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Atomic manipulation of polarizable atoms by electric field directional diffusion

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Abstract. We present a brief summary of the properties of alkali metals on III–V(110) surfaces, as studied with the scanning tunneling microscope (STM). These include the non-metallic properties found in the one- and two-dimensional phases, and the directional diffusion of the alkali atoms due to the electric field gradient in the STM junction.

The ability to position the probe tip of a scanning tunneling microscope (STM) has opened the door to manipulation of atoms on the nanometer scale [1]. In this work we have shown that alkali atoms on III–V semiconductor surfaces can be induced to move by the application of a voltage pulse between the tip and the surface. The alkali atoms undergo a directional diffusion towards the region of highest field due to the interaction of the alkali atom dipole moment and the intense electric field in the STM junction [2]. This mechanism is to be distinguished from other manipulation schemes, which involved the transfer of atoms between the tip and surface or direct sliding of atoms across the surface using the force between the probe tip and adatom [1]. In this extended abstract the properties of Cs on GaAs and InSb(110) are described, followed by a description of the observation of the directional diffusion of Cs under the action of the electric field gradient in the STM junction.

We have studied the properties of alkali atoms on semiconductor surfaces because they represent model systems for understanding metal–semiconductor interfaces. The experiments were performed on clean GaAs and InSb(110) surfaces obtained by cleaving wafers in ultrahigh vacuum. Both p-type and n-type doping were used. Our initial work has shown that Cs forms one-dimensional (1D) zig-zag structures on GaAs and InSb(110) surfaces, as shown in figure 1 [3]. The nearest neighbor (NN) bond distances in these structures were 6.9 Å on GaAs(110) and 8.0 Å on InSb(110). At higher alkali densities, 2D and 3D structures were also observed [3, 4]. The 2D phases on both GaAs and InSb surfaces consisted of superstructures of Cs(110)-like polygon clusters (five-atom polygons on GaAs and four-atom polygons on InSb) [3, 4]. These structures resemble the planar clusters observed in gas phase alkali clusters, and have NN bonding distances close to the value of solid bulk Cs (5.2 Å).

The evolution from 1D to 3D structures in the alkali phases offers a unique situation to examine the evolution of the electronic properties. This is particularly interesting since bulk Cs lies near the metal–insulator transition [5]. We would expect the metal–insulator behavior to be sensitive to coordination and expanded lattices. To probe for metallic characteristics we have measured the tunneling conductivity at zero bias, which is proportional to the density of states at the Fermi level. Tunneling versus voltage characteristics for the various Cs phases on GaAs(110) are shown in figure 2. Both the 1D and 2D Cs phases show insulating current–voltage characteristics. On GaAs(110) the tunneling gap narrows from 1.1 to 0.6 eV in going from the 1D to the 2D phase (the tunneling gap on the bare GaAs(110) surface is 1.45 eV) [3]. On InSb(110) the Cs 1D phase shows a tunneling gap equal to the bare surface gap of 0.15 eV, as shown in [4]. The absence of a larger band gap over the Cs structure may be due to the pickup of InSb states in the measurement, which would obscure the larger 1D Cs band gap. Note that on GaAs the 1D Cs structure narrows the band gap from that of the clean surface and hence it is easier to see in the current versus voltage measurements. Interestingly, the 2D Cs phase on InSb(110) shows a tunneling gap of 0.6 eV, which is larger than the underlying substrate band gap of 0.15 eV [4]. This band gap is similar to that observed for the 2D phase on GaAs(110) and suggests that this may be a characteristic of the 2D Cs phase. On both surfaces, 3D clustering is observed following second-layer adsorption of Cs, which displays clear metallic current versus voltage characteristics. These

