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LETTER TO THE EDITOR

Interaction of scanning tunneling microscopy tip with mesoscopic islands at the atomic-scale

R Z Huang, V S Stepanyuk and J Kirschner

Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

E-mail: rzhuang@mpi-halle.de

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Abstract

Performing atomic-scale simulations, we study the interaction of the scanning tunneling microscopy (STM) tip with mesoscopic islands at zero bias voltage. Our calculations reveal tip-induced shape transitions in Co islands on Cu(100) as the tip approaches the surface. The structure of the islands and of the tip are found to depend strongly on the tip–substrate distance. A significant influence of the tip on atomic diffusion on the top and at the edges of the islands is demonstrated. The size-dependent strain relief in the islands caused by the tip and by the substrate is found to play a key role in atomistic processes on islands. Our results show that, for certain tip–surface separations, the hopping diffusion of Co adatoms on the top of Co islands and the upward mass transport at the edge of the islands can be strongly enhanced. Our findings point out the possibility of manipulating atomic motion on mesoscopic islands using the STM tip.

(Some figures in this article are in colour only in the electronic version)

Progress in atomic engineering now makes it possible to produce nanostructures on metal surfaces that are tailor-made on the atomic scale [1–4]. As the size of nanostructures shrinks into the mesoscale, control of the individual atomic events involved in their formation becomes crucial. The STM has been proven to be one of the best experimental tools to study and manipulate matter at the atomic scale [4, 5]. The STM can be used to create artificial atomic-scale nanostructures with novel electronic and magnetic properties [4, 6–8]. By adjusting the tip–adatom distance, one can affect diffusion barriers of adatoms [9] and control their dynamics [10]. An atomic switch (reversible transfer of atoms between tip and surfaces) was realized using the STM [11].

Normally, the tip–sample distance is not accessible to direct measurements and could be inferred from measurements of the current, voltage, and displacement of the piezoelectric scanner tube [12]. Recent studies have demonstrated [13] that the real separation between

the tip and the surface can differ substantially from the value estimated from the experimental setup, due to relaxations of the surface atoms and the tip. Atomic relaxations are very important in a distance range where the onset of a short-range chemical interaction between the tip apex and the surface atoms takes place [14]. Very recent work of Limot *et al* [15] has revealed that the tip–adatom interaction is significantly different from the interaction of the tip with a flat surface.

Here, we demonstrate the effect of the tip on structure and atomistic processes on mesoscopic islands. We perform realistic atomistic modeling for the tip interaction with Co islands on Cu(100) at zero bias voltage, i.e. without any electric field effects. The tip-induced shape transitions in islands are revealed. We show that, at small tip–sample distances, structure of islands exhibits strong changes, which significantly influences the atomistic motion on the top and at the edges of the islands. Hopping diffusion on the top of the islands and upward mass transport at the edges of islands are predicted to depend strongly on the tip–surface separations. Tip-enhanced diffusion is found to take place for certain tip–substrate separations. Our studies show that the tip-induced strain relief in islands and atomic relaxations in the tip can drastically affect atomic motion on islands.

Atomic-scale simulations are performed using *ab initio* fitted many-body potentials formulated in the second moment approximation of the tight binding theory [16, 17]. The Korringa–Kohn–Rostoker (KKR) Green's function method [18] is used to create an *ab initio* data pool for fitting parameters of potentials. Surface properties (the binding energies of supported Co clusters of different sizes, the Hellmann–Feynmann forces acting on the Co adatom for different positions above the surface) and bulk properties (bulk modulus, lattice constants, cohesive energies, and elastic constants) are used in our model. The reliability of these potentials for different atomic configurations has been demonstrated [19–24]. Recent studies [25] have shown that our method describes atomic relaxations in nanostructures in very good agreement with fully *ab initio* calculations. The calculation technique based on *ab initio* interatomic potentials is preferred over first-principle calculations, because a full optimization of the structure of the tip, islands and the substrate at each step of the tip approach to islands is beyond the accessible computation time. For technical details, we refer to our former studies [16, 18, 25].

