STM and STS study of endohedral metallofullerenes adsorbed on Si(111)-(7×7) surfaces

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Structures and physical properties of metallofullerenes have hardly been studied because of the difficulty in obtaining amounts of samples enough to study them. Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) are powerful techniques to study structures and electronic properties of metallofullerenes. In the present study, we have investigated structures and electronic properties of $M@C_{82}$ (M: Ba, Ce and Dy) and $Dy@C_{60}$ adsorbed on Si(111)-(7×7) surface at 295 and 100 K by using an ultra-high vacuum STM system.

The Si(111) substrate was degassed at 600 ˚C for 12 h, and repeated a flash-annealing up to 1100 ˚C for 10 s several times. After these procedure, the Si(111) substrate was maintained at 700 ˚C for 3 min, and was slowly cooled down to room temperature. The STM image of the well-ordered 7×7 reconstruction with few defects was clearly observed in the Si(111). The metallofullerene powder was introduced into a small quartz-made evaporator. After degassing, metallofullerene was deposited at about 650 ˚C on the well-defined Si(111)-(7×7) surface which was held at room temperature.

Figure 1 shows STM topographic image of the Si(111)-(7×7) surface covered with almost one monolayer of $Dy@C_{82}$ at 295 K. The dim blobs on the Si surface are assigned to the $Dy@C_{82}$ molecules in the first layer, and the bright near-circular features are to the individual $Dy@C_{82}$ molecules in the second layer. The STM image showed no specific nucleation in the first layer. Moreover, the first layer is disordered and any second layer islands are not observed before the completion of the first layer, which indicate that the substrate-adsorbate interaction is stronger than the intermolecular interaction. The height of the $Dy@C_{82}$ molecule on the first layer is 11.3 Å which is close to that, ~ 12 Å, of $Nd@C_{82}$ adsorbed on the closed-packed C_{60} thin-film.[1] The value is also close to the van der Waals diameters of two long axes of the $Dy@C_{82}$ molecule (11.3 – 11.4 Å).[2] Consequently, it has been concluded that the long axis of $Dy@C_{82}$ is oriented along the direction perpendicular to the surface. This molecule has a dipole moment because the Dy is displaced from the center of the C_{82} cage. The dipole moment should affect the orientation of the molecule. The STS shows that the energy gap of the multilayer of $Dy@C_{82}$ is 0.1 eV at 295 K, which is consistent with the gap for the thin-film of $Dy@C_{82}$ estimated by temperature dependence of resistivity.[2] Figure 2 shows the image of the surface after multilayer deposition of the $Dy@C_{60}$ adsorbed on the Si(111)-(7×7) surface held at room temperature. The height of the $Dy@C_{60}$ molecule is about 8 Å. We will present the density of states for metallofullerenes determined by STS at 295 and 100 K. The STS measurement of metallofullerenes in applying the gate voltage is tried to realize the nanoscale FET.

1) N. Lin *et al*., *Phys. Rev. B* 58, 2126 (1998).
2) Y. Kubozono *et al*., *Phys. Rev. B* submitted.

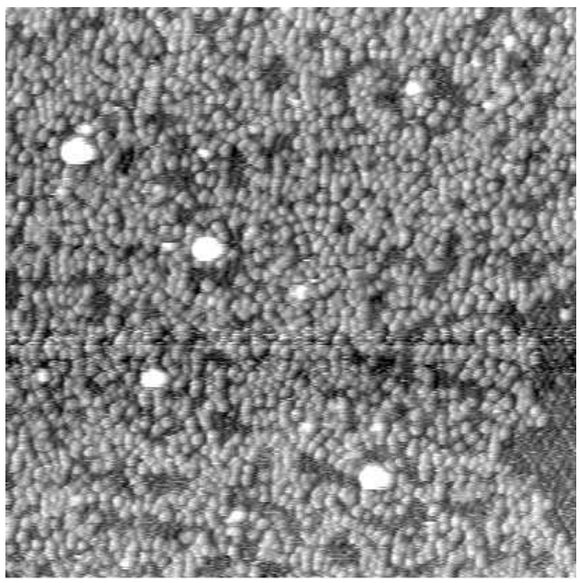

Figure 1. The STM image (80 nm × 80 nm) of ~ 1 monolayer of $Dy@C_{82}$ adsorbed on the Si(111)-(7×7) surface. The tunneling current is 0.25 nA and the bias voltage is –2.61 V. The dark regions are still unfilled bare Si surfaces.

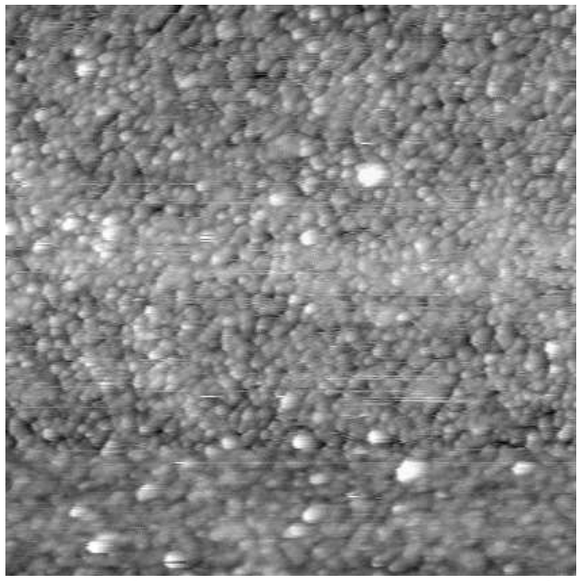

Figure 2. The STM image (80 nm × 80 nm) of a multilayer of $Dy@C_{60}$ molecules adsorbed on the Si(111)-(7×7) surface. The tunneling current is 0.25 nA and the bias voltage is –2.75 V.