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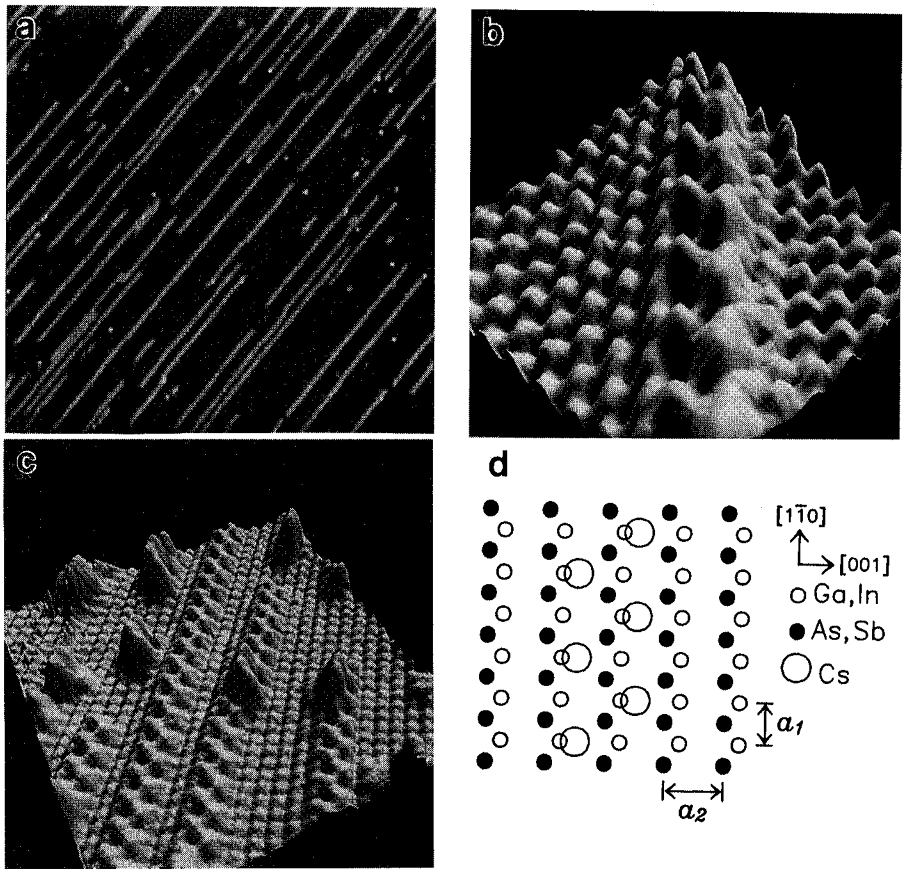

Figure 1. STM images recorded at negative sample bias showing one-dimensional Cs zig-zag chain structures on GaAs(110) and InSb(110): (*a*) 1370 × 1370 Å image of 1D Cs chains on GaAs(110); (*b*) 70 × 70 Å image of a single Cs chain on GaAs(110); (*c*) 200 × 200 Å image of Cs chains on InSb(110); (*d*) schematic drawing of the Cs zig-zag chains; the lattice constants for GaAs (InSb) are $a_1 = 4.00$ (4.58) Å and $a_2 = 5.65$ (6.48) Å.