The Cu(100) substrate is represented by a seven-layer thick slab. Each layer contains 512 atoms. Periodic boundary conditions are applied in the surface plane. We model the tip by a Cu pyramid consisting of 14 atoms arranged in fcc(001) stacking. The two bottom layers in the substrate and the basis layer of the tip pyramid are fixed at each given distance. Fully relaxed calculations are performed at each step of the tip approach towards island. Our studies have shown that the size of the tip practically does not affect the main results of the present work.

First, we discuss the tip-induced structural changes in mesoscopic islands. An adatom is positioned at the central hollow site above the islands (cf figure 1). As an example, in figure 1 we show atomic relaxations in the square $Co_{8\times8}$ island for different tip–substrate separations. Here the tip–substrate distance h is defined as the distance between the tip apex atom and the surface atoms of the substrate (cf figure 1). When the tip apex is about 8–9 Å away from the surface, the atomic relaxations in the island are mainly determined by the island–substrate interaction. To understand the results presented in figure 1(a), we recall recent studies on mesoscopic relaxations at metal interfaces [19, 26, 27]. Usually, strain relaxations are predicted on the basis of the macroscopic lattice mismatch between the two materials. However, if the deposited system is of mesoscopic size, the size-dependent mesoscopic mismatch, rather than the macroscopic one, is the driving force for strain-relieving effects. For small islands, the mesoscopic mismatch can be unexpectedly large. Therefore, the strain induced at the interface can be locally larger than expected from macroscopic considerations. The mesoscopic islands locally distort the surface and induce strongly inhomogeneous displacement patterns in the

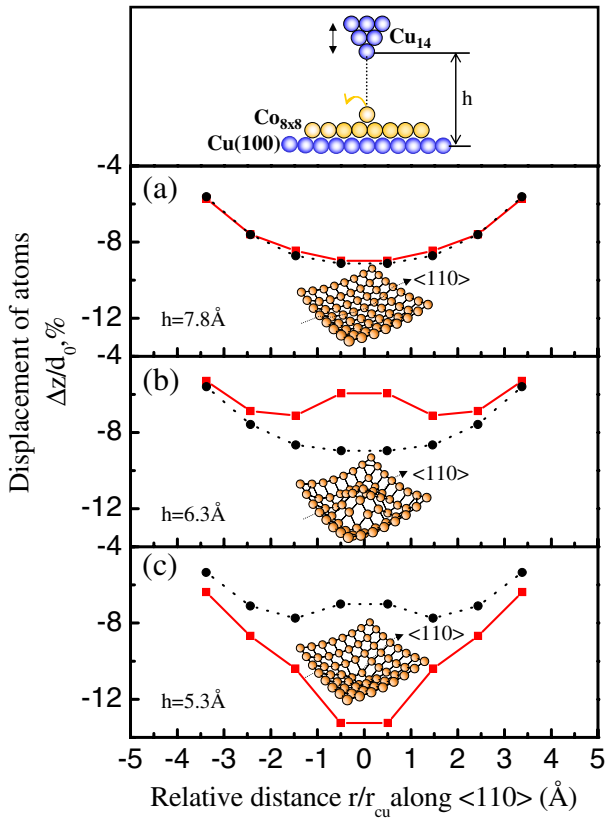

Figure 1. Tip-induced shape transitions (solid line) in Co islands. Vertical displacements in Co island on Cu(001) surface in ⟨110⟩ direction are shown. $\Delta z = z - d_0$ is the displacement of the atoms in Co island. z is the height above the surface level and $d_0 = 1.8075$ Å is the interlayer distance in bulk Cu. r is the distance between atoms. $r_0 = 2.5562$ Å is the bond length in bulk Cu. h is the tip–substrate distance. The results for the system without Co adatom are also shown (dashed line) for comparison.

