Influence of resonant tunneling on the imaging of atomic defects on InAs(110) surfaces by low-temperature scanning tunneling microscopy

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We have used a low-temperature scanning tunneling microscope (STM) to study the surface of heavily doped semiconductor InAs crystals. The crystals are cleaved in situ along the (110) plane. Apart from atomically flat areas, we also observe two major types of atomic scale defects which can be identified as S dopant atoms and As vacancies, respectively. The strong bias voltage dependence of the STM image of the impurities can be explained in terms of resonant tunneling through localized states which are present near the impurity.

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With the advent of the scanning tunneling microscopy (STM) and the decrease of system sizes down to the nanometer scale, experimental results can often no longer be interpreted in terms of the standard model for STM imaging. This is generally caused by the following reasons. (i) For system sizes comparable to the atomic scale, the local density of states in the contact area can be strongly altered by the tunneling current (tip-sample interaction), resulting in the appearance of additional localized states near the Fermi level. (ii) Individual localized states start to dominate the tunneling current, because the radii of the localized states become comparable to the area of the contact size. (iii) In the presence of localized states, the finite relaxation rate of the nonequilibrium electrons has to be taken into account, especially at low temperatures where the relaxation rate may become smaller than the tunneling rate.

In a recent publication we could already show that the STM imaging and scanning tunneling spectroscopy of InAs(110) surfaces is strongly affected by tip induced band bending due to charges which are present on localized states at the tip apex. Here, we present a series of additional experimental results which demonstrate the role played by individual localized states related to atomic defects. In order to identify this role, we have imaged dopant atoms and vacancies appearing at the surface of the InAs compound semiconductor at a temperature of 4.2 K. All the experiments have been performed with a home built low-temperature STM with an in situ sample cleavage mechanism. The samples used in the experiments are n-type InAs monocrystals which have been heavily doped with S atoms ($n \approx 5 \times 10^{17} \text{ cm}^{-3}$). The crystals are cleaved in situ along the (110) plane. Since the STM is cooled far below the boiling point of oxygen, the partial vapor pressure of oxygen is extremely low. Therefore, surfaces such as GaAs(110) and InAs(110), which normally tend to oxidize very quickly, will stay clean under these conditions for many days.

Figure 1 shows a typical image of a InAs(110) surface. The atomic rows can be clearly observed. The images are similar to those obtained by Feenstra et al. on GaAs(110). The image depends on the polarity of the applied bias voltage. For negative sample bias voltage electrons tunneling out of the occupied surface states carry the current. These states are located near the As lattice sites (Fig. 1a). For positive sample bias voltage electrons tunnel into the empty states which are located near the In lattice sites (Fig. 1b). For clarity the As sublattice in Fig. 1a has been copied on the In sublattice in Fig. 1b.

Apart from the different energy dependence of the density of states for both type of atoms, relaxation of the surface atomic structure results in a tilt of the As atoms in the vertical direction. The tilt is described in terms of a buckling angle and gives rise to a lateral shift between the two sublattices in the [001] direction which is easily observed in Fig. 1. We also observe a shift in the [110] direction which has been reported earlier for GaAs by Lengel et al. and might be explained in terms of a slightly different tip-to-sample distance at different sample bias voltage.

We have also obtained detailed STM images of single dopant atoms and vacancies at different polarities and values of the applied bias voltage and low constant tunneling current ($\approx 20 \text{ pA}$). Figure 2 shows a series of STM images of an atomic impurity at different values of sample bias voltage. From the observed frequency of this kind of atomic defects, we conclude that the defect shown in Fig. 2 is a single S dopant atom. For negative bias voltage not exceeding a threshold value of about $-0.9 \text{ V}$, the STM image of the impurity appears as a depression (dark spot) between two neighboring atomic As rows (Fig. 2d). When increasing the bias voltage above the threshold value, the impurity suddenly appears as a hillock (bright spot) rather than as a depression (Fig. 2a-c). When the bias voltage exceeds $-2.5 \text{ V}$, the bright spot corresponding to the impurity again disappears. A comparable behavior is observed for positive bias voltage, with a different threshold value of about $+0.45 \text{ V}$ at which the impurity starts to appear as a
hillock (Fig. 2e-h).

In order to identify the origin of the pronounced bias voltage dependence of the STM image of the impurity in Fig. 2, we also imaged a neighboring defect at different applied bias voltage (Fig. 3). From the appearance of this defect at different bias voltage, we conclude that it corresponds to a vacancy in the As sublattice. At more elevated bias voltage, the defect image does not suddenly change from a depression to a hillock. On the other hand, at higher bias voltage the defect becomes surrounded by a cloud which indicates a decrease of the occupied density of states (Fig. 3f) and an increase of the empty density of states. In agreement with our experiments, we see that atomic defects of distinct nature behave different when imaged at different bias voltage.

