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Transport in single atomic junctions: strong correlation and Coulomb blockade

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Abstract. We report here the first observation of the strong correlation and Coulomb blockade effects in a single-atomic junction (single tungsten-atom STM tip). In contrast to previous work [1, 2], the use of an atomic-scale central island makes the change in the electrostatic potential due to the variation of the number of electrons in the island greater than 1 eV and thus the electron correlation effect is made more controllable and stable even at room temperature.

1 Experimental setup

The experiment was performed using an ultra-high vacuum (UHV) STM (JSTM-4500XT) with an operating pressure of 2×10^{-8} Pa at 77 K and 300 K. The STM tip was made from a single crystal tungsten wire with (111) orientation. An STM tip with a pyramidal structure well protruded about 2 nm on the tip apex with a single tungsten atom at the end of the apex, which is followed by the three and six tungsten atoms in the second and third layers, respectively, was prepared by the field evaporation plus field emission technique [3]. In contrast to the previous method [4], this new technique allows us to in situ fabricate a single-atom tip inside the STM chamber. Direct observation of the tip apex by field ion microscope (FIM) confirmed that there is a single tungsten atom at the end the tip apex. Such a single atom STM tip is stable and robust for high field (≤ 1 V/Å) operation, so a silicon atom and hydrogen atom can be extracted and redeposited routinely and repeatedly on a Si(100)2×1 surface [4].

2 Experimental results

The current-voltage characteristics between the single tungsten-atom STM tip and Au(111) or Si(100)2×1 surface. The normalized differential conductances $(dI/dV)/(I/V)$ vs. the applied voltage featured five to six periodic oscillation peaks in both (sample) positive and negative bias voltages, which is the unique characteristics of a Coulomb staircase in a double barrier tunnel junction. The voltage separation of adjacent oscillation peaks was ~ 1.1 eV. This oscillation period was independent of tip-sample separation, temperature and substrate material.

The negative differential conductance ($dI/dV < 0$) was observed between the oscillation peaks. This feature existed for both Si(100)2×1 and Au(111) surfaces but is more pronounced for the Au(111) surface at 77 K.

If we apply a strong field (> 2 V/Å) on the tip apex, the single tungsten atom at the end of the tip apex eventually evaporates. Such a truncated configuration without

an apex atom was also observed by FIM. Such a truncated tip did not feature any oscillatory behavior in the normalized differential conductance.

3 Theoretical model

A tight-binding (TB) calculation for the electronic states of a single-atom tip, taking into account field-induced energy shift of each constituent atom, shows the presence of two narrow peaks in the local density of states in the apex atom: one is below the Fermi level and the other is above it. This means that there are localized states into the apex atom which are electrically decoupled from the underlying layers by an effective tunnel barrier. The present numerical result is consistent with the previous measurements of the field emission spectrum from a single tungsten-atom tip [4].

The localized electronic state in the apex atom is thus regarded as the central island which capacitively couples to the two electrodes, the rest of the tungsten tip and the sample surface. We estimated the charging energy for the highest occupied energy level (5d) of a tungsten atom by the ab initio calculation and compared with the experimental value determined from the linearly increasing third-to-sixth photoionization energies [5]. The charging energy of the localized state in the pyramidal structure is $U \sim 1.1$ eV, which is compared with the charging energy of ~ 12 eV for an isolated tungsten atom.

In our experiment, the tunnel current is governed by the slower apex atom-sample tunneling event. As a positive bias voltages is applied, the Fermi level of the sample moves downward relative to the energy levels of the localized state which are split equally by U due to the charging effect [6]. When the sample Fermi level goes across each one of the resonances, the sample starts extracting an electron from the localized state and new channels for tunnel current open up one by one, which results in the observed periodic oscillation peaks in the positive sample voltage. If a negative sample voltage is applied, the Fermi level of the sample moves upward to cross each one of the resonance energy levels of the localized states and the sample starts supplying the localized state with an additional electron, which results in the observed periodic oscillation peaks in the negative sample voltage.

The observed negative differential conductance between the oscillation peaks is attributed to the coherent multiple tunneling effect between the localized state in the apex atom and the sample. This was confirmed by the theoretical analysis for the Anderson model of a single atom point contact.

4 Conclusion

The result reported here is the first proof of the existence of Coulomb blockade oscillation and negative differential conductance in a single atomic junction. Various mesoscopic devices based on the Coulomb blockade effect and active devices based on the negative differential conductance should be realized on an atomic scale.

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