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On the use of NEXAFS and PSID SEXAFS in the study of adsorbate–semiconductor coordination

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Abstract. Using Si(111)7 × 7–Cl as a model system, we have investigated the use of polarisation-dependent NEXAFS and ion yield SEXAFS in the determination of adsorbate–semiconductor coordination. Cl K-edge Cl^+ yield data indicate a Cl–Si bond length of 2.01± 0.03 Å, in agreement with Cl KLL Auger yield SEXAFS data. The polarisation-dependent behaviour of the 'white line' in Auger yield NEXAFS data is found to be consistent with a recently proposed pseudo-intra-molecular σ^*-resonance model.

There has been debate in the literature recently concerning the validity of using photon-stimulated ion desorption (PSID) surface extended x-ray absorption fine structure (SEXAFS) as a means of determining surface bond geometries [1]. In the present work we explored the use of PSID SEXAFS at an adsorbate (Cl) edge in a simple way, i.e.

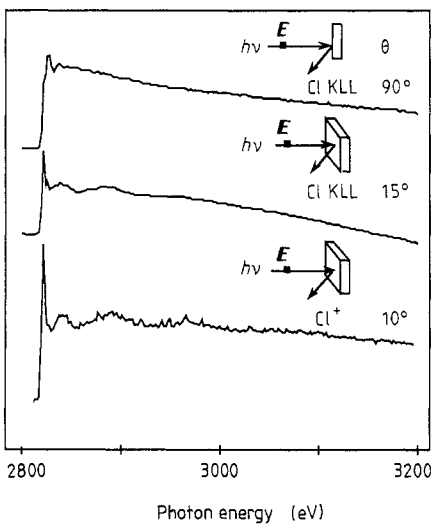

Figure 1. Cl K-edge Auger and ion yield SEXAFS data for Si(111)7 × 7–Cl at angle of incidence $\theta°$.

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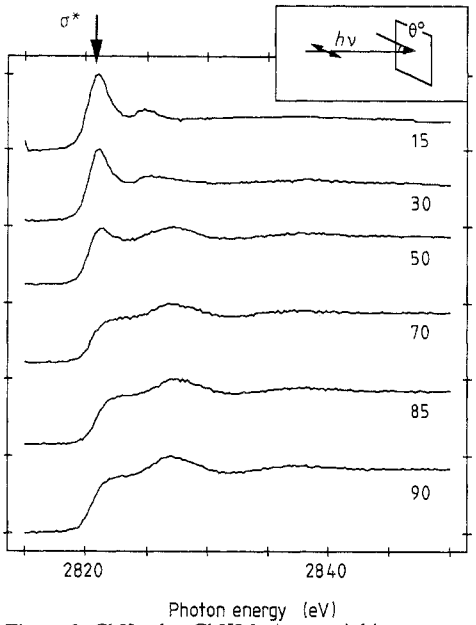

Figure 2. Cl K-edge Cl KLL Auger yield NEXAFS for Si(111)7 × 7–Cl as a function of photon incidence angle, $\theta°$. The pseudo-intra-molecular σ^*-resonance is indicated.

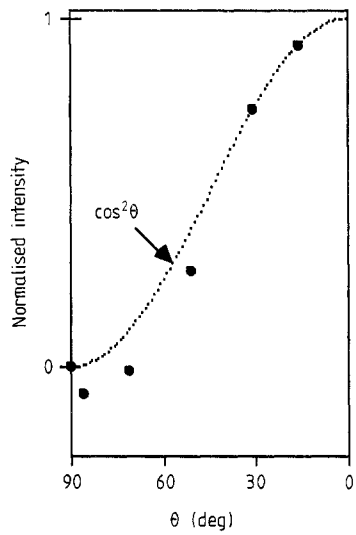

Figure 3. The normalised intensity of the σ^*-resonance obtained from figure 2 (●).

by determining whether the ion yield data indicate the same geometry as the more conventional Auger yield method. The results, which were obtained from a conventionally prepared Si(111)7 × 7–Cl surface (which has Cl bonded atop Si [2]) using station 6.3 at the SRS, Daresbury Laboratory, are shown in figure 1. Analysis yields the same Cl–Si bond distance and coordination number from ion and Auger yield, showing that for this system at least the ion yield represents a valid SEXAFS measurement technique.

As for the near-edge x-ray absorption fine structure (NEXAFS), we recently suggested the possibility of using adsorbate–semiconductor σ^*-resonances to evaluate the adsorbate bond angle [3]. The validity of this seems to be confirmed by our more recent work, where the intensity of the σ^*-resonance has been recorded as a function of photon incidence (***E***-vector) angle with respect to the Si–Cl bond (figure 2). After accounting for an atomic-like background, the intensity has the expected [4] $\cos^2\theta$ dependence (figure 3).

References

[1] McGrath R, McGovern I T, Thornton G, Warburton D R, Norman D and Cimino R 1988 *Vacuum* **38** 424–5

[2] Citrin P H, Rowe J E and Eisenberger P 1983 *Phys. Rev.* B **28** 2299–301

[3] Thornton G, Wincott P L, McGrath R, McGovern I T, Quinn F M, Norman D and Vvedensky D D 1989 *Surf. Sci* **211 + 212** 959–68

[4] Stöhr J and Jaeger R 1982 *Phys. Rev.* B **26** 4111–31