Determination of anomalous scattering factor near Ge-K absorption edge used by phase change method

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The anomalous scattering factor ($f'+if''$) (ASF) of X-ray resonant scattering changes remarkably near an absorption edge of an atom. It is well known that this change is significant for the phase determination of crystal structure factor and the study of X-ray magnetic scattering. ASF near the absorption edge is so sensitive to the conduction band structure and the lifetime of intermediate transition process that it is not easy to evaluate it theoretically. Thus, it is interesting to investigate the consistency between the calculated ASF and the measured one. When the sign of Fourier coefficient χ_{hr} (χ_{hi}) of real (imaginary) part of X-ray polarizabilty changes, a conspicuous change of asymmetry in rocking curves (Fig.1) can be seen in a perfect crystal. We have studied the phase changes of χ_{hr} (or f^0+f', f^0 is the normal atomic scattering factor) using rocking curves for 660, 555 and 844 reflections of Ge at BL-15C in KEK-PF. At the boundary of the phase change, the condition of $f^0+f'=0$ can be found experimentally. Then the value of f' can be determined with good precision using the well-known calculated value of f^0.

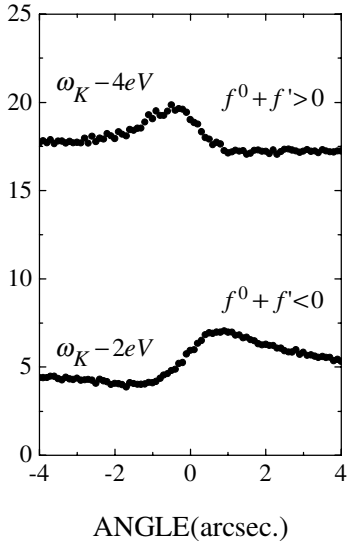

Fig.1 Observed rocking curves of Transmitted-beam for Ge 844. ω_K is the energy of Ge K-absorption edge (11103.6eV).

The calculated and measured ASFs are shown in Fig.2. The thin solid line (corrected by lifetime) and the dotted one (without correction) are obtained according to the isolated atom model (IAM). The thick solid line and the open circles are obtained as follows. f' for the former is determined by the dispersion relation (DR)[1)] and for the latter by the phase change method (PCM), whereas f'' is determined from the measured XAFS in both cases. It is clear that the value of f' determined by the PCM is different from that calculated by the IAM , but is in excellent agreement with that obtained by the DR.

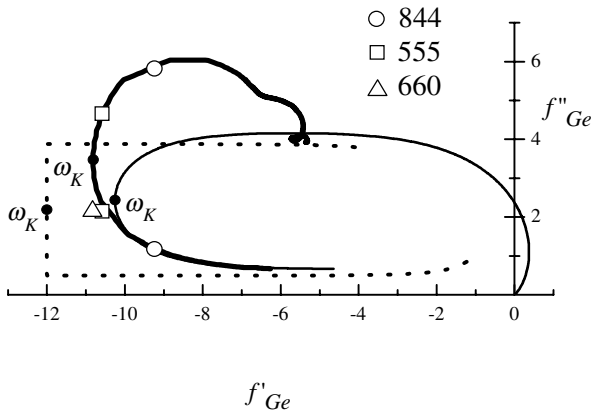

Fig.2 The calculated and measured ASF. The thin solid line is calculated by Parratt and Hempstead formula[2)]. The dotted line is calculated by Sasaki[3)].

References

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