be $1\text{-}2 \text{ \AA}$ greater than that shown there.

Let us now consider models which may account for our observations of Fig. 3. We clearly observe some band bending in the semiconductor. In the zero-current limit we can compute this band bending simply by solving Poisson's equation for the three-dimensional tip-semiconductor system.¹⁷ The two main parameters in such a computation are the radius-of-curvature of the probe tip and the contact potential (difference in work-functions) between tip and sample. The opening angle of the tip shank can also be varied,¹⁷ but we keep this fixed at 90° for the results shown here. We use for the computation the established photoemission result for the energy of the rest-atom state of 0.7 eV below the VB maximum.¹² We initially assume zero contact potential (*i.e.* flat band conditions for zero sample-tip voltage) which is consistent with our observed tunneling spectra. We compute band bending for a range of sample voltages, and search for the voltage at which the rest-atom states is aligned with the tip Fermi-level, as pictured in Fig. 4. Results are shown in Fig. 3 for tip radii of 1 , 10 and 100 nm respectively. In all cases the agreement between the experimental results (for any given temperature) and the computations is poor. If we make the somewhat unrealistic assumption of 0.3 eV contact potential (tip work-function largest) for the 100 nm radius case then that result is shifted to lower-magnitude voltages, as shown, but the agreement with the data is still poor. We have also considered more complicated tip shapes, *e.g.* with flat spots or with small-radius hemispherical protrusions on the apex, but in no case do they produce improved agreement with the data of Fig. 3.

Summarizing the results of Fig. 3, we find in the computations a *gradual* increase in rest-atom peak shift with decreasing tip-sample separation, but the observed results at each temperature vary 4-5 times faster. Also, the computational results contain no significant temperature dependence; the theoretical results of Fig. 3 are for 0 K , and the only effect of changing temperature is a small increase (14 meV at 61 K) in the position of the sample Fermi-level that produces a shift in the rest-atom peak *opposite* to that observed. We therefore conclude that some new aspect of the physics is required to account for our observations of the rest-atom peak shift.

We adopt a model similar to that previously presented for $\text{Ge}(111)\text{c}(2\times 8)$ by Dujardin *et al.*³ We assume that there is an accumulation of carriers, holes in the present case, at the semiconductor surface and/or in the near-surface region, due to the tunnel current. The charge density of these nonequilibrium carriers will produce changes to the

electrostatic potential profile, in particular, producing additional band bending which may be temperature dependent. Furthermore, the high-current density and/or high-fields in the tunnel junction may produce energy shifts to the rest-atom energy band which go beyond that expected from the simple electrostatic considerations discussed above.^{18,19} Thus, although we have not identified the precise mechanism which gives rise to the shifts in the rest-atom band, we feel that the data clearly indicates the need for a new mechanism and one which likely involves limited transport through the rest-atom band.³ A full understanding of this mechanism must also include explanations for (i) the relatively slow dependence of the observed shift with tunnel current (approximately logarithmic for currents above some critical value, as seen in the data of Fig. 3) and (ii) why we do not observe similar shifts in the location of the adatom spectral peaks (at positive voltages), *i.e.* these appear to have different behavior than the rest-atom peak.

The experimental results presented here are in good accord with those discussed previously by Dujardin *et al.*³ for both clean and H-covered Ge(111)c(2×8) surfaces. As temperature is reduced they observed a large decrease in the tunnel current between about -0.5 and -0.1 V, the region we identify as being VB derived. We see a similar decrease, but as a function of increasing tunnel current (in Fig. 2, the ratio of conductance near -0.5 V compared to that at, say, $+2.0$ V decreases greatly with increasing current). The temperature dependence in our results is relatively small since the range of varied temperatures is restricted, but if we include the prior room temperature results of Feenstra and Slavin⁶ then this trend of decreasing VB current with decreasing temperature is apparent, in agreement with the data of Dujardin *et al.* Importantly, we identify the decrease in VB current as arising from the shifting of the rest-atom state while the surface bandgap (energies ranging from the VB maximum to the onset of the adatom states) remains *constant* in size, a small but significant modification on the interpretation of Dujardin *et al.*

We return for a moment to the spectra of Fig. 1 and 2 to comment upon an additional feature not mentioned above, namely, the occurrence of a discontinuity in the conductance at a voltage near -1.8 V. This feature is seen in nearly all the spectra we have acquired. Detailed voltage-dependent imaging reveals that for sample voltages between -1.8 V and 0 V the STM images reveal the rest-atom states, as expected,^{6,10} whereas for voltages below -1.8 V the images actually reveal the *adatom* states. (The adatom states are also seen at positive sample voltages, as expected).^{6,10} We interpret the results in terms of *inversion* of the occupation of the adatom states, *i.e.* by electrons tunneling directly from valence band states into the adatom band. This observation conclusively demonstrates that electrostatic tip-induced band bending is indeed occurring in the Ge. The magnitude of this tip-induced band bending is consistent with the computed results of Fig. 3, as will be discussed in detail elsewhere.²⁰ But again, the observed shifts of the rest-atom band are found to be much greater than can be accounted for by this tip-induced band bending.

