Pis'ma v ZhETF, vol.67, iss.2, pp.130 - 135 © 1998 January 25

SCANNING TUNNELING SPECTROSCOPY OF CHARGE EFFECTS ON SEMICONDUCTOR SURFACES AND ATOMIC CLUSTERS

N.S.Maslova, S.I.Oreshkin, V.I.Panov, S.V.Savinov, A.Depuydt, C.Van Haesendonck**

Chair of Quantum Radio Physics, Moscow State University
119899 Moscow, Russia

**Laboratorium voor Vaste-Stoffysica en Magnetisme, Katholieke Universiteit Leuven*
B-3001 Leuven, Belgium

Submitted 15 December 1997

We have used scanning tunneling microscopy and scanning tunneling spectroscopy at liquid helium temperature to study the electronic structure of in situ cleaved, (110) oriented surfaces of InAs single crystals. Both unperturbed, atomically flat areas and areas with an atomic size defect cluster have been investigated. We show that the anomalous behavior of the local tunneling conductivity which indicates a pronounced enhancement of the semiconductor band gap for the flat areas, is consistent with band bending induced by charges localized at the tip apex. Atomic size defect clusters contain additional charges which modify the band bending, explaining the different behavior of the tunneling conductivity near the defect cluster. The experimentally observed oscillations of the tunneling conductivity near the band gap edges can be directly related to resonant tunneling through quantized surface states which appear because of the band bending.

PACS: 61.16.Ch, 68.35.Dv, 71.55.Eq, 73.20.Hb

Measurements with scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) are usually interpreted in terms of standard models for electron tunneling [1]. However, the STM and STS data often also reveal anomalous features which can not be explained in this way. These STM and STS anomalies tend to become more pronounced when lowering the temperature.

With the decrease of the tunneling contact area and the temperature, nonequilibrium processes start to play a significant role. If the relaxation rate for the electron states is not infinitely large, a non-equilibrium occupation of the electron states will appear in the presence of a non-zero tunneling voltage, even for macroscopic systems [2 – 4]. For nanometer scale tunneling contacts the non-equilibrium effects can drastically change the expected tunneling conductivity, especially in the presence of localized states. In this article we show that the importance of the non-equilibrium effects is supported by our STS measurements on InAs semiconductor surfaces.

The relaxation rate for the electron states in the vicinity of the tunneling contact usually incorporates all possible sources of inelastic scattering. At low temperatures, where inelastic scattering processes are strongly suppressed the finite relaxation rate will induce a non-equilibrium steady-state distribution in energy space in the contact area. The important decrease of the relaxation rate at liquid helium temperatures implies that the standard expression for the tunneling current has to be modified to

$$I \propto 2\pi e \int d\varepsilon \frac{(n_t^0(\varepsilon) - n_s^0(\varepsilon))V^2\rho_t\rho_s\Gamma_t\Gamma_s}{V^2\rho_t\Gamma_t + V^2\rho_s\Gamma_s + \Gamma_t\Gamma_s}, \tag{1}$$

where Γ_t and Γ_s are the relaxation rates in the tip and in the sample, respectively, and ρ_t and ρ_s are the corresponding tip and sample density of states, V – is the tunneling transfer matrix element, while $n_t^0(\varepsilon)$ and $n_s^0(\varepsilon)$ are the equilibrium electron distribution functions for the tip and sample, respectively.

When the relaxation rate for the non-equilibrium electrons in the tip or in the sample is smaller than the tunneling rate, the current will be determined by the electron relaxation processes which become very slow at liquid helium temperatures [5]. This explains why typical values for the tunneling current in low temperature STM measurements tend to be much smaller than at room temperature for the same tip-sample separation. For our measurements on InAs surfaces, which are discussed in more detail below, typical tunneling currents at room temperature are in the 1 nA range. At liquid helium temperatures a typical tunneling current is 10 pA.