To understand qualitatively the changes in the STM image of a dopant atom we used a simple model which describes the effects in terms of switching on and off a channel for resonant tunneling and see e.g. [14]). Such channels are formed by localized states present near the impurities. Figure 4 illustrates the tunneling process via a localized state. The position of the energy level associated with the localized state is assumed to depend on the applied bias voltage in a rather complicated way. This dependence may be affected by an important modification of the unperturbed energy spectrum by the tip-sample interaction, charging effects or the complex configuration of the electric field in the contact area. For bias voltage smaller than the threshold value, a localized state does not participate in the resonant tunneling process, as illustrated in Fig. 4a (initial position $\varepsilon_d^0$). The impurity appears as a dark spot in the STM image, indicating an important reduction of the local density of states near the impurity.

The threshold value $V_{th}$ of the bias voltage, above which resonant tunneling sets in, can be estimated by relying on the simple condition

$$\varepsilon_d = \varepsilon_d^0 + f(V_{th}) = E_F$$

(1)

where $\varepsilon_d^0$ corresponds to the unperturbed position of the localized impurity level. The function $f(V)$ describes the dependence of the position of the impurity level on applied bias voltage. A resonant tunneling current will start to flow for bias voltage larger or equal than $V_{th}$, i.e., when $\varepsilon_d$ is located between $E_F$ and $E_F - eV$ (Fig. 4a, position 2 of the level $\varepsilon_d$). When the impurity level $\varepsilon_d$ is located above the conduction band edge, the current is determined by the tunneling rate. Because of the heavy n-type doping, free electron states are available between the conduction band edge $E_c$ and the Fermi level $E_F$. We assume that the relaxation rate for the nonequilibrium electrons on the localized state exceeds the tunneling rate for the energy levels in the conduction band. When further increasing the applied bias voltage, $\varepsilon_d$ is located within the semiconductor band gap (Fig. 4a, position 3 of the level $\varepsilon_d$) and the resonant tunneling current will now be determined by the relaxation rate for the electrons occupying the localized level. This relaxation rate is smaller than the tunneling rate for energies within the band gap. Therefore, the tunneling current decreases and the bright spot corresponding to the impurity image disappears (Fig. 2).

As already indicated above, the exact location of the energy level $\varepsilon_d$ relative to the band gap edges is strongly affected by charging effects, tip-induced band bending and modifications of the initial density of states by the tunneling processes. Therefore, a complicated and possibly nonmonotonic dependence of the location of the energy level $\varepsilon_d$ on the applied bias voltage $V$ will emerge, resulting in a switching on and off of the resonant tunneling channel. Moreover, it is possible that there is more than one localized state connected to the impurity. For positive applied bias voltage the situation remains very similar (Fig. 4b). For a complicated dependence $f(V)$ of the energy level $\varepsilon_d$, one single impurity level can be responsible for switching on and off the resonance channel at different threshold values $V_{th}$ for positive and negative bias voltage. For positive bias voltage the resonant tunneling current starts to flow when $\varepsilon_d$ is located between $E_F$ and $E_F - eV$.

Other possible mechanisms for switching on or off the resonant tunneling channel may be related to changes of the effective potential well near the impurity which are induced by the applied bias voltage. In quantum mechanics the presence of localized states in a symmetric quantum well is well known and there exists a critical value for the asymmetry at which the localized states disappear. The applied bias voltage changes the symmetry of the effective potential well. Therefore, the localized energy levels present in the well can disappear at high bias voltage.

In conclusion, we have found that the STM images of an individual atomic defect (doping atoms) on an InAs(110) surface strongly depend on the value of the applied tunneling bias voltage. Moreover, there exist threshold values for both positive and negative polarities of the tunneling bias voltage. When the bias voltage reaches these threshold values, the STM image of the defect drastically changes from appearing as a depression (low density of states) towards a hillock (high density of states). We can explain the observed behavior in terms of the formation of resonant tunneling channels which are connected to localized energy states near the atomic defect. The exact position of these localized states is determined by tip-sample interactions, charging effects and relaxation processes which all depend on the applied bias voltage. The possibility to have resonant tunneling may therefore depend in a very complicated and even nonmonotonic way on the applied bias voltage. Our model supports the idea that in low-temperature STM experiments, the nanometer size of the tunneling contact strongly enhances the influence of individual localized states.
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Fig. 1. Constant-current STM images acquired at sample bias voltage of (a) −1.5 V and (b) +1.5 V. The scanned area is 26 Å × 14 Å and the tunnel current is fixed at 20 pA.

Fig. 2. Constant-current STM images of a dopant atom on the InAs(110) surface acquired at different sample bias voltage. The scanned area is 44 Å × 44 Å and the tunnel current is fixed at 20 pA.

Fig. 3. Constant-current STM images of a As vacancy on the InAs(110) surface acquired at different sample bias voltage. The scanned area is 70 Å × 70 Å and the tunnel current is fixed at 20 pA.

Fig. 4. Schematic diagram for localized state assisted tunneling (a) for negative sample bias voltage, and (b) for positive sample bias voltage.
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