Nanostructuring surfaces: Deconstruction of the Pt(110)-(1×2) surface by C₆₀

The interactions at the interface between large molecules and metallic substrates have attracted considerable interest due to the development of new devices based on organic films and/or functionalized inorganic molecules. When deposited on metal surfaces, the C₆₀ (fullerene) molecule creates regularly ordered, nanometre scale holes (“nanoholes”). Grazing incidence X-ray diffraction reveals a c(4x4) reconstruction induced by C₆₀ on a Platinum (110) surface that had initially a (1x2) type reconstruction. While the initial missing row of the (1x2) surface structure is partially deconstructed, under each fullerene we find a double atomic vacancy involving the topmost Pt layers. The resulting interface is deeply modified with 75% occupancy of Pt and regularly distributed double vacancies. The orientation of the C₆₀ molecule is compatible with a cm symmetry of the local surface, with one of the molecule’s pentagonal rings of carbons almost parallel to the surface and its hexagonal rings almost parallel to the (111) facets of the Pt nanohole.

We studied the c(4×4) reconstruction obtained by depositing a single layer of fullerene on the Pt(110)-(1×2), missing row reconstruction, using grazing incidence X-ray diffraction at the European Synchrotron Radiation Facility in Grenoble. The substrate was maintained at about 800 K during deposition, and the saturation coverage was determined by monitoring one superstructure reflection during the growth. A set of 45 fractional rods and nine crystal truncation rods were measured to optimize calculation of the structure (Figure 1 shows a few of them).

The strong interaction of the C₆₀ molecules with the Pt-substrate is shown by the high number of C-Pt bonds participating in the anchoring of the molecules to the substrate. The most stable configuration yields 15 C-Pt bonds with an average bond distance of 2.4 Å, which is an indication of charge delocalization from the molecule to the substrate over a rather large contact interface area.

This work was done in collaboration with the Institut de Ciència de Materials de Barcelona and the Physics Department of the Universitat Autònoma de Barcelona.

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FURTHER READING

The X-Ray Diffraction data analysis agrees with a surface substrate ordering where the initial (1x2) missing row is “de-reconstructed” by a partial filling (50%) of the missing rows, due to the interaction of the C₆₀ with the substrate (Fig. 2). The resulting surface consists of a Pt top layer where complete rows alternate with half-filled ones, yielding a 75% occupancy, with double vacancies alternating with Pt doublets which generates the new c(4x4) surface periodicity. The unit cell contains a single bi-atomic Pt-surface hole used to host the C₆₀ molecule and forming a regular, dense quasi-hexagonal molecular phase.

Figure 1 : X-Ray diffraction intensities measured when rocking the crystal sample in a multiple directions were used to determine the c(2x2) structure of C₆₀ molecules on Pt(110). Data shown here are for some fractional rods and crystal truncation rods. The continuous lines correspond to the best fit model.

Figure 2 : Top and lateral view of the C₆₀/Pt(110)-c(4×4): Darker color atoms correspond to deeper surface atoms.