

New insights in the c(4x2) reconstruction of hexadecanethiol on Au(111) revealed by GIXRD

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Abstract

Alkanethiols are attractive candidates to establish linkages between an underlying substrate with different molecular species. On single crystalline substrates, alkanethiols self-assemble into structurally well defined domains, thus beyond their technological interest, they are also considered as model systems for self assembled monolayers. The nature of the interaction between these molecular chains as well as those with the substrate plays an important role to model these types of self-assembled structures.

The c(4x2) structure of C₁₆H₃₃SH alkanethiol monolayers self-assembled on Au(111) has been studied by Grazing Incidence X-Ray Diffraction (GIXRD). This structure coexist on the surface with the ($\sqrt{3}\times\sqrt{3}$)R30° phase. The surface unit cell consists of four symmetry-independent molecules with atomic displacements related by couples, so only two non-equivalent chains are present in the surface cell. The analysis of the experimental data shows that the stability between neighbor chains is due to Van der Waals interactions while the substrate also plays an important and non-negligible role in the stabilization of the c(4x2) reconstruction. The lateral and normal substrate relaxations to the surface plane are small, gold displacements are lower than 0.25 Å, but contribute very strongly to the fractional order intensities. The molecular chains form a close packed structure tilted approximately 37° from the surface normal. The best fit does not provide indications of dimer formation between closest S-atoms.

The experimental results obtained from the experimental data analysis are compared with those supplied from the most plausible model available in the literature for this system [1].

References

- [1] P.Fenter, A. Eberhardt and P.Heisenberg, Science, 266 (1994), 1216.