Multiple-wave X-ray Diffraction at Resonance: An Iterative Born Approximation

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The experiments were carried out at wiggler beamline, 17B, NSRRC and SP12B2 Spring 8. A $[111]$ cut GaAs single crystal is used as a sample crystal. The diffracted intensity of three-beam $(222)/(1\bar{1}3)$ case, as well as fluorescence yield was measured for the photon energies covering the Ga K and As K edges. Consider a three-wave (O,G,L) X-ray diffraction, in which O, G and L are incident, primary and secondary reflections, respectively. The fundamental equation can be expressed in terms of the electric displacement $\vec{D}$:

$$\begin{cases} 2\varepsilon_0 D_0 = x_0 D_{0[0]} + x_{0-G} D_{G[0]} + x_{0-L} D_{L[0]} \\ 2\varepsilon_0 D_G = x_{G-0} D_{0[G]} + x_0 D_{G[G]} + x_{G-L} D_{L[G]} \\ 2\varepsilon_L D_L = x_{L-0} D_{0[L]} + x_{L-G} D_{G[L]} + x_0 D_{L[L]} \\ where \\ D_{Hi[Hj]} = -[\overrightarrow{K_{Hj}} \times (\overrightarrow{K_{Hj}} \times \overrightarrow{D_{Hi}})] \end{cases}$$

With a third-order Born approximation:

$$D_G^{(3)} \cong A_G x_{G-O} D_G^{(2)} + A_G A_L |x_{L-O}\| x_{G-L}| D^{(2)}_{O[L][G]} - A_G A_O A_L |x_{G-O}\| x_{L-O}\| x_{O-L}| D^{(2)}_{O[L][O][G]} - A_G^2 A_L |x_{G-O}\| x_{L-G}\| x_{G-L}| D^{(2)}_{O[G][L][G]}$$

Where the resonance tem $A_H = \dfrac{1}{2\varepsilon_0 - \chi_0}$, $2\varepsilon_H = \dfrac{K_H^2 - k^2}{K_H^2}$ $(H \equiv O,G,L)$

k is the magnitude of the incident wavevector in vacuum and K_H are the magnitudes of diffracted waves in the crystal. The three-wave intensity is then given by:

$$I_G^{(3)}(\psi_u) = I_G^{(2)} + I_D(\delta_3, \psi_u) + I_I(\psi_u) \quad (3)$$

$I_G^{(2)}$ is the two-wave intensity, $I_D(\delta_3, \psi_u)$ is the phase dependent part of the three-wave intensity and $I_I(\psi_u)$ is its phase independent part. Experimentally, the fluorescence yield and multiple-wave diffraction intensities as a function of the Bragg angle and azimuth angle of rotation of a symmetric Bragg primary reflection were measured. The asymmetric intensity ratio Rv of three-wave diffraction is defined as $R_V = (I_2 - I_{\min})/(I_{\max} - I_2)$, where $I_{\max}$ and $I_{\min}$ are the maximum and minimum intensities of three-wave diffraction measured. Rv is used for both theoretical and experimental analysis. The real part f' and imaginary f'' of dispersion corrections on the atomic scattering factors versus the photon energy are deduced then from Rv (See Fig.1), where f' can be obtained via 2-dimension interpolating surface splines. Finally, the fine structure function χ can be determined from f' and f''. The experimental and theoretical x 's are shown in Fig. 2.

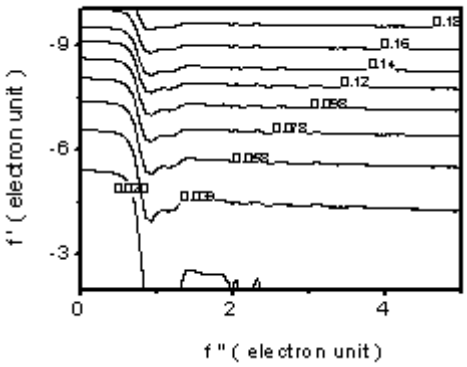

Figure 1. 3-Dimension distribution of theoretical Rv

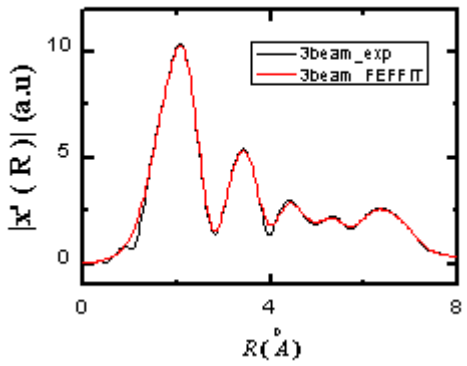

Figure 2. The structure function x.