substrate. The vertical displacements in the Co island presented in figure 1(a) demonstrate the impact of mesoscopic strain relief on the structure of the island. One can see that the island is not flat any more: the atoms at the centre of the island are pushed down, while the edge atoms exhibit strong upward relaxations. When the tip approaches the island, the tip–island interaction begins to play an important role. Our results show that the shape of islands strongly depends on the distance between the tip and the island. For example, in the range of tip–substrate distances between 7.8 Å and 6.3 Å (cf figure 1(b)), the atoms at the centre of the island exhibit a strong upward relaxations. Here we should mention that the distance between the tip apex atom and the Co adatom is in the range between 4.5 Å and 3.0 Å, which is exactly in the range of the chemical interaction distance. When the tip–substrate distance decreases from 6.3 Å to 5.3 Å (cf figure 1(c)), the atoms at the centre of the island are strongly pushed down. Comparing the displacements in the islands for the system with and without the adatom (cf figure 1), one can see that the existence of the adatom strengthens the tip–substrate interaction, especially for short distances.

Noticeable atomic relaxations are also found in the tip during its approach towards the island. Figure 2 shows that, in the range between 7.7 Å and 5.7 Å, the tip length increases,

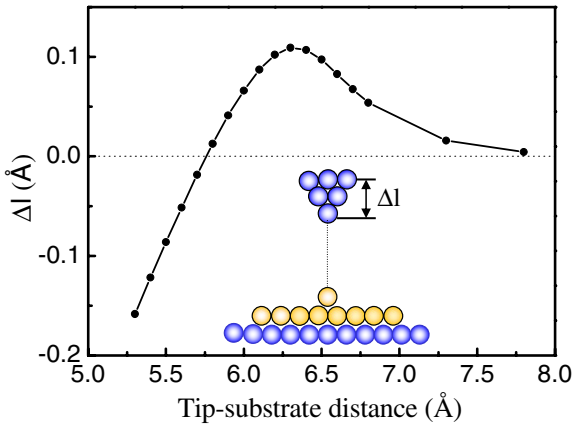

Figure 2. The atomic relaxations in the tip during vertical manipulation. Here, $\Delta l = l - l_0$. l and l_0 are the tip length with and without tip–island interaction.

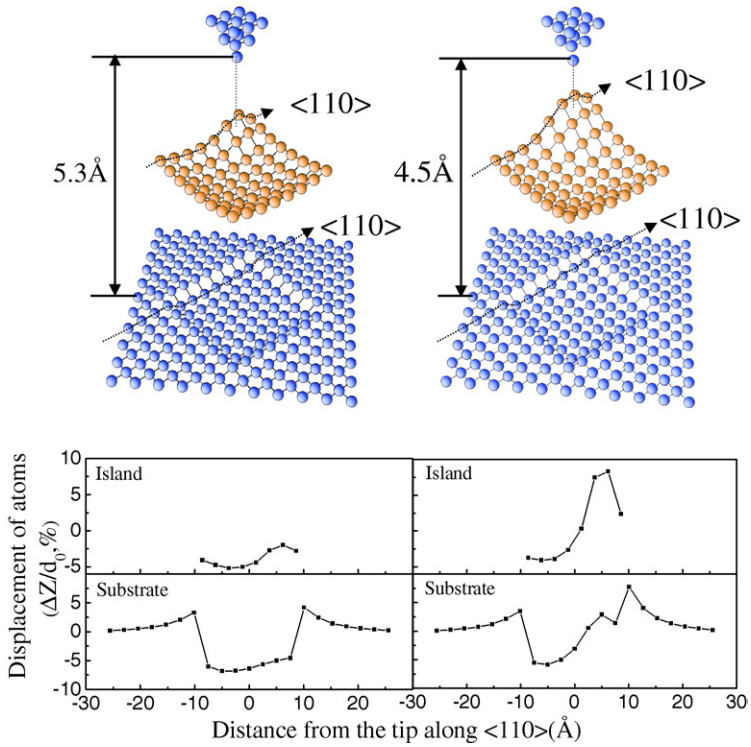

Figure 3. Vertical displacements of the edge atoms in $Co_{8\times8}$ island on Cu(001) surface in the ⟨110⟩ direction induced by the tip. The meaning of the symbols in this figure is the same as in figure 1.