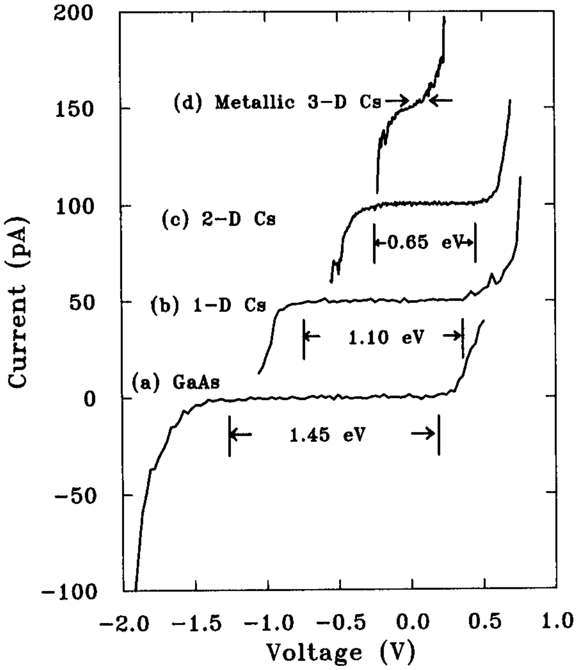

Figure 2. Current versus voltage measurements over various Cs structures on GaAs(110): curve (*a*), region of clean n-GaAs(110); curve (*b*), 1D zig-zag chain on n-GaAs(110); curve (*c*), 2D Cs phase on p-GaAs(110); curve (*d*), saturation 3D bilayer on p-GaAs(110). Note that curves (*b*)–(*d*) are offset vertically for clarity.

observations are suggestive of a description based on a Mott–Hubbard insulator [4, 6]. This would account, for example, for the narrowing of the band gap observed in going from the 1D to the 2D Cs phase on GaAs; the Cs density and coordination increase, which would be expected to reduce any electron correlation effects [4].

In the above STM measurements, images could only be obtained at negative sample bias on p-type material. On n-type material stable images could also be obtained at low positive sample biases (< 2 V). We discovered that the reason for this was that under positive sample bias the Cs atoms were *moving* over the surface, as shown in figure 3. This was shown by recording images of the low-density 1D Cs chain structures at negative sample bias, where the structures are observed to be stable (figures 3 (*a*), (*b*), and (*c*)). The tip was then positioned in the center of the imaged area and the voltage was switched to a positive value for a selected time period. The area was then re-imaged at negative sample bias. As observed in figures 3(*d*), (*e*), and (*f*), the density of Cs chains increased in the image, and was concentrated in the center region where the tip was positioned during the voltage pulse [1, 2]. The Cs density showed a monatomic increase as a function of voltage pulse length. Thresholds were observed at approximately 0.5 V on p-type material and 2 V on n-type. The Cs density also increased with higher voltages at a fixed pulse length.

