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Lateral and vertical manipulations of single atoms on the Ag(1 1 1) surface with the copper single-atom and trimer-apex tips

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ABSTRACT

We study the lateral and vertical manipulations of single Ag and Cu atoms on the Ag(1 1 1) surface with the Cu single-atom and trimer-apex tips using molecular statics simulations. The reliability of the lateral manipulation with the Cu single-atom tip is investigated, and compared with that for the Ag tips. We find that overall the manipulation reliability (MR) increases with the decreasing tip height, and in a wide tip-height range the MR is better than those for both the Ag single-atom and trimer-apex tips. This is due to the stronger attractive force of the Cu tip and its better stability against the interactions with the Ag surface. With the Cu trimer-apex tip, the single Ag and Cu adatoms can be picked up from the flat Ag(1 1 1) surface, and moreover a reversible vertical manipulation of single Ag atoms on the stepped Ag(1 1 1) surface is possible, suggesting a method to modify two-dimensional Ag nanostructures on the Ag(1 1 1) surface with the Cu trimer-apex tip.

1. Introduction

Single atoms on surfaces can be manipulated both laterally and vertically in a controlled way by the scanning tunneling microscope(STM) [1–20] and the atomic force microscope [21–23]. This technique provides a bottom-up way to build atomic structures and has been proved to be a powerful tool in many scientific fields. For the lateral manipulations a substantial portion are devoted to those on the metal surfaces with the STM at a cryogenic temperature [3–16]. Three basic models of the lateral manipulation, i.e., the sliding, pulling and pushing, have been revealed by Meyer et al. [3] during the manipulation of individual Cu, Pb atoms on a Cu(2 1 1) surface. It also has been achieved that [10,15,16] the atomic force between the tip and the atoms is the driving force for the lateral manipulation, while for the vertical single-atom manipulation on the metal surfaces, the strong electric field plays an dominant role for picking up and releasing atoms between the tip and the surface [2,6].

In our previous work we have studied theoretically the lateral and vertical manipulations of single atoms on the Cu, Ag and Al(1 1 1) surfaces, focused mainly on how to improve the manipulation reliability (MR) of the lateral manipulation [26,27] and to achieve the reversible vertical manipulation using atomic force [28]. The systems considered are homo-systems in which the tip, surface and the manipulated atoms are of the same species. However, the tip compositions can affect largely the manipulation as is generally achieved [14,17], which suggests that the single-atom manipulation on the hetero-system is also of an general interest. Thus in this work we mainly dealt with the lateral and vertical single-atom manipulations on the hetero-system, i.e., the Ag and Cu adatoms on the Ag(1 1 1) surface with the copper tip. A better MR is achieved and the reversible vertical single-atom manipulation is also possible, as compared to the homo-system of Ag/Ag(1 1 1) with the Ag tips.

2. Model system and theoretical methods

For the lateral manipulation we considered the flat Ag(1 1 1) surface where a Ag or Cu adatom adsorbed on the fcc site [Fig. 1(a)], while for the vertical manipulation both the flat and stepped surfaces are considered [Fig. 1(b)]. The copper tip atoms are arranged in fcc(1 1 1) pyramid-like stacks containing six layers. The single-atom [Fig. 1(a)] and trimer-apex [Fig. 1(b)] tips have one and three atom(s) in the apex, respectively. The substrate is represented by a nine-layer slab, with each layer containing 10×16 atoms, and periodic boundary conditions are applied in the two directions parallel to the surface plane. The stepped surface consists of upper and lower terraces separated by a (1 1 1)-microfacetted mono-atomic step. Manipulations are simulated by molecular statics method employing parallel molecular dynamics code LAMMPS [30], and the interactions between the Ag and Cu atoms are described by

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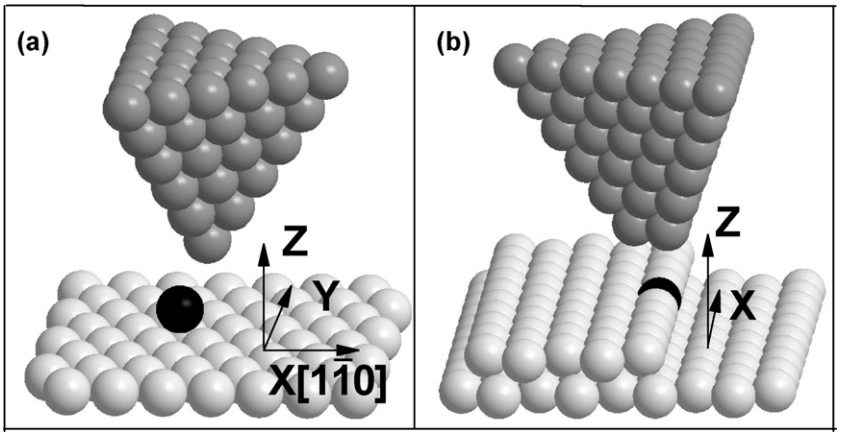

Fig. 1. (a) Model for simulating the lateral manipulation of Ag and Cu adatoms on the flat Ag(1 1 1) surface with the Cu single-atom tip, and (b) for the vertical manipulation of single Ag atom from the Ag(1 1 1) stepped surface with the Cu trimer-apex tip.

the embedded-atom-method potential provided by Williams et al. [31]. During the manipulation process, the tip is initially placed at a certain height(vertical distance between the tip–apex atom(s) and the surface atoms), and is then moved along the X([1 $\bar{1}$ 0]) or Z direction in small steps. At each step, the system is relaxed to the nearest local minimum-energy configuration, in which the atoms in the topmost layer of the tip and in the bottom two layers of the substrate are frozen to mimic a semi-infinite crystal.

