In order to develop a method to reconstruct the density of unoccupied electronic states in between Fermi energy and vacuum level, we performed combined anisotropic anomalous scattering and diffraction anomalous fine structure (AAS-DAFS) scans. For a model of the polarization dependence of resonant X-ray scattering (AAS) as well as dedicated nomenclature see e.g. [1]. Examining the energy dependence of the dipole-dipole transition near the Ti-$K$ absorption edge in rutile TiO$_2$ [2], special interest was given to the stability of the symmetry restrictions imposed by the Ti site symmetry $m\cdot m\cdot m$ on the dipole-dipole transition. Here we present new results, extending former findings from studying the sample orientation dependent, diffracted intensity on different allowed and forbidden reflections at the specific resonance photon energy of $E = 4985$ eV exclusively [3], in respect to the energy dependence.

Experiments were performed at beamline C1 (CEMO) and E2 (RÖMO) using a Si (111) double crystal monochromator and $\sigma$-polarized X-rays. An energy range of 4900 eV to 5200 eV was chosen. As samples we used 10 x 10 x 1 mm$^3$ rutile single crystal wafers provided by Crystec GmbH in (001) and (111) orientation. For a two dimensional intensity surface, in dependence of energy and $\Psi$-rotation about the scattering vector, we measured rocking curves at each grid point. The integrated intensities for the “forbidden” 001 and for the allowed 111 reflection are plotted in Fig. 1.

The overall shape of the $\Psi$-dependent intensity modulation does not change along the energy axis except by an energy dependent factor accounting for the oscillating contributions to the Ti atomic
scattering factor $f'_{ao}(E)$ and $f''_{ao}(E)$ of isotropic DAFS. Thus, the deformation tensors $D'(E)$ and $D''(E)$ of the atomic scattering factor tensor seem to change only slightly with varying energy.

Considering the diffraction anomalous fine structure the statement of constant deformation tensors $D(E)$ implies a scaling of the oscillating part of the normalized integrated reflection intensity with $Ψ$. For a detailed comparison we performed DAFS scans with an energy resolution of 1 eV along the principal directions [100] at $Ψ = 0°$ and [110] at $Ψ = 45°$ while simultaneously measuring the fluorescence X-ray absorption fine structure (XAFS) signal. The results, shown in Fig. 2, further support these findings.

The results of our experiments give strong evidence of constant second rank deformation tensors $D'(E)$ and $D''(E)$ for the Ti atomic scattering factor tensor in rutile following the AAS model of [1]. The scaling of the diffraction anomalous fine structure induced by these tensors does not alter the general modulation over energy.

References