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Atomic Manipulation by Mechanical Resonance

Byungsoo Kim† and Takashi Hikihara‡,* and Vakhtang Putkaradze†

†Department of Mathematics, Colorado State University, Fort Collins, CO 80523 USA
‡Department of Electrical Engineering, Kyoto University
Katsura, Nishikyo, Kyoto 615-8510, JAPAN
∗ Photonics and Electronics Science and Engineering Center, Kyoto University
Katsura, Nishikyo, Kyoto 615-8510, JAPAN

Abstract—Manipulation of single atom has come into realization with the development of non-optical microscope technology like scanning tunneling microscope or atomic force microscope (AFM). Especially the recent experiments using AFM have demonstrated surprisingly diverse controllability of single atoms. Classical mechanical simulation is studied to support the resonant effect in the atomic manipulation using AFM.

1. Introduction

Recent development of dynamic force microscopy has demonstrated its capability of manipulating single atoms and building nano structures with single atoms [1, 2, 3, 4, 5, 6]. Scanning tunneling microscopy and AFM have been applied intensively on the semiconductor surfaces and demonstrated their capability of the image resolution for atomic scale and direct controllability of single atoms. Recent experiments conducted in Osaka University have shown that the ultra high vacuum non contacting AFM (UHV-NCAFM) could realize very diverse manipulation of single atoms [4, 5, 6]. Such diverse controllability has immense potential importance of application in the fields of bio science and material science. Upon the observation of the experimental possibility, theoretical studies have followed to illuminate the mechanism of atomic manipulation using NCAFM [7, 8, 9, 10]. There are two points of view on the atomic control, quantum mechanical view and classical mechanical one. The solid silicon (Si) surface is formed as a regular lattice structure of Si atoms and many electrons are filling the space between those atoms. Thus the Si surface is a very complicated system consisting of many atomic particles and the manipulation of a single atom could be a very challenging process. Despite such challenges, amazingly diverse possibility of manipulation has been experimentally realized. Based on the experimental results, our study tries to illuminate the process under the view of mechanical resonance and shows that the dynamic interaction of atoms could results in such manipulation of single atoms.

2. Review: experimental results

Most experiments of manipulation using AFM are conducted on the silicon surface since the material is of high interest in the semiconductor industry. The solid silicon is formed as a very regular diamond lattice with four outermost electrons for an atom and they form covalent bonds between atoms. Even though the atoms form a regular lattice, they vibrate in their lattice position and the covalent bonds can break and form to make structural changes. The atomic resolution of image made by AFM could show the change in the atomic lattice structure through the direct interaction between the atoms in Si surface and those in the AFM tip, which is a very sharp solid structure of silicon or other material by itself. The approach of the AFM tip is delicately controlled by electronic circuit so that the surface lattice is not damaged under the interaction with tip (NCAFM). Very sensitive variation of the interaction between the AFM tip and the Si surface atoms results in many interesting and diverse manipulations of surface atoms. The experiments tried the extraction of a single atom embedded in the surface lattice and it was successful. Then repeated experiments revealed that the extracted or an atom from the AFM tip could be deposited back into the defect hole in the surface lattice [4]. And for a surface with mixed atoms, indium (In) atoms doped on the silicon surface, similar experiments with NCAFM showed that two different type of neighboring atoms could interchange their lattice position [5]. And further experiments succeeded in interchanging two atoms between an atom in the surface and one in the AFM tip [6]. So literally the experiments have shown that most of imaginable manipulations are possible.

3. Statics or dynamics

Even though the experiments have been very successful, the related theory and explanation of those experiments are not completely illuminated. The complicated many body system of lattice atoms with even more complicated electronic distribution escapes from any exact theory. The density functional theory in quantum mechanical approach has been applied to calculate the electronic structure of the system and to calculate the force balance between atoms [7, 8].