In summary we have performed STS experiments on Ge(111)c(2×8) surfaces. We observed significant shifts in the position of the rest-atom spectral peak as a function of the current setpoint. These shifts are found to be much larger than that expected on the

basis of simple electrostatic tip-induced band bending. Some new mechanism is required to account for the data; this mechanism likely involves limited transport of the carriers in the rest-atom band, as previously suggested by Dujardin *et al.*³

Discussions with J. A. Northrup and G. Dujardin are gratefully acknowledged. This work has been supported by the A. von Humboldt Foundation and by the U.S. National Science Foundation.

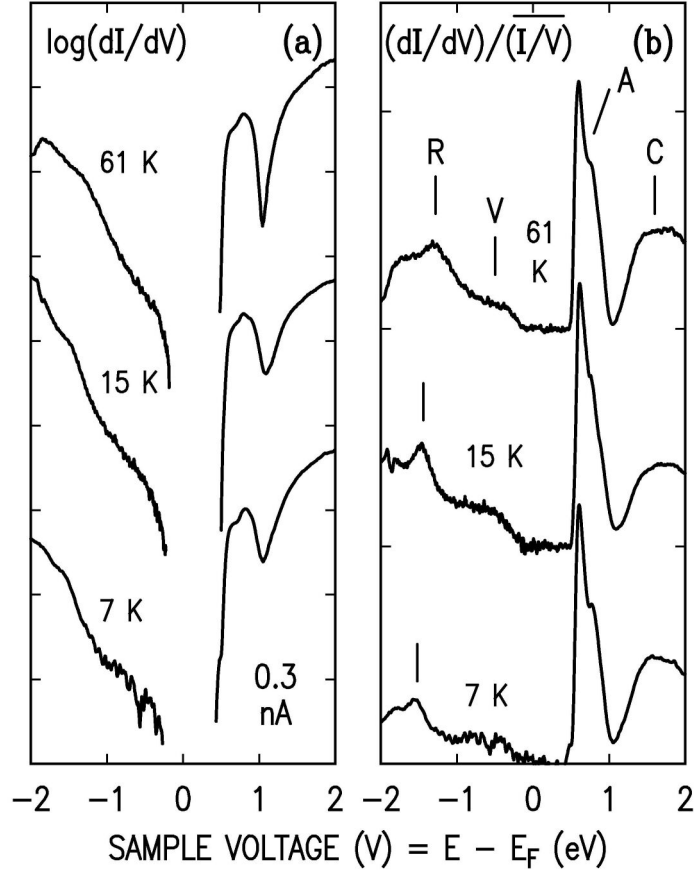


FIG. 1. Tunneling spectra obtained from the Ge(111)c(2×8) surface at various temperatures and with a current setpoint of 0.3 nA. Spectra are shown as (a) dI/dV at constant tip-sample separation on a logarithmic scale (one order-of-magnitude per division) and (b) normalized conductance on a linear scale. The spectra at different temperatures are shifted vertically, for clarity. Adatom (A), rest-atom (R), valence band (V) and conduction band (C) components in the spectra are indicated.

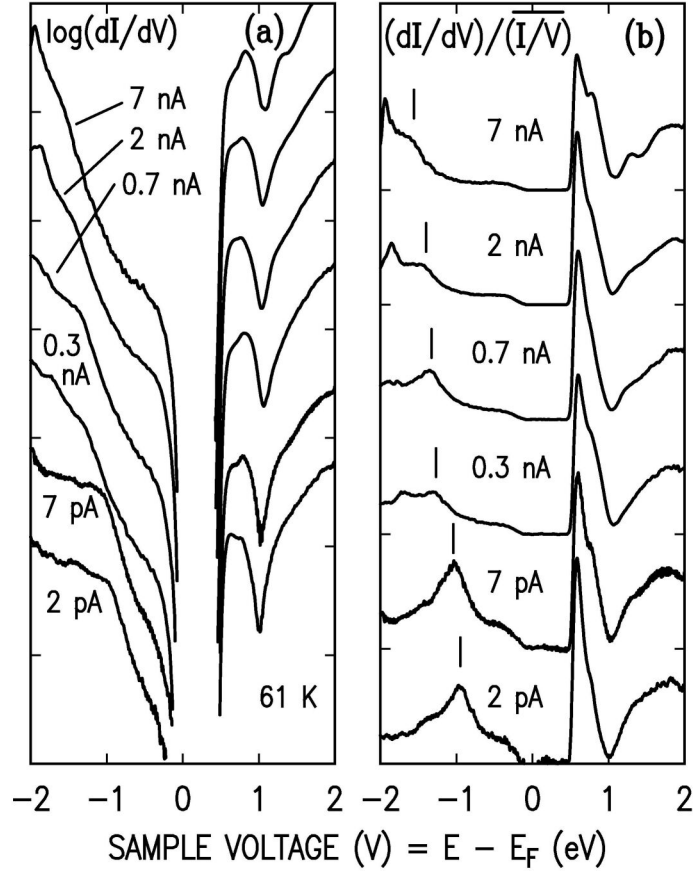


FIG. 2. Tunneling spectra for a temperature of 61 K and at various current setpoints. The rest-atom spectral peak is indicated by the ticmarks in (b).

