The adsorption structures of C_{60} on graphite and Al(111)

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Fullerene-based molecular crystals and films are of considerable interest because of their very rich electronic properties, including superconductivity with high critical temperatures, ferromagnetism and metal-insulator transitions. The interfaces of C_{60} films with metal surfaces are of particular interest for molecular electronics applications. The electronic properties of these films are known to depend strongly on their structures and the relative molecular orientations of the C_{60} molecules, yet there are few detailed structure determinations for C_{60} films.

Earlier studies of C_{60} on highly-oriented pyrolytic graphite (HOPG) indicated that it is weakly bound to the surface and forms a probably-incommensurate hexagonal structure. The LEED studies presented here on single crystal graphite concur with that finding, and further show that there is no preferred orientation of the C_{60} monolayer for temperatures down to 50 K, i.e. its diffraction pattern consists of uniform rings. This somewhat surprising result indicates that the corrugation of the C_{60}-graphite potential is extremely small. Large-scale molecular dynamics (MD) simulations using potentials based on averaged pair potentials reproduce this result. Smaller all-atom MD simulations were performed to elucidate the detailed behavior of the adsorbate within one of the larger domains.

C_{60} on Al(111) forms either a $(2\sqrt{3}x2\sqrt{3})R30°$ structure or a 6x6 structure (Fig. 1) on Al(111), depending on the temperature. Earlier STM studies suggested a temperature-activated substrate reconstruction that leads to different adsorption sites in the annealed monolayer[1], and a DFT study suggested that this structure consists of two molecules in surface vacancies and one on top of an ad-dimer[2]. We present a LEED study for this adsorption system.

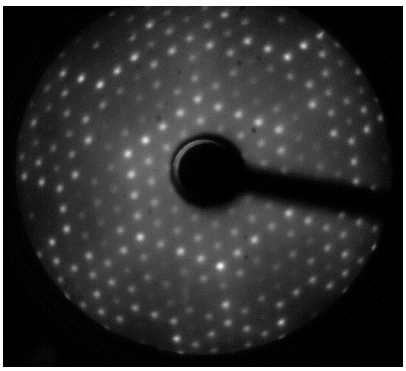

Fig 1. LEED pattern from Al(111)-(6x6)-3C_{60} at T = 143 K and using a beam energy of 115 eV.

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