

# X-ray resonant Raman scattering in Si at 1s absorption edge

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## Introduction

The application of the total reflection x-ray fluorescence (TXRF) method [1] combined with intense synchrotron x-ray sources offers new possibilities for measuring very low concentrations of light element impurities on the surface of Si wafers. Several experiments [2, 3] have shown that the detection limit of Al impurities on Si surface is limited by the presence of the x-ray resonant Raman scattering (RRS). For excitation energies tuned below the Si K-absorption edge to avoid the intense Si K fluorescence x-ray line the RRS structure of Si is indeed overlapping with the Al K x-ray peak. In the analysis of low-resolution data a precise knowledge of the background profile that is mainly due to the x-ray Raman scattering is therefore crucial.

## Experiment

The x-ray resonant Raman scattering spectra of Si were measured at the ESRF beamline ID21 by means of high-resolution x-ray spectroscopy, using a von Hamos Bragg-type curved crystal spectrometer [4]. As the Bragg angle domain covered by this instrument extends from 24.4° to 61.1°, for the observation of the 1400 – 1800 eV x-ray spectra of interest the spectrometer was equipped with an ADP (101) crystal ( $2d = 10.642\text{\AA}$ ). The diffracted x-rays were recorded with a 26.8 mm long and 8 mm high position-sensitive back illuminated CCD detector consisting of 1340 columns and 400 rows with a pixel size of  $20 \times 20 \mu\text{m}^2$ . The schematic drawing of the von Hamos spectrometer geometry is presented in Fig. 1a. At ID21 the spectrometer was installed downstream of the STXM chamber to which it was connected through a ~200 cm long evacuated pipe (Fig. 1b).

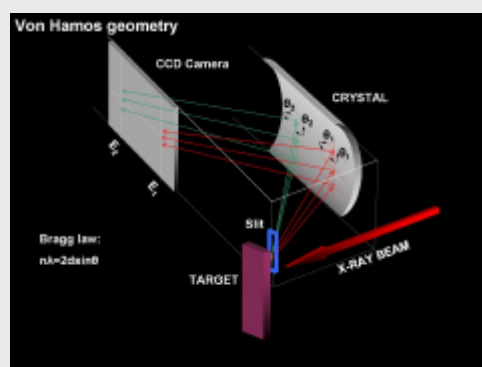


Fig. 1a: Schematic drawing of the von Hamos geometry.



Fig. 1b: Photograph of the von Hamos spectrometer as installed at the ESRF beamline ID21.

The x-ray beam was monochromatized by means of two  $20\text{\AA}$  Ni/B<sub>4</sub>C multilayers. Thanks to this monochromator  $10^{12} - 10^{13}$  incident photons/s were obtained on the target with an energy resolution of ~6 eV. The angle between the incoming beam and the target surface was 20°. The target consisted of a 25 mm high x 12 mm wide x 1 mm thick polycrystalline Si sheet.

## Results

The Si RRS spectra were measured at several excitation energies between 1790 eV and 1900 eV. The beam energy calibration was determined from measurements of the K-absorption edges of Al and Si. The energy calibration of the crystal spectrometer was deduced from measurements of the  $K\alpha_{1,2}$  x-ray lines of Al and Si. These measurements were also employed to determine the instrumental broadening of the spectrometer. Examples of the measured x-ray RRS spectra are shown in Fig. 2a (data taken at beam energies tuned below the 1s absorption edge) and in Fig. 2b (data taken at beam energies tuned across the edge with 2 eV steps).

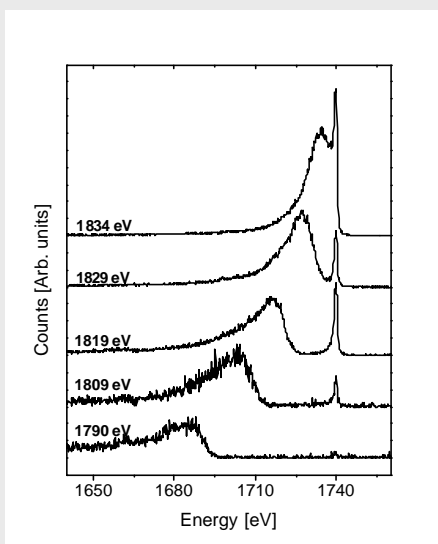


Fig. 2a: High resolution x-ray RRS spectra for excitation energies tuned below the 1s absorption edge.