This approach could regenerate accurate atomic structure and force balance. However its simulation involves intensive calculation for the electronic density and could not reproduce the reversibility of the extraction and deposition of atoms [7]. This could be understood as that the static force balance could impose some preference to one process between the extraction and the deposition. In the density functional theory, the kinetic energy of atoms has often been repressed for the simplicity of electronic density calculation. However, total exclusion of the kinetic energy of the atoms could be unrealistic considering such diverse controllability of atoms [14]. Thus we focus more attention on the atomic vibration and dynamic interaction between the surface atoms and the AFM tip atoms. In our approach, the possibility of increased kinetic energy of the manipulated target atoms and related resonance effect is the key factor of consideration for explaining the diverse manipulation possibilities. The increased energy of the target atom could be suspected as a resonant effect induced by several causes. First cause could be the direct atomic vibrational interaction between the target atom in the surface and atoms in the AFM tip. The second cause could be that the vibrational energy of the neighboring surface atoms could be locally transferred and focused on the target atom under the distorted potential energy structure induced by the proximity of the AFM tip. In both cases the locally excited atomic vibration of the target atom may be activated and lead to such atomic manipulations. This is our proposing scenario for the atomic manipulation using NCAFM. The intrinsic localized modes have been the study of interest for many scientific fields and it may be applied in the atomic vibration of the silicon lattice. In our dynamic approach for atomic vibration and resonance, simple and idealized interatomic potential energies have been used to simulate the atomic motion. Even though there are several flaws for simulating atomic system with a predefined empirical potential, for example, the Lennard-Jones potential cannot reproduce the diamond lattice structure of the silicon, it is more computationally favorable to simulate atomic movement under the Newtonian dynamics. There are several proposed empirical potentials [13] and we uses LJ potential (1) for the simplicity of simulation setting. Ideally the combined simulation is possible under the Car-Parrinello molecular dynamics (CPMD) scheme, but the inclusion of atomic vibration for the simulation of a big atomic system is still not realistic even in this scheme and the attention has been paid on the electronic density calculation for the most part and the atomic motion is minimized to find minimum potential configuration in this approach of illuminating the manipulation process of the single atoms.

4. Simulations

In the simulation with predefined interatomic potential energy, the goal is set on the demonstration of the possibility of the diverse manipulations of the target atoms under atomic interaction and their vibration. Simulated processes are the extraction of the target atom from the surface lattice under the vibrational interaction with tip atoms, the deposition of the target atom into the defect hole on the surface. The atomic parameters of silicon atom are used for the extraction and deposition simulations and for the interchange simulations. The Lennard-Jones (LJ) potential energy is used for the empirical interatomic potential as in the equation (1).

$$V_{LJ} = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]. \quad (1)$$

For the extraction and deposition simulation, a double layer lattice as in fig.1 is formed under the LJ potential and the atoms are free to move under the potential field and initially they form a stable lattice equilibrium. A target atom in the lattice is approached by a group of vibrating atoms forming a pyramid shape and this approaching atoms imitate the AFM tip. The free atoms in the lattice interact with the AFM atoms under the LJ potential. The simulation aims to confirm that the external excitation of the AFM tip atoms could extract the target atom without damaging the lattice structure except extracting the one atom. And for the deposition simulation, a defect hole is created in the lattice and a free atom on the AFM tip is brought near the defect hole to mimic the deposition. The atomic vibration of the tip atoms is simulated about 5×10^{12} Hz and the period of the tip oscillation is simulated as $T = 10^{-10}$ seconds to speed up the simulation.