i.e. the apex-atom of the tip is relaxing towards the island. However, for smaller tip–substrate separations, the repulsive forces between the tip–apex and the adatom cause an upward relaxation of the tip–apex, i.e. the tip length decreases.

We have also found that islands exhibit strong shape changes at their edges. For example, in figure 3 we depict the shape of the Co island and the substrate underneath when the tip is

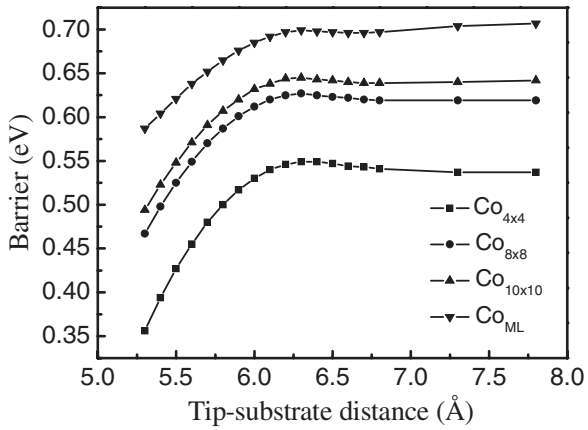

Figure 4. Hopping barrier of the Co adatom on top of the Co islands, as a function of tip–substrate distance. Results for Co monolayer on Cu(001) surface (Co_{ML}) are also shown.

placed at the edge of the island. Due to decreased coordination of the edge atoms (compared to the atoms at the centre of the island), they are strongly affected by the interaction with the tip. Pronounced tip-induced displacement patterns in the substrate are also seen in figure 3. These results prove unambiguously that mesoscopic islands react dynamically to the presence of the tip, its distance and position.

The complicated strain relaxations in mesoscopic islands and their strong dependence on the tip position revealed by our calculations could have important implications for atomistic processes on the top and at the edges of islands. For example, the tip-enhanced hopping diffusion on the top of islands has been found in our simulations. Figure 4 shows that the hopping barrier on the top of islands is strongly decreased when the tip approaches the islands. Additionally, the strong size-effect is well seen: the diffusion barrier depends strongly on the size of islands. Our analysis shows that tip-induced strain relaxations in islands, atomic relaxation in the tip, and tip–adatom interaction are factors that determine the observed behaviour of the hopping diffusion. For example, if calculations are performed for the ideal tip and the tip-induced relaxations in islands are ignored, the hopping barrier increases drastically (up to 1 eV) for tip–substrate distances smaller than 5.5 Å. This is a consequence of strong bonding which occurs between the tip–apex and the adatom at such short distances. However, in a fully relaxed geometry, the tip–apex moves away from the island (cf figure 2), and the island atoms under the tip relax towards the surface (cf figure 1(c)). In other words, the distance between the apex atom and the adatom increases, and the adatom experiences an attractive force in the direction of the tip. As a consequence, the hopping barrier reduces during the tip approach. A strong dependence of the barrier on the island size can be attributed to the size-dependent mesoscopic relaxations in islands [19, 26]. If the tip is far away from the island, the hopping barrier is determined by the size-dependent mesoscopic mismatch between the island and the substrate [26]. It was shown that the diffusion of adatoms on small islands having large mesoscopic mismatch can be a few orders of magnitude faster than on large ones. When the tip is in close proximity to islands, small islands exhibit stronger downward atomic relaxations than large islands. Consequently, the tip-induced reduction of the diffusion barrier on small islands is more appreciable. If we assume that the diffusivity D is related to the hopping barrier of single adatoms by $D = D_0 \cdot \exp(-E_d/kT)$, where E_d is the energy barrier for hopping and D_0 is the prefactor, we obtain that the diffusion coefficient of Co adatoms at room temperature

