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Anomalous Scattering Factor near Absorption Edge of Ge

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The measured anomalous scattering factor (ASF, $f' + if''$) near Ge K absorption edge traces a circular arc as shown in Fig.1[1)]. According to the quantum theory of X-ray resonant scattering, ASF can be given by the following equation in case of only one resonant mode,[2)]

$$f' + if'' \propto -1 / (\Delta\omega + i\Gamma / 2) \quad . \qquad (1)$$

Where, $\Delta\omega = \omega_n - \omega$, ω_n is resonant energy and Γ is the natural width of spectrum. The circle-like locus of $f' + if''$ in Fig.1 can be obtained by changing $\Delta\omega$. If the energy of the initial peak just above the edge in f'' curve in Fig.2 is assigned to be ω_M and its height $\Delta f''_M$ after subtracting the background to be the diameter of the circle in Fig.1, the following equation can be derived from equation (1)

$$\Delta f' + i\Delta f'' = -\Delta f''_M / (x + i) \quad . \qquad (2)$$

Where $x = 2(\omega_M - \omega) / \Gamma$ and $\omega_M = \omega_K + \Gamma / 2$. Equation (2) is rewritten as

$$\Delta f' = -x\,\Delta f''_M / (x^2 + 1), \quad \Delta f'' = \Delta f''_M / (x^2 + 1). \qquad (3a,b)$$

In order to get the ASF ($f'_C + if''_C$) in a real crystal, it is necessary to add $\Delta f' + \Delta f''$ to the values calculated by the isolated atom model (IAM). That is

$$f'_C = \Delta f' + f'_{atom}, f''_C = \Delta f'' + f''_{atom} . \qquad (4a,b)$$

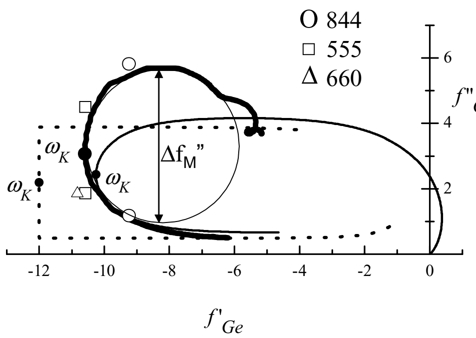

Fig.1 The Locus of the ASF in Ge. O □ Δ (zero crossing method) and thick solid line (dispersion relation) are measured values. The dashed line and solid line are calculated values of the IAM with CLS[3)] and PH[4)].

Here f'_{atom} and f''_{atom} are the real and imaginary parts of ASF given by the IAM. In the ASF of Ge crystal, $\Delta f''_M$ is determined to be 5.38 and $\Gamma / 2$ is evaluated to be 2.5±0.5 eV. This value is five times larger than the calculated value (0.5eV) by using classical damping. From this result, the lifetime ($\tau = h / 2\pi\Gamma$) of the intermediate state is estimated to be 0.13±0.03 fs. Then f'_C and f''_C (thick solid line) are obtained and shown in Fig.2. The ASFs determined by zero crossing method , the dispersion relation method (solid line) and the IAM[3)] (dashed line) are shown in Fig.2. It is clear that the values of f'_C obtained by the present method are in good agreement with the zero crossing method and the dispersion method.

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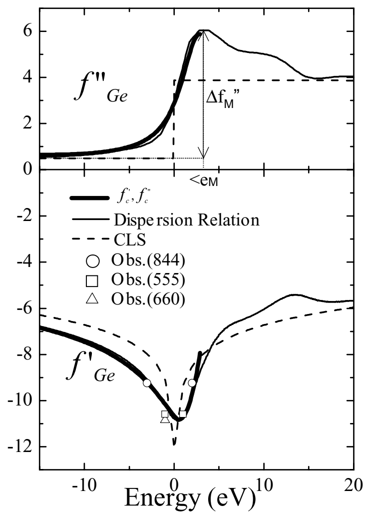

Fig. 2 The measured and the calculated ASF.

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