Experimental and theoretical studies of electron transport properties in the mesoscopic regime have revealed that low temperature properties of very small structures not only depend on material properties such as the atomic composition, the lattice structure or the electron effective mass. Transport and tunneling phenomena in mesoscopic systems also strongly depend on the relevant dimensionality and on the specific geometry and configuration of the system. As indicated in [6], transport phenomena which are related to electron tunneling in nanostructures have to be treated in terms of a total transmission probability. The latter probability has to include the tunneling process as well as all other relaxation and scattering processes in the system, similar to the Landauer approach for quantum transport phenomena [7].

In order to test the relevance of the above mentioned non-standard tunneling phenomena, we have performed detailed STM and STS measurements at liquid helium temperature on InAs(110) surface for atomically flat areas as well as for areas which contain an atomic size defect cluster. The experimental results allow us to demonstrate the influence of charging effects which occur in the vicinity of the STM tunnel junction. The STM and STS data have been obtained with a home built low temperature microscope with an in situ cleavage mechanism to obtain a clean sample surface at low temperature [8]. The samples are n-type InAs semiconductor monocrystals which have been highly doped with Sn ($n \simeq 5 \cdot 10^{17}\,\mathrm{cm}^{-3}$) and are cleaved along the (110) plane after cooling down to liquid helium temperature.

It is well known that the STM topography of III-V compound semiconductor surfaces, including the InAs(110) surface, depends on the polarity of the applied bias voltage [9]. For negative sample voltages the STM image is determined by the As sublattice, while for positive sample voltages the In sublattice becomes visible. Relaxation of the surface atomic structure results in a tilt of the As atoms in vertical direction, which can be described in terms of buckling angle and gives rise to a lateral shift between In and As sublattices [10]. Our most striking observations for the STS measurements can be summerized as follows. (i) A strongly enhanced semiconductor band gap (about 1.8 eV) is observed for atomically flat surface regions. (ii) The Fermi level is shifted from the conduction band edge inside the band gap despite the high doping level. (iii) In the vicinity of an atomic size defect cluster the band gap is considerably reduced, but the Fermi level remains to be pinned in the band gap. A strongly enhanced band gap has been reported previously for low temperature STS measurements on the InAs(110) surface [11]. Even

5*

at room temperature the value and position of the measured band gap can be different from the values for the bulk material [12].

In order to explain the unusual behavior of the tunneling conductivity, we rely on the above mentioned theoretical approach and take into account the finite relaxation rate for the electrons in the tunneling contact which induces a non-equilibrium steady-state electron distribution in the presence of an applied bias voltage. We will argue that for nanometer scale junctions the non-equilibrium electron distribution results in charging effects and can drastically change the experimentally observed $I(V)$ characteristics.

The inset in Fig.1 shows a typical $I(V)$ characteristic for an atomically flat area on the InAs(110) surface. The presence of a wide band gap $\simeq 1.8$ eV can be clearly observed. This measured band gap value strongly differs from the bulk value which is 0.43 eV at 4.2 K. Moreover, the Fermi level E_f is located inside the measured band gap. Another result shown in Fig.1 are the oscillations of the tunneling conductivity which appear in the $dI/dV(V)$ curves near the band gap edges. The period of the oscillations is 0.14 eV for both polarities of the applied voltage.

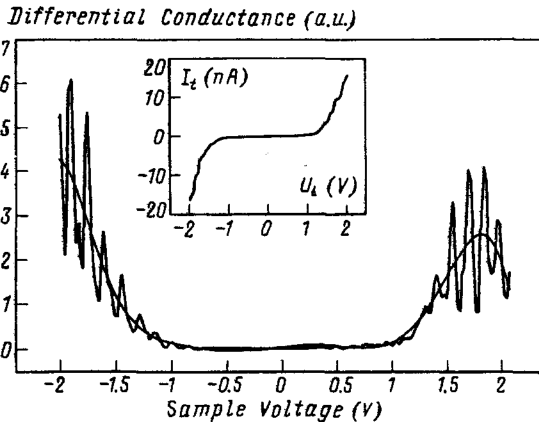
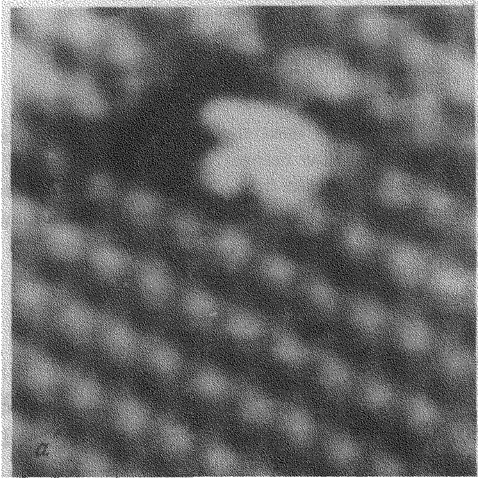