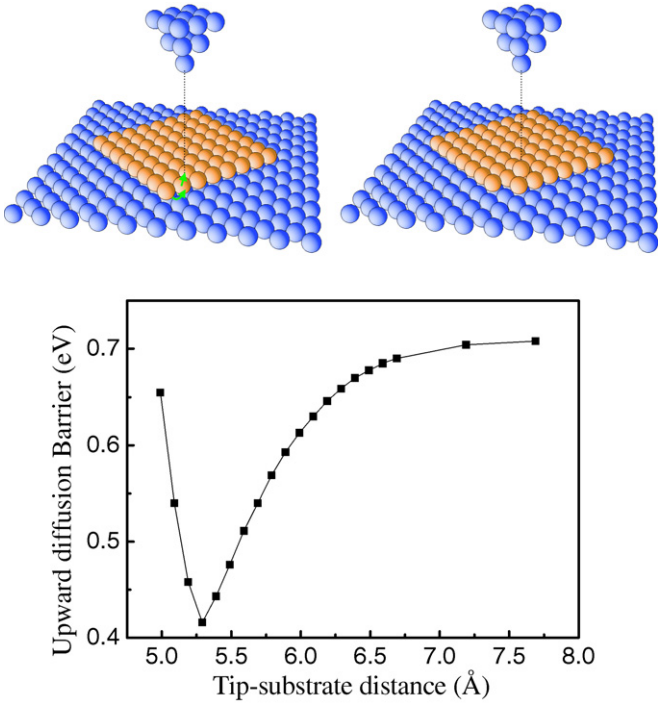

Figure 5. Effect of the tip on an upward mass transport at the edge of $Co_{8\times8}$ island.

in the presence of the tip can be enhanced by two to three orders of magnitude compared to that on islands without the tip.

Finally, we discuss the effect of the tip on atomic motion at the edge of the islands. We have calculated the Ehrlich–Schwoebel (ES) barrier and the edge exchange barrier for Co adatoms on Co islands. These two barriers determine a downward mass transport. We have found that both the ES and the exchange barriers are very large (about 1 eV) when the tip is away from the edge of square islands. Approaching the tip towards the island edge only slightly reduces these barriers (to about 0.9 eV, depending on the tip position). However, we have found that the tip can have a strong impact on upward mass transport at the edge of islands. An upward mass transport near Co islands on Cu(100) has been predicted recently by Miron and Fichthorn [28]. Performing accelerated molecular dynamics simulations they have found that a Co adatom that has landed on top of a Co island on Cu(100) diffuses until it reaches a kink or corner, where it pulls up another Co atom from the edge onto the second layer. Our calculations have revealed that the tip placed at the edge of the square Co island can strongly facilitate the upward mass transport. We depict this mechanism in figure 5: the edge atom is pushed onto the second layer and another Co atom from the island corner takes its position, because it is strongly influenced by tip–island interaction. The barrier of this process is significantly reduced from 0.7 eV (the tip is far away) to 0.4 eV for the tip–substrate distance about 5.3 Å. This is due to the fact that the edge atom has been pushed up to a high position by the tip approach before its upward diffusion (cf figure 3). However, for smaller tip–substrate distances (for example, at 4.5 Å, cf figure 3) the barrier for this process strongly increases mainly due to the increasing repulsive tip–island interaction in the process.

In conclusion, we have demonstrated tip-induced shape transitions in mesoscopic islands. Complete calculations of the tip–island–surface structure during tip approach have enabled us

to reveal the main features of tip–island interaction at the atomic scale. The size-dependent strain relaxations in islands are shown to play a key role in the tip-induced atomistic processes on islands. Our studies suggest that atomic motion on top of islands and at their edges can be manipulated by the STM tip.