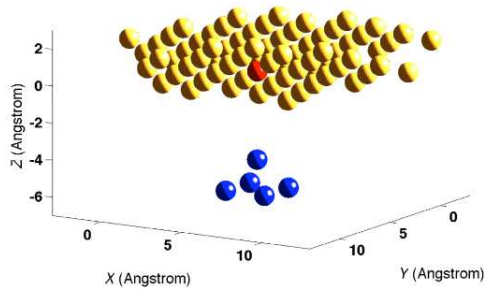

Figure 1: Initial arrangement of the lattice atoms (yellow), target atom (red) and AFM tip atoms (blue) for simulations. The tip atoms are considered as fast 5×10^{12} Hz oscillators with fixed amplitude. To model the oscillations of the AFM tip itself, we also prescribe the motion of the tip atoms, bringing them closer to surface and taking them away from the surface with much slower frequency $\sim 10^{10}$ Hz. The dynamics of all 72 target and lattice atoms is then computed according to the rules of Newtonian mechanics, taking into account all the inter-atomic forces.

In the simulation, both scenarios for extraction and deposition could be realized. This rather simple many body simulation shows that the target atom could move between the double well of potential energy with increased kinetic

energy when the potential barrier is small enough. And this could imply that the target atom could overcome a preferred force balance or energy minimum state when it could cross the energy barrier with its increased kinetic energy. The simulation results are shown in the fig. 2 and 3. This scenario of atomic motion can resolve the reversibility of the extraction and deposition control. The possibility of resonance in the atomic vibration and its application on the atomic control has been suggested regarding various interests [11, 12]. In those studies, electromagnetic wave or infrared laser of resonant frequency has been suggested for the atomic control. Interestingly, there is such a possibility of resonant excitation in the mechanical control using NCAFM. For the external resonant excitation on the target atom, the atomic vibration of the atoms in the tip of AFM can be considered as having the resonant frequency for the target atom in the material surface. Hence in our consideration, the resonant excitation is replaced from the electromagnetic wave frequency to the mechanical vibrational frequency of the atoms. Another distinct difference between those resonant excitations is that the AFM tip can distort the potential energy landscape around the target atom. Such a possibility has not been clarified yet in the experimental setting and thus we try to provide basic simulation setting and to find preliminary conditions for making atomic manipulations under the resonance effect.

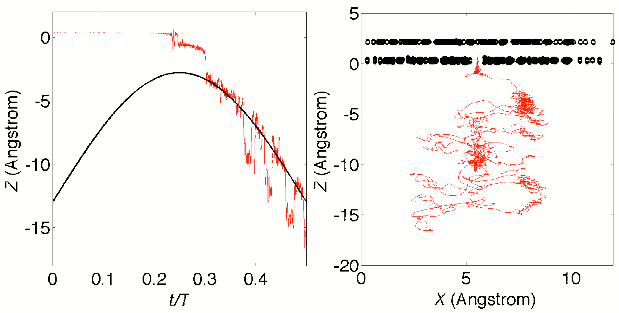

Figure 2: Dynamical description of the process of extraction. *Left*: The target atom (thin red line) gets extracted from the lattice under the approach of AFM tip atom, shown in black. Time scale is shown in units of the period T of AFM oscillation. Only the first half of AFM oscillation is shown, as it demonstrates the approach to the lattice. The second half of AFM oscillation plays no role in the dynamics. The target atom follows the tip, escaping the bonds with the lattice. *Right*: The motion of lattice atoms, shown in black, and the target atom, shown in red, as seen from the side. Coordinate X is along the surface, and Z is normal to the surface.

The simulation showed that the periodic excitation could extract the target atom without damaging the surrounding lattice and thus the excitation could be very localized. And also the tip creates the double well potential structure around the target atom so that the target atom could find another stable equilibrium near the tip. Hence the simulation result suggests that the presence of the AFM tip in the manipulation process can offer two important environment for the atomic control, which are the resonant excitation and the local distortion of energy landscape. In the simulation, the kinetic energy of neighboring atoms shows increased kinetic energy as in fig.5, but it was small compared to that of the target atom in fig.4.

