First-Principles Study on Microscopic Mechanism of Atom Manipulation by Atomic Force Microscope

論 文 の 内 容 の 要 旨

論文題目　First-Principles Study on Microscopic Mechanism of Atom Manipulation by Atomic Force Microscope
（第一原理計算に立脚した原子間力顕微鏡原子操作の微視的な機構の研究）

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We report first-principles total-energy electronic-structure calculations that clarify the microscopic mechanisms of four types of atom manipulations [i.e. the lateral manipulation of Si atom on Si(111)-7×7 surface; the lateral interchange manipulations of Sn and Ge atoms on the Sn-covered Ge(111)-c(2×8) surface, and Sb and Si atoms on the Sb-covered Si(111)-(7×7) surface; the vertical interchange manipulation of Sn and Si atoms on the Sn-covered Si(111)-($\sqrt{3}$x$\sqrt{3}$)R30° surface, and atom gating manipulation of Ag atom on the Si(111)-(7×7) surface] by atomic force microscope. We determine the reaction pathways and the corresponding reaction barriers for each atom manipulation. The manipulations in the lateral manipulation, the lateral interchange manipulation and the atom gating manipulation take place due to the diffusion barrier modification of the surface atom by the probing tip. The formation of bond between the surface and tip atoms is the essential physics for the barrier modification. The tip reduces the diffusion barrier of the surface atom and stabilizes the intermediate metastable structures of the reaction. We have discovered that either spontaneous or tip-assisted formation of dimer structure of two surface adatoms, when they are close to each other, is the precursor for the lateral interchange manipulation on the Ge and Si surfaces. There are multiple metastable dimer structures of Sn-Ge and Sb-Si on the Ge and Si surfaces, respectively. The lateral interchange occurs due to the dimer-dimer transition between the metastable dimer structures. The calculated energy barrier of the lateral interchange manipulation is less than 0.6 eV. Similar dimer structures of tip apex atom and surface adatom are also found

to be the precursor for the vertical interchange manipulation. The dimer structures form due to the structure relaxation of tip apex and surface adatom, when the tip makes contact with the surface. We have studied the atom gating manipulation with two types of tips, i.e. Si and Pt tips. Both the tips trap the diffusing atom near the tip apices by forming bond(s) with it. We have clarified that the asymmetric lateral position of the tip between the half unit cells creates asymmetric potential well that prevents the backward diffusion of the adatom.