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References

[1] Eigler D M and Schweizer E K 1990 *Nature* **344** 524
[2] Bartels L, Meyer G and Rieder K H 1997 *Phys. Rev. Lett.* **79** 697
[3] Li J, Berndt R and Schneider W-D 1996 *Phys. Rev. Lett.* **76** 1888
[4] Crommie M F 2000 *J. Electron Spectrosc. Relat. Phenom.* **109** 1
[5] Wiesendanger R and Güntherodt H-J (ed) 1996 *Scanning Tunneling Microscopy* vol 1–2 (Berlin: Springer)
[6] Crommie M F, Lutz C P and Eigler D M 1993 *Phys. Rev.* B **48** 2851
[7] Manoharan H C, Lutz C P and Eigler D M 2000 *Nature* **403** 512
[8] Hla S W, Braun K F and Rieder K H 2003 *Phys. Rev.* B **67** 201402
[9] Kürpick U and Rahman T S 1999 *Phys. Rev. Lett.* **83** 2765
[10] Stroscio J A and Celotta R J 2004 *Science* **306** 242
[11] Eigler D M, Lutz C P and Rudge W E 1991 *Nature* **352** 600
[12] Hansen O, Ravnkilde J T, Quaade U, Stokbro K and Grey F 1998 *Phys. Rev. Lett.* **81** 5572
[13] Hofer W A, Fisher A J, Wolkow R A and Grütter P 2001 *Phys. Rev. Lett.* **87** 236104
[14] Blanco J M, González C, Jelínek P, Ortega J, Flores F and Pérez R 2004 *Phys. Rev.* B **70** 085405
[15] Limot L, Kröger J, Berndt R, Garcia-Lekue A and Hofer W A 2005 *Phys. Rev. Lett.* **94** 126102
[16] Levanov N A, Stepanyuk V S, Hergert W, Bazhanov D I, Dederichs P H, Katsnelson A A and Massobrio C 2000 *Phys. Rev.* B **61** 2230
[17] Cleri F and Rosato V 1993 *Phys. Rev.* B **48** 22
Rosato V, Guillope B and Legrand B 1989 *Phil. Mag.* A **59** 321
[18] Wildberger K, Stepanyuk V S, Lang P, Zeller R and Dederichs P H 1995 *Phys. Rev. Lett.* **75** 509
[19] Stepanyuk V S, Bazhanov D I, Baranov A N, Hergert W, Dederichs P H and Kirschner J 2000 *Phys. Rev.* B **62** 15398
[20] Stepanyuk V S, Klavsyuk A L, Hergert W, Saletsky A M, Bruno P and Mertig I 2004 *Phys. Rev.* B **70** 195420
[21] Pick Ŝ, Stepanyuk V S, Klavsyuk A L, Niebergall L, Hergert W, Kirschner J and Bruno P 2004 *Phys. Rev.* B **70** 224419
[22] Miron R A and Fichthorn K A 2004 *Phys. Rev. Lett.* **93** 128301
[23] Sastry K, Johnson D D, Goldberg D E and Bellon P 2005 *Phys. Rev.* B **72** 085438
[24] Ju S P, Lo Y C, Sun S J and Chang J G 2005 *J. Phys. Chem.* B **109** 20805
[25] Stepanyuk V S, Klavsyuk A L, Niebergall L, Saletsky A M, Hergert W and Bruno P 2005 *Phase Transit.* **78** 61
[26] Stepanyuk V S, Bazhanov D I, Hergert W and Kirschner J 2001 *Phys. Rev.* B **63** 153406
[27] Lysenko O V, Stepanyuk V S, Hergert W and Kirschner J 2002 *Phys. Rev. Lett.* **89** 126102
[28] Miron R A and Fichthorn K A 2005 *Phys. Rev.* B **72** 035415