Fig.1. Differential conductance curve measured above the atomically flat area of the InAs(110) surface, the current-voltage characteristic is shown in the inset

In our topographic STM images we also observe atomic size defect clusters (see Fig.2). The lateral size of the cluster image is about 1 nm and its height is less than 0.5 nm. The measured band gap value above the cluster is 0.4 eV, which is significantly smaller than the observed band gap value for the flat surface regions. We note that the gap structure in $dI/dV(V)$ is much less pronounced when compared to the atomically flat areas (see Fig.1). On the other hand, E_f is still located inside the band gap and again we observe oscillations of the tunneling conductivity near the gap edges. The period of these oscillations is about 0.09 eV which is different from the oscillations observed on the flat surface. As discussed in more detail below, we can link in both cases the anomalous behavior of the tunneling conductivity directly to the band bending which is induced by charging effects.

In Fig.3*a* we illustrate how the anomalously large experimental value for the InAs band gap can be explained for the atomically flat surface regions. We assume the band bending is induced by charges which are occupying localized states present at the tip apex. This charge depends on the polarity and the magnitude of the applied voltage. That is why the commonly used model for tip induced band bending [13] has to be modified.



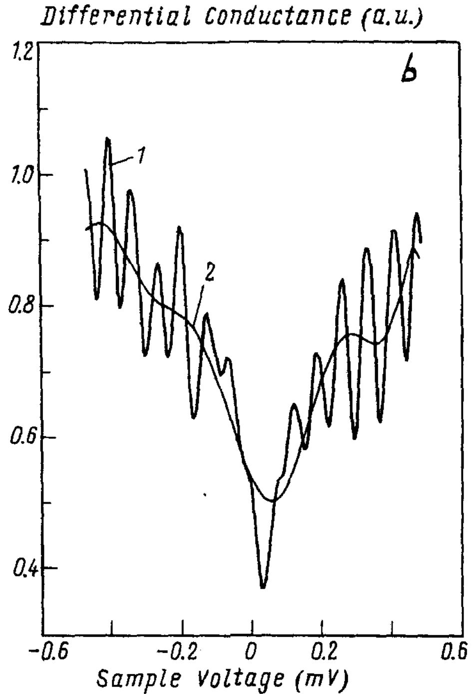


Fig.2. (*a*) STM image of an atomic scale defect cluster appearing on the InAs surface. The scanned area measures 44 × 44 Å. The tunnel current is fixed at 20 pA, while the sample is biased at −500 mV. (*b*) Differential conductance curve measured above the defect cluster shown in Fig.2*a*. The curve marked *1* corresponds to the measured curve, while the curve marked *2* corresponds to a fitted 9th order polynomial. The latter curve allows to estimate the width of the semiconductor band gap

The external charge appearing on the tip apex is proportional to the difference between the non-equilibrium distribution function for the electrons in the presence of the tunneling current and the distribution function at zero applied voltage. So, the sign of the extra charge at the tip apex follows the changes in polarity and value of applied voltage bias. As discussed above, the non-equilibrium distribution appears because of the finite relaxation rate for the electrons, implying that the electron distribution function in the tunneling contact area can be different from the Fermi – Dirac distribution which is present in the macroscopic leads. Therefore, in the presence of a tunneling current, the non-equilibrium electron distribution in the contact area result in a negative charge at the tip apex for positive sample voltages and in a positive charge for negative sample voltages. The shape of band edges follows the dependence of additional charge vs. applied bias voltage as obtained in [14]. Each localized state at the tip apex can not have charge more than $2e$, so the saturation of the charge dependence on applied bias voltage occurs.