3. Results and discussions

3.1. Lateral manipulation of single Ag and Cu adatoms on the Ag(1 1 1) surface with the Cu single-atom tip

According to the theoretical investigations, the Cu tips are more effective than the Pt and Ag tips in lowering the energy barrier for moving atoms during the lateral manipulation [14]. This indicates that the Cu tip may improve the MR of the lateral manipulation of Ag adatoms on the Ag(1 1 1) surface, as compared to the Ag tips. Thus, in the following we present the results on the lateral manipulation with the Cu single-atom tip on the Ag(1 1 1) surface.

For the lateral manipulation of the Ag adatom on the Ag(1 1 1) surface, the manipulation can be successful in the tip-height range from 1.0 to 4.9 Å. During the manipulation, the Ag adatom moves forward following the tip, i.e., in a pulling model. We use X_{ada} and X_{tip} to denote the X coordinates of the adatom and one frozen atom of the tip, respectively. When the tip moves along the X([1 $\bar{1}$ 0]) direction in the manipulation, the distance $\Delta X = X_{tip} - X_{ada}$ varies as shown in Fig. 2. The fluctuation amplitude of ΔX is denoted by $\Delta X_0 = \max(\Delta X) - \min(\Delta X)$ (see illustration in Fig. 2). As described in our previous study [26,27], ΔX_0 can be used to evaluate roughly the MR of the manipulation: the less the ΔX_0 is, the more reliable the manipulation will be.

The variation of ΔX_0 with tip height is given in Fig. 3(a), which shows that the MR increases in overall trend as the tip height decreases. Note that the MR is determined by the two opposite effects, the tip attraction and the surface attraction on the adatom. A larger tip attraction or a weaker surface attraction will leads to a better MR [26,27]. In the lateral manipulation with the single-atom tip, MR is mainly determined by the tip attraction (the tip potential), since the surface attraction can be taken as approximately the same for different tip heights [26,27]. Calculations show that at 4.9 Å the tip potential has a single well under the tip–apex, while below it the potential curve has double wells separated symmetrically by a saddle point located under the tip–apex [Fig. 4(a)]. In our simulation, the adatom always stays behind the tip throughout the manipulation process, indicating that the adatom is trapped in the left well. The potential well gets sharper as the tip height decreases [see Fig. 4(a)]. A sharp well implies a large attractive force on the adatom exerted by the tip in the X direction. Hence at the lower tip heights the MR is better than that at higher heights.

This trend of the MR with the tip height is similar to that for the homo-systems of Ag/Ag(1 1 1) with the Ag single-atom tip [27], as is given in Fig. 3(a). For comparisons, the MR for the lateral

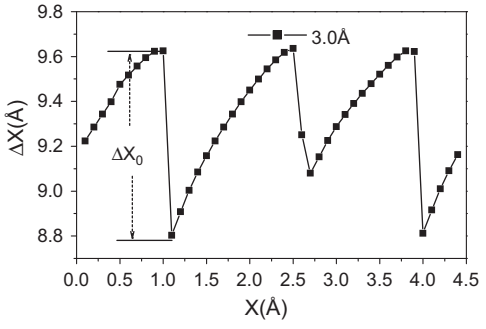

Fig. 2. Variation of the lateral distance between the Ag atom and one top-layer atom of the tip in the X direction (ΔX) during the lateral manipulation with the Cu single-atom tip at 3.0 Å. The fluctuation amplitude of the curve is denoted by $\triangle X_0$.

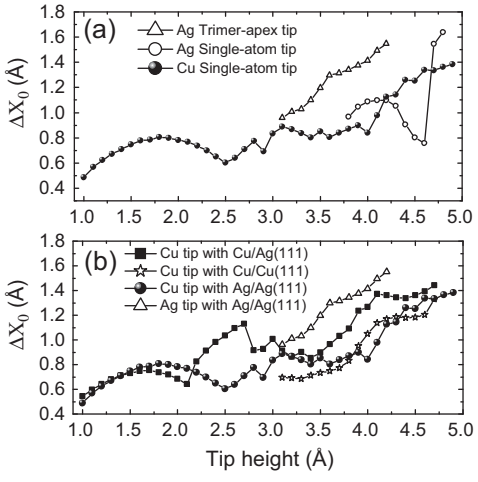

Fig. 3. (a) In lateral manipulation, the variation of $\triangle X_0$ with the tip height for the Ag/Ag(1 1 1) system with the Cu single-atom tip, and those with the Ag single-atom and trimer-apex tips. (b) Comparison of the MR for the Ag/Ag(1 1 1), Cu/Ag(1 1 1) and Cu/Cu(1 1 1) with the Ag and Cu single-atom tips, respectively.