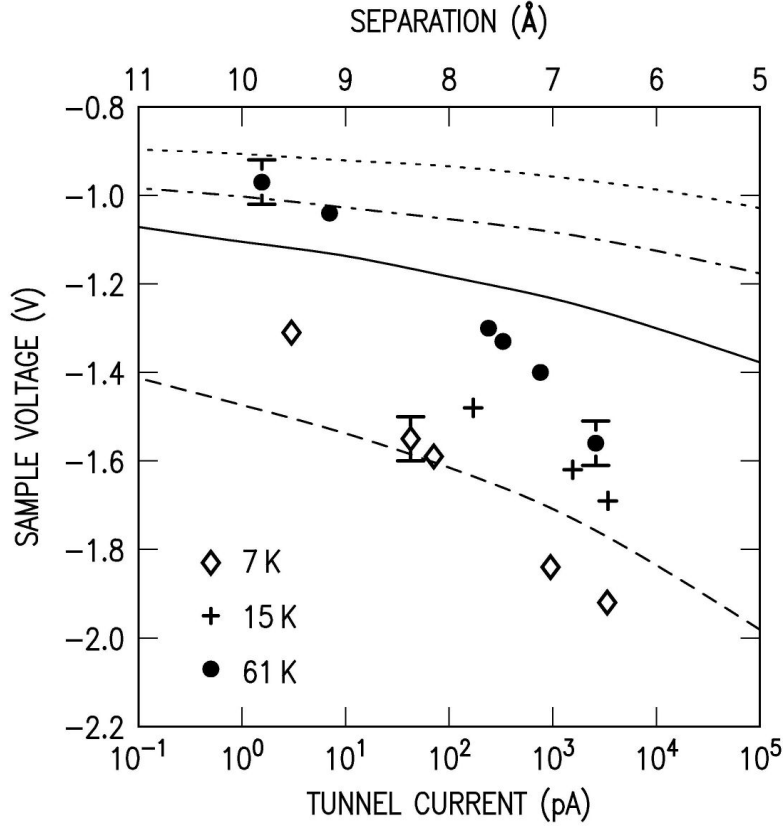


FIG. 3. Observed position of the rest-atom peak, as a function of tunnel current and for various temperatures. Typical error bars are shown on a few points, indicating the variation in the results at different points on the surface and due to small (unintentional) variations in tip shape. Theoretical results for the peak position are shown by the lines, using a contact potential of 0 eV and probe-tip radii of 1 nm (dotted line), 10 nm (dot-dashed line), and 100 nm (dashed line), and a contact potential of 0.3 eV and tip radius of 100 nm (solid line).

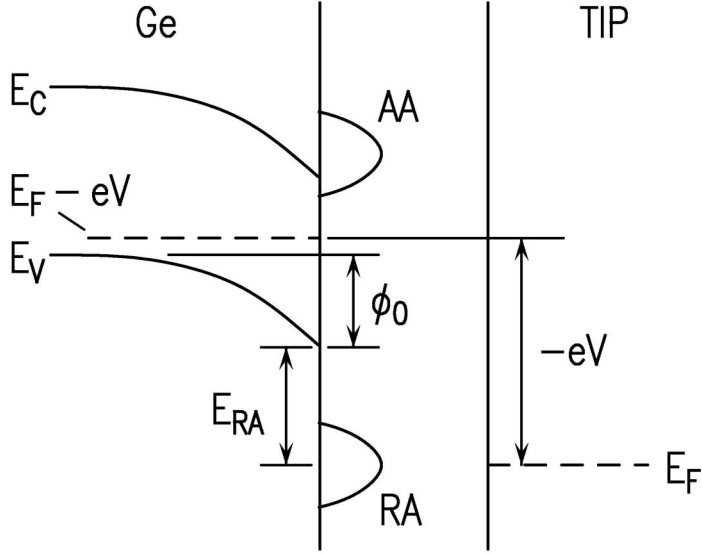


FIG. 4. Schematic energy band diagram for observation of the rest-atom (RA) surface band. The Ge bulk VB and CB edges are indicated by E_V and E_C , respectively, and the adatom surface band is denoted AA. Fermi-levels of tip and sample are separated by an energy $-eV$ where $V < 0$ is the sample voltage relative to the tip. The semiconductor band bending at the surface is denoted by ϕ_0 . The energy of the rest-atom band below E_V is $E_{RA} = 0.7 \text{ eV}$.

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