The oscillations of the tunneling conductivity cannot be explained in terms of Coulomb blockade or Coulomb staircase effects. If the oscillations are caused by Coulomb charging effects, the period of these oscillations can be directly related to the size a of the relevant particle which is being charged. The oscillation period should be $\Delta E \sim e^2/a$. For $a \sim 0.5 - 1.0\,\mathrm{nm}$ we obtain $\Delta E \sim 1 - 0.5\,\mathrm{eV}$, which does not agree with the experimental data.

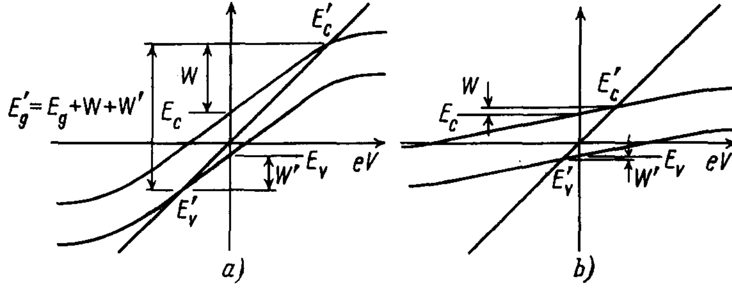


Fig.3. Schematic view of the tip induced band bending which occurs near the InAs surface. E_c and E_v correspond to the conduction and valence bands edges at zero bias respectively, while E_c' and E_v' correspond to the measured position of the band edges. Straight line in the first quadrant corresponds to the position of the tip Fermi level relative to the sample Fermi level. W and W' gives the band bending. (a) above atomically flat InAs surface (b) above atomic size cluster

The observed oscillations can also not be explained by interference effects. For a tip to sample separation $b \sim 0.5\,\text{nm}$, the period of the electron density oscillations ΔE should be much larger than the period obtained from our experimental results. Indeed, $\Delta E \sim (2\pi\hbar p_F)/(mb)$, where m is the effective mass of the electron and $p_F \sim \hbar/a_0$ is the electron wave vector at the Fermi level with a_0 the InAs lattice constant. This implies that $\Delta E \sim \hbar^2/mba_0 \sim 1\,\text{eV}$, in clear disagreement with our experimental result $\Delta E \sim 0.09\,\text{eV}$. A period of 0.09 eV would imply an unrealistic tip to sample separation of more than 5 nm.

The band bending values W and W' indicated in Fig.3 can be estimated to be $W \sim \sim W' \sim e^2/b$, where as before b is the tip to sample separation. For $b \sim 0.5 - 1.0\,\text{nm}$, we obtain $W \sim W' \sim 1 - 0.5\,\text{eV}$. These values are comparable to usual band bending values [14]. The essential feature of our model (see Fig.3) is the fact that due to the voltage dependence of the localized charge, the exact values of W and W' now depend on the polarity as well as on the amplitude of the applied voltage in our case. The experimentally observed band gap will be $E_g \sim W + W' + E_{gb}$, where $E_{gb} \sim 0.43\,\text{eV}$ is the bulk value of the InAs band gap. Therefore, the band bending induced by a charged tip apex can account for the experimentally observed increase of the band gap.

In the presence of an atomic defect cluster, the band bending will be modified in the vicinity of the defect cluster [15]. This occurs because of the additional charging of the localized states which are associated with the defect cluster. For negative sample voltages a negative charge is expected to appear near the cluster, while for positive sample voltages the defect cluster should acquire a positive charge. Similar to the case of a charged tip apex, the external charge appearing on the cluster is proportional to the difference between the electron distribution function in the presence of a tunneling current and the distribution function at zero applied voltage. The charge on the defect cluster causes a band bending which partially compensates the band bending induced by the charged tip. The gap edges position now weakly depends on applied bias voltage as it is shown on (see Fig.3b). Consequently, the experimentally observed band gap above the defect cluster will be reduced when compared to the band gap which is observed for atomically flat surface areas. However, E_f remains in the band gap. This can be explained by the

fact that the band bending is asymmetric: the bending of the conduction band differs from the valence band bending. The decrease of the band gap above a defect cluster was also observed in [16] for a GaAs(110) surface, but the effect was less pronounced than for our InAs(110) surfaces.