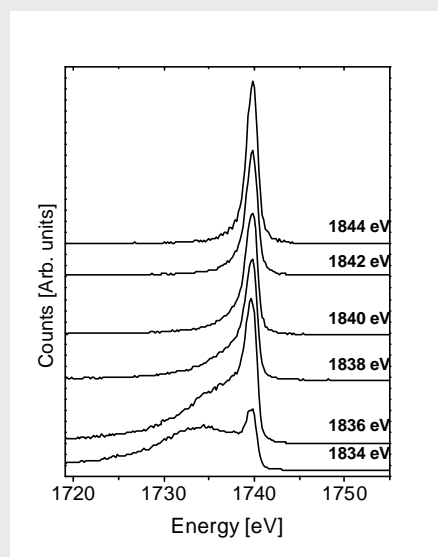


Fig. 2b: High resolution x-ray RRS spectra for excitation energies tuned across the 1s absorption edge.

## Interpretation

In order to better understand the structures of the measured RRS x-ray spectra, calculations of the resonant Raman scattering around the K absorption edge with a 2p vacancy in the final state were performed, using the formula of Kramers-Heisenberg [5, 6, 7]. For comparison with experimental data the theoretical RRS spectra were convoluted with the Gaussian instrumental broadening of the spectrometer ( $\sigma = 0.5$  eV) and the beam energy profile, assuming for the latter a Gaussian shape with a full width at half maximum of ~6 eV.

As an example, the Si RRS spectrum observed at an excitation energy of 1829 eV is compared with the corresponding convoluted theoretical spectrum (solid line) in Fig. 3. The cross sections of the different processes contributing to the observed profiles were also determined as a function of the beam energy, using the same theoretical calculations (Fig.4).

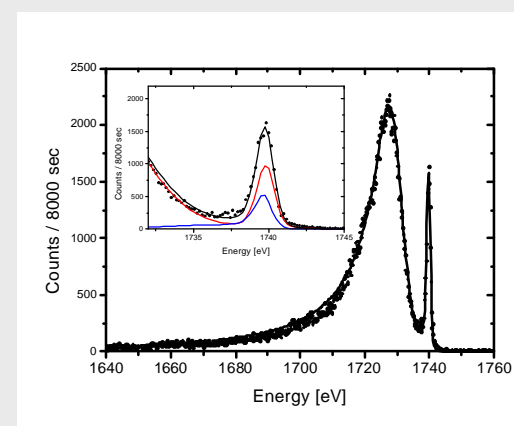


Fig. 3: High-resolution RRS spectrum of Si for an excitation energy of 1829 eV. The dots correspond to the experimental data, the thick solid line to the theoretical shape obtained from the calculations [6]. The inset shows the fluorescence line region with results of calculations for excitations to discrete (blue line) and continuum (red line) states.

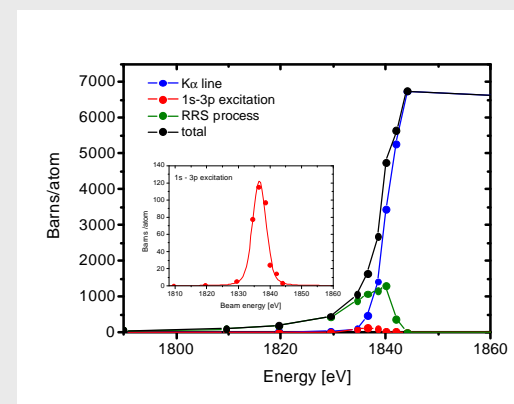


Fig. 4: Cross sections of interest around the 1s absorption edge. The 1s-3p excitation which could be fitted with a Voigt profile is shown enlarged in the inset.

In order to probe the influence of the chemical environment on the RRS x-ray spectra, similar high-resolution measurements were also performed with SiO<sub>2</sub>, Al and Al<sub>2</sub>O<sub>3</sub> samples. These data are being analysed. Significant differences are clearly observed between the metal and semiconductor samples, as well as between the elemental and oxide samples.

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