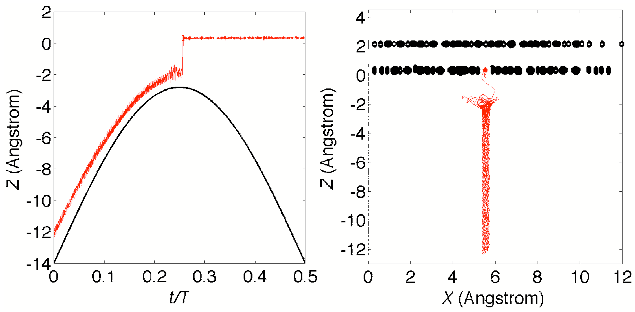

Figure 3: Dynamical description of the process of deposition. *Left*: The target atom (red) follows the AFM tip (black) until it approaches the lattice, positioned at $Z = 0.2$ Å. Time is scaled by the period of AFM oscillation T. The increase in kinetic energy of the target atom due to the interaction with the lattice atoms allows it to escape the potential well of the tip and bond to the lattice. *Right*: The motion of lattice atoms, shown in black, and the target atom, shown in red, as seen from the side.

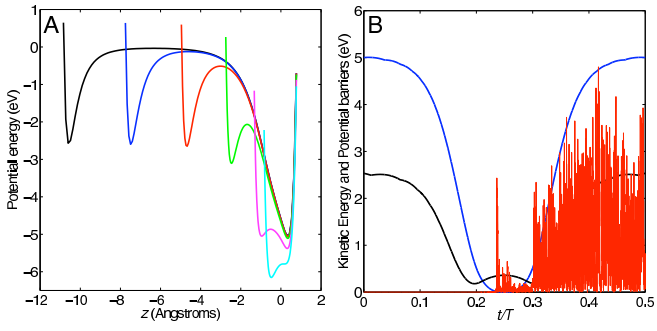

Figure 4: *Left*: The double well potential created by the tip. *Right*: The kinetic energy of the target atom (red) and the change of the energy barrier in the double well potential.

5. Concluding Remarks

In this paper we discussed a simple model for illuminating the manipulation of single atoms under the scenario of atomic resonance. The actual atomic system of Si lattice is very complicated system of nano-meter scale. On such an intricate system, the successful manipulation experiments have been monumental achievements and it promises very

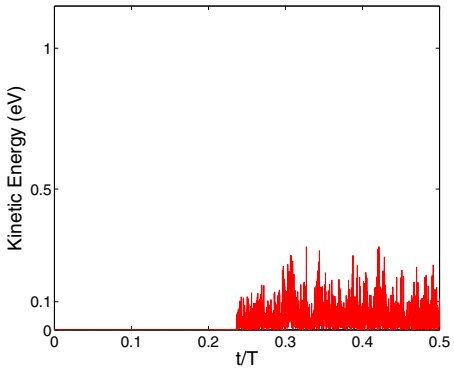

Figure 5: The kinetic energy of a neighboring atom under the extraction simulation. The excitation by the tip atoms increases the atomic vibration of local neighborhood of the target atom.

important potential applications. However, there have been some difficulties in explaining such diverse manipulations. To resolve it from the approach of electronic density computation, we proposed the inclusion of more dynamic aspect of atomic motion and its kinetic energy into the picture of manipulation process. The atomic control using the resonant excitation has been repeatedly proposed. The novelty of our study lies in that our proposal for the resonant excitation is the mechanical resonance under the AFM tip's presence. Even though our simulation models cannot exactly represent the real lattice and AFM system, they could reproduce such a diverse movement of particles and those diverse manipulations possibility in our picture is strongly suggestive to the experimental realizations. Hence such an inclusion of more dynamic motion of atoms into the existing picture of the manipulation process will add more flexibility for correct understanding of those phenomena in such an extremely small world. Our future work will be investigating the possibility of resonant atomic vibration under more sophisticated potential interactions or under the CPMD scheme and also designing an experimental setting for studying the vibrational effect on such manipulation processes.

Acknowledgments

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