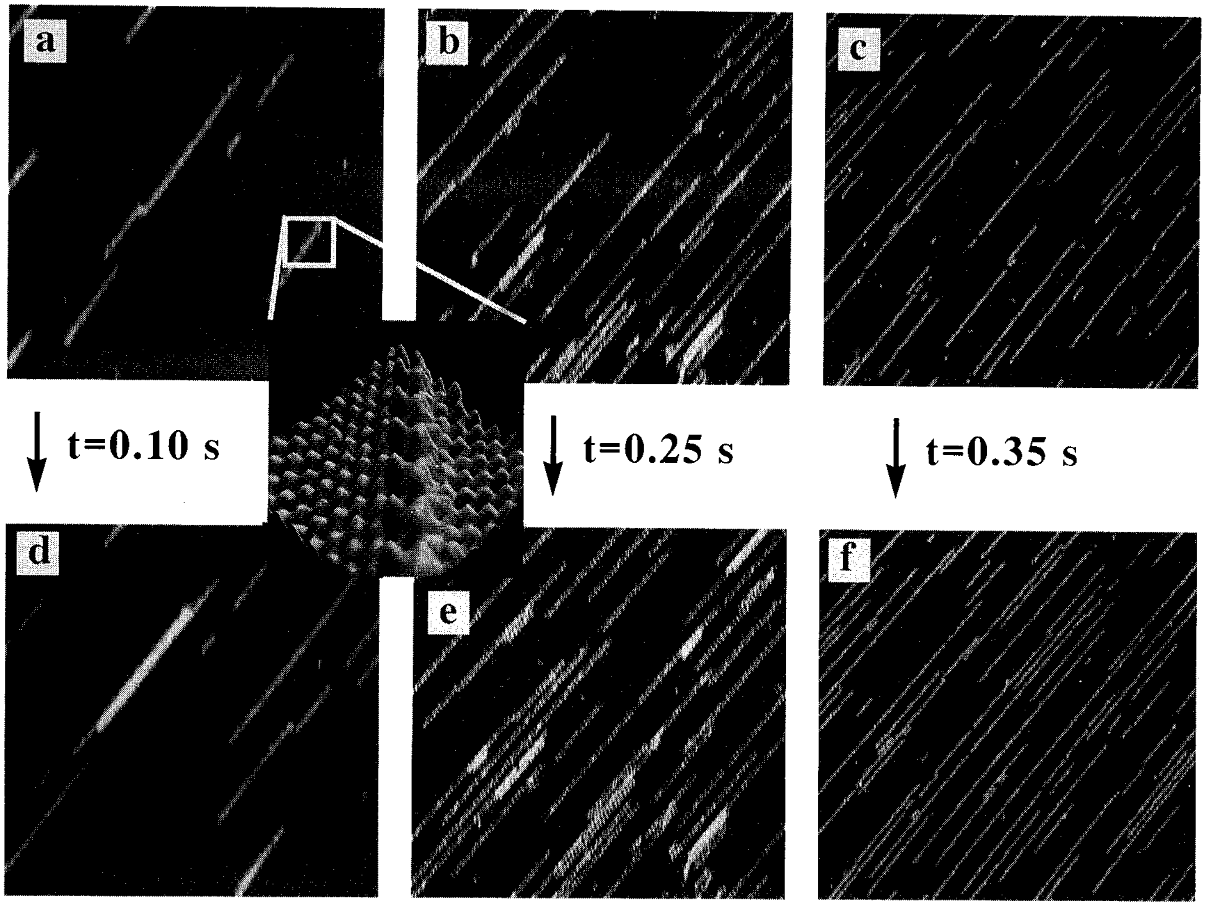

Figure 3. STM images of Cs on p-type GaAs(110). (*a*)–(*c*) Images recorded at -2 V sample bias showing the initial state before pulsing the sample voltage. (*d*)–(*f*) Images recorded at -2 V after pulsing the sample voltage to $+1$ V, with the tip positioned in the center of the image for 0.15, 0.25, and 0.35 s, respectively. All of the images are 1400×1400 Å, except (*a*) and (*d*), which are 1000×1000 Å.

The mobility of the alkali atoms in the STM junction can be understood by considering the interaction energy of an atom in an inhomogeneous electric field. The interaction energy contains two terms: the product of the electric field with the static dipole moment of the atom and the product of the electric field with the induced dipole moment. The induced dipole moment itself is proportional to the electric field through the atom's polarizability. Only one of these two terms depends on the polarity of the electric field; at positive sample bias the two terms add whereas at negative sample bias they cancel. Taking suitable parameters for the static dipole moment and polarizability for Cs, we estimate a potential well under the probe tip of approximately 1 eV at 3 V sample bias and 5 Å tip–sample separation. This can be compared to the surface corrugation potential of GaAs(110) which is about 0.8 eV perpendicular to the GaAs rows (along the [100] direction) and 0.1–0.2 eV along the GaAs rows [7]. At negative sample bias of -3 V the interaction potential is <0.1 eV for a polarizability of 50 Å^3. This technique thus gives a measure of the atom's polarizability, similar to the field induced directional diffusion studies analyzed with field ion microscopy [8].

With higher voltage pulses it is possible to induce a sufficient force on the alkali atoms to close pack them together. This leads to the exciting regime of the synthesis or creation of new structures or phases of matter. With higher-voltage pulses we succeeded in creating small nanoclusters of Cs atoms and complete close packed 2D phases [1, 2]. The 2D phases were not the same ones observed following simple room temperature adsorption. This technique is only in its infancy and the future awaits more creative uses of it, both as a way to study the interaction forces in the STM junction and a method of atomic manipulation.

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