SEXAFS-Study of the K/Si(111) Interface

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The interface between K and Si(111) was investigated by means of surface EXAFS at the K-1s threshold. The intention of this study was to clarify coverage-dependent structural aspects of K adsorption on Si(111). The x-ray absorption spectra in the energy range 3580 eV $\leq h\nu \leq$ 3900 eV were recorded at the EXAFS-II beam line for different polar angles using a partial-electron-yield detector positioned below the sample. Such an arrangement yields a high edge jump ratio independent of the orientation of the surface relative to the beam. The interfaces were prepared in an UHV chamber using commercial n-type Si(111) wafers as substrates, which - after annealing at 1100 °C - displayed well-ordered 7x7 LEED patterns. The K overlayers were deposited with commercial SAES getter sources.

SEXAFS measurements on overlayers in the monolayer-range require high stability, a condition that is, unfortunately, not well fulfilled at the EXAFS-II beam line of HASYLAB. These intensity fluctuations of the monochromatized beam cause the quality of the spectra to be relatively poor.

The analysis of the SEXAFS spectra followed well-established paths. Fig. 1a shows the polarization-dependent spectra after Fourier transform (FT) for a coverage of 1/4 ML K on Si(111) at T = 130 K. There is no scattering neighbor for normal incidence (ϑ = 90°, in-plane scattering), but the out-of-plane spectrum (ϑ = 35°) indicates a scattering contribution from the substrate. The corresponding K-Si bond length given by peak A in the FT was found to be r = 2.86 ± 0.08 Å. This value is shorter than the one given by Kendelewicz et al. /1/ for the K/Si(100) interface, r = 3.14 ± 0.10 Å; the latter is approximately the sum of the covalent radii. The polarization dependence indicates that the K atoms adsorb on top positions above Si atoms, which agrees with findings from STM images /2/.

With increasing K coverage, the edge jump grows progressively, however, not the amplitude of the SEXAFS oscillations. Fig. 1b shows the FT spectrum for a K coverage of 10 ML, with a wide peak (B). The phase shifted position of this peak corresponds to the nearest-neighbor bond length in bulk K metal (r = 4.54 Å). However, the observed broadening indicates that K condensation took place in a rather irregular way.

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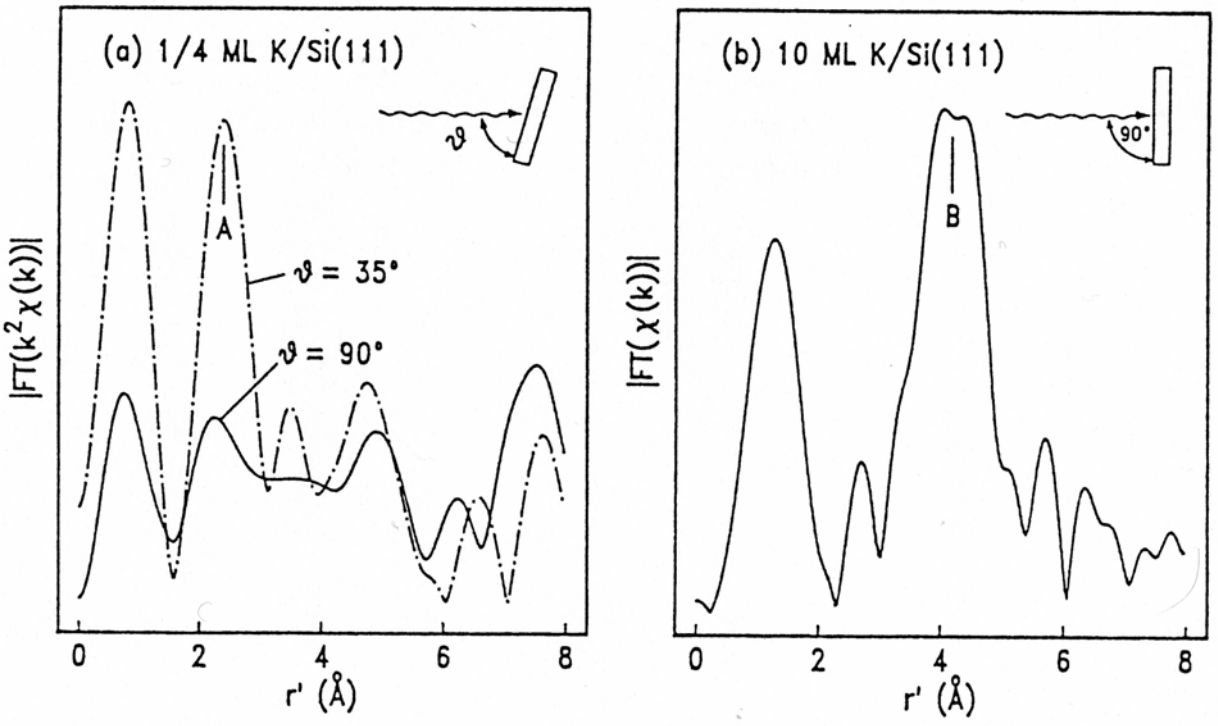

Fig. 1. Modulus of Fourier transform of the EXAFS function, χ(k), for various K coverages on Si(111) at T = 130 K.