In general additional localized states can appear in the band gap due to tip-sample interaction [17]. In this case the common model for tunneling processes has to be considerably changed [18] and the tunneling current can be completely dominated by these additional localized states for bias voltages less than the band gap value, provided the finite relaxation time for the non-equilibrium electrons is taken into account.

In conclusion, our scanning tunneling spectroscopy measurements of the InAs(110) surface confirm the importance of band bending which is induced by localized charges which are present near the tunneling contact. We have presented theoretical arguments which rely on the finite relaxation time for the electrons at the tip apex and on the sample surface as well as on a non-equilibrium electron distribution at finite voltages. This model consistently explains our main experimental observations, including an enhancement of the semiconductor band gap and the appearance of oscillations in the tunneling conductivity near the band gap edges. The presence of an additional charge on atomic size defect clusters accounts for the different behavior when compared to atomically flat areas.

The work in Moscow has been supported by the Russian Ministry of Research (Surface atomic Structures, grant 95-1.22; Nanostructures, grant 1-032) and the Russian Foundation of Basic Research (RFBR, grants 96-0219640a and 96-15-96420). The work at the KULeuven has been supported by the Fund for Scientific Research - Flanders (FWO) as well as by the Flemish Concerted Action (GOA) and the Belgian Inter-University Attraction Poles (IUAP) research programs. The collaboration between Moscow and Leuven has been funded by the European Commission (INTAS, project 94-3562).

---

1. J.Tersoff and D.R.Haman, Phys. Rev. B **31**, 805 (1985).
2. E.L.Wolf, *Principles of electron tunneling spectroscopy*, Oxford Universitary Press, 1985.
3. P.N.Trofimenkoff, H.J.Kreuzer, W.J.Wattamaniuk, and J.G.Adler, Phys. Rev. Lett. **29**, 597 (1972).
4. J.G.Aoller, H.J.Kreuzer, and J.Straus, Phys. Rev. **13**, 2812 (1975).
5. *Quantum Transport in nano-structured semiconductors*, Kluwer Academic Publishers, 1996.
6. O.Agam, N.S.Wingreen, and B.L.Altshuler, Phys. Rev. Lett. **78**, 1956 (1997).
7. R.Landauer, Springer Ser. Sol. St. Sci. **61**, 38 (1985).
8. S.I.Oreshkin, V.I.Panov, S.V.Savinov et al., Pribory i technica experim. **4**, 145 (1997).
9. R.M.Feenstra, J.A.Stroscio, J.Tersoff, and A.P.Fein, Phys. Rev. Lett. **58**, 1192 (1987).
10. N.S.Maslova, S.I.Oreshkin, V.I.Panov et al., *Charge effects on InAs(110) surfaces by low temperature scanning tunneling spectroscopy*, STM-97, July 20-25, Hamburg, 1997.
11. J.Wildöer, *Low temperature scanning tunneling microscopy on mesoscopic systems*, Ph.D. thesis, Delft University of Technology, 1996.
12. R.M.Feenstra and J.A.Stroscio, J. Vac. Sci. Technol. **B5**, 923 (1987).
13. H.W.M.Salemink, M.B.Johnson, and O.Albrektsen, J. Vac. Sci. Technol. **B12**, 362 (1994); H.W.M.Salemink and O. Albrektsen, Phys. Rev. **B47**, 16044 (1993).
14. P.I.Arseev, N.S.Maslova, V.I.Panov, and S.V.Savinov, *Role of charge effects in tunneling investigations of semiconductors, Semiconductors-97*, December 1-5, Moscow, 1997.
15. J.F.Zheng, X.Liu, N. Newman, E.R. Weber et al., Phys. Rev. Lett. **72**, 1490 (1994).
16. R.S.Goldman, R.M.Feenstra, B.G. Briner et al., Appl. Phys. Lett. **69**, 3698 (1996).
17. N.S.Maslova, Yu.N. Moiseev, V.I. Panov et al., Sov. Phys. JETP **75**, 505 (1992).
18. P.I.Arseyev and N.S.Maslova, Sov. Phys. JETP **75**, 575 (1992).