PS15.03.02 ANISOTROPY OF ANOMALOUS SCATTER-ING: NEW EXPERIMENTAL EVIDENCE. A. Kirfel, Mineralogical Institute, University of Würzburg, and T. Lippmann, HASYLAB/DESY, Hamburg, FRG

Anisotropy of Anomalous Scattering (AAS) is caused by resonant X-ray scattering occurring in the vicinity of an absorption edge and giving rise to X-ray optical effects in both transmission and diffraction. The description requires a generalized scattering model which predicts the intensity variation and polarization properties of the scattered radiation upon rotation ψ of the crystal about the scattering vector [1]. As a special consequence, the excitement of 'forbidden' reflections systematically extinct due to screw axes and/or glide planes is of particular interest, because the observed signal allows direct experimental proof of the model, independent of size and complexity of the non-resonant scattering structure. This selectivity of scattering provides the opportunity of partial structure analysis, site discrimination in structures possessing non-equivalent cation sites, and the distinction of resonance type. New experimental evidence of the model validity is obtained by synchrotron radiation experiments. For Cuprite, Cu_2O, (Pn$\bar{3}$m), reflection *300* , by i) rotation of the polarization direction of the incident radiation about the beam axis, i.e. rotation of the scattering plane, and ii) direct polarization analysis by secondary reflection using Ge analyzer crystals. For orthorhombic Sodium Nitroprusside, $Na_2[Fe(CN)_5(NO)]$ $2H_2O$ (Pnnm), the intensity variations, $I(\psi)$, of several 'forbidden' axial reflections are used for an ab initio structure determination. Finally, the intensity patterns of AAS induced 'forbidden' reflections in cubic Magnetite, Fe_3O_4 (Fd$\bar{3}$m), clearly reveal that the observed signals are solely due to a mixed dipole-quadrupole transition in Fe^{3+} occupying the tetrahedral position ($\bar{4}$3m), whereas the octahedral site ($\bar{3}$m) fails to contribute significantly.

[1] KIRFEL, A., PETCOV, A. & EICHHORN, K. (1991). Acta Cryst. A47, 180-195.

PS15.03.03 INELASTIC X-RAY SCATTERING INVESTIGATION OF ELECTRON CORRELATIONS IN ALUMINUM. * B. C. Larson, Oak Ridge National Laboratory (ORNL); J. Z. Tischler, ORNL; E. D. Isaacs, AT&T Bell Labs; P. Zschack, Oak Ridge Associated Universities; A. Fleszar, Universität Würzburg; and A. G. Eguiluz, University of Tennessee and ORNL.

We have made inelastic x-ray scattering measurements of the dynamical structure factor $S(q,\omega)$ for aluminum using the X-14 beam line at the National Synchrotron Light Source (NSLS); these measurements have been used to make the first large-q determination of the many-body local-field factor $G(q,\omega)$ for this simple metal. Within a Hubbard-like model, the local field-factor (LFF) provides a measure of short-range electron-electron correlations, which have been the subject of extensive theoretical interest for over forty years. Experimental information on $G(q,\omega)$ at large-q has been lacking; however, we have used *ab initio* calculations of the electronic-response for non-interacting electron-hole pairs $\chi^{(0)}(q,\omega)$, including the band structure, to extract the real and imaginary parts of the LFF directly from inelastic x-ray scattering measurements. $G(q,\omega)$ has been found to be largely real and much stronger than predicted by theory, reaching a value ~2 for q ~ 2k$_F$. In addition, we have observed the polarizability for *non-interacting* electron-hole pairs, $\chi^{(0)}(q,\omega)$, at the "critical" wave vector for which $G(q,\omega) \approx 1$, and at large q, for which the effects of the electron-electron interactions become negligible. The analysis of $S(q,\omega)$ measurements made along the [013] and [001] directions for wave vectors from 0.7k$_F$ to 2.5k$_F$ will be discussed. RPA and $\chi^{(0)}(q,\omega)$ calculations will be used to illustrate the impact of long-range Coulomb interactions and short-range exchange-correlation effects on $S(q,\omega)$ as a function of wave vector.

PS15.03.04 ANISOTROPY OF ANOMALOUS SCATTER-ING: INVESTIGATION OF POLARIZED ABSORPTION BY FLUORESCENCE MEASUREMENTS. T. Lippmann, HASYLAB/DESY, Hamburg, A. Kirfel, University of Wurzburg, K. Fischer, University of Saarbrücken, FRG

Polarized X-ray absorption is examined both theoretically and experimentally by fluorescence measurements. Using the dipole approximation, the conventional scalar resonant scattering factors (and hence the absorption coefficient) are replaced by second-rank tensors. By application of the Jones-calculus an algorithm is developed, which includes both linear birefringence and dichroism, and provides a detailed representation of the fluorescence intensity for crystals exhibiting large faces. Moreover, neglecting birefringence and assuming not a too large relative dichroism, an adequate approximation is presented, which is applicable for most practical cases [1].

The experimental setup for a simultaneous determination of the absorption tensor elements depends on crystal system and face investigated. For the orthorhombic system, the geometrical prerequisites are discussed, and a fluorescence intensity function is developed and illustrated by model calculations.

Test experiments concerning various experimental geometries and polarization states of the primary radiation are carried out on different crystal faces of $LiHSeO_3$, showing results in good agreement with the theoretical considerations.

Additionally, polarized absorption spectra of $(NH_4)_9[Cu(S_2O_3)_4]Br_2$ as a further example of a synthetic compound and of two Amphiboles (Edenite and Hastingsite) as examples for iron bearing minerals are presented. The detection of orientational dispersion of the absorption tensor in these monoclinic crystals supports both the model and the experimental method.

[1] Lippmann, T., Kirfel, A., Fischer, K. (1996) J. Appl. Cryst. **29**, 1-12

PS15.03.05 RESONANT RAMAN SCATTERING: SPECTROSCOPY AND CRYSTALLOGRAPHY. C. J. Sparks, G. E. Ice, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6118, USA

Resonant Raman scattering which occurs near absorption edges can be both a useful spectroscopy of the chemical state and a background nuisance in the measurement of weak diffuse scattering. This resonant inelastic scattering arises from the promotion of a bound electron into an unfilled bound state and is a measure of the unfilled density of states in the presence of a core hole. Some applications of this new spectroscopy will be reviewed and compared with other spectroscopies. This resonant radiation emission has a nonradiative counterpart in Auger electron emission which is also developing into a useful spectroscopy. Those interested in the measurement of diffusely distributed intensity associated with liquids, amorphous solids, short-range order and defects need be aware of this inelastic scattering contribution to your signal; Resonant Raman scattering is most intense when the incident radiation is just below the absorption threshold to maximize elemental contrast with the resonant (dispersion) terms of the x-ray atomic scattering factor. The magnitude of resonant Raman scattering will be illustrated by comparing its cross section to the cross section for Compton and elastic scattering. Means to deal with the inelastic scattering are described.