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Temperature diffuse scattering for cubic powder patterns.*

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In measuring the short range order diffuse scattering from powder patterns of binary alloys, the correction for temperature diffuse scattering becomes very important, particularly if the sample is held above the critical temperature. The correction is sometimes made by assuming that for powder patterns the approximation of independent vibrations is adequate:

$$I_{TD} = NI_e f^2(1-e^{-2M}) . \quad (1)$$

The rigorous theory of temperature diffuse scattering of X-rays is available (James, 1948), and by a few approximations it is possible to compute a temperature diffuse scattering curve for cubic powder patterns which is a much better approximation than equation (1).

From James, equation (5·45),

$$I_{TD} = NI_e f^2 e^{-2M} \frac{kT}{m} \frac{|\mathbf{R}|^2}{|\mathbf{g}|^2} \sum_j \frac{\cos^2 \alpha_{Rj}}{V_{\varphi j}^2} , \quad (2)$$

where, for an element: N is the number of atoms, I_e the Thomson scattering per electron, f the atomic scattering factor, $2M$ the usual Debye factor, k the Boltzman constant, T the absolute temperature, m the mass of the atom, $|\mathbf{R}|$ $(= 2 \sin\theta/\lambda)$ the diffraction vector drawn from the origin of the reciprocal lattice to the position of measurement, $|\mathbf{g}|$ $(= 1/\Lambda)$ the vector from the nearest relevant reciprocal-lattice point to the position of measurement and equal to the reciprocal of the wavelength of the elastic wave, $V_{\varphi j}$ the velocity of the elastic wave φj, α_{Rj} the angle between $\mathbf{R}$ and the vibration direction of wave φj, and $\sum_j$ the summation over the three independent waves. By assuming that all elastic waves have the same average velocity V, that $2M$ is small, and that each Brillouin zone can be replaced by a sphere of equal volume, (2) becomes

$$I_{TD} = NI_e f^2(1-e^{-2M}) g_{\max.}^2/3g^2 . \quad (3)$$

Within any Brillouin zone, g is expressed by $g^2 = R^2+R_{hkl}^2-2RR_{hkl}\cos\varphi$, where R_{hkl} is the vector from the origin to the center of zone hkl. The contribution to the powder pattern intensity, at fixed $|\mathbf{R}| = 2\sin\theta/\lambda$, from one Brillouin zone is then given by

$$I_{TD} = NI_e f^2(1-e^{-2M}) \frac{g_{\max.}^2}{6} \int_0^{\varphi_0} \frac{\sin\varphi d\varphi}{R^2+R_{hkl}^2-2RR_{hkl}\cos\varphi} , \quad (4)$$

where φ_0 is determined by $g_{\max.}^2 = R^2+R_{hkl}^2-2RR_{hkl}\cos\varphi_0$. Multiplying by the appropriate multiplicity factor j_{hkl}, and adding values from all Brillouin zones which contribute at a fixed value of $|\mathbf{R}|$, gives the powder pattern intensity.

As an example consider a face-centered cubic element. In this case $g_{\max.} = (3/\pi)^{1/3}/a$, where a is the edge of the cubic cell. In terms of the general variable $x = 2a\sin\theta/\lambda$ and the values $x_{hkl} = 2a\sin\theta_{hkl}/\lambda$ for each unmixed hkl, the ratio of I_{TD} to that for independent vibrations is given by

$$\frac{I_{TD}}{NI_e f^2(1-e^{-2M})} = \frac{(3/\pi)^{2/3}}{6x} \sum_{hkl} \frac{j_{hkl}}{x_{hkl}} \ln\left[\frac{(3/\pi)^{1/3}}{|x-x_{hkl}|}\right] . \quad (5)$$

Fig. 1 is a plot of (5). Within the accuracy of the approximations used, it is a general temperature diffuse scattering curve for the powder pattern of any face-centered cubic element. The old theory involving independent vibrations of the atoms is represented on this plot by the horizontal line at height unity. Averaged over wide ranges of 2θ, the computed intensity is roughly equal to that for independent vibrations. In the immediate vicinity of each hkl reflection, the diffuse intensity rises to high sharp peaks, which are of course hidden by the powder-pattern lines. Outside of the hidden region, there is a modulation of the order of 30% above and below the independent scattering curve. Since short-range order and size-effect determinations (Warren, Averbach & Roberts, 1951) are based on modulations in the diffuse intensity, it is obvious that the approximation of independent vibrations represented by (1) is in many cases inadequate for correcting powder-pattern intensities. For body-centered cubic elements, a curve similar to Fig. 1 is readily constructed. By using an appropriate average $\langle f^2 \rangle$, the curves can be used for correcting the temperature diffuse scattering from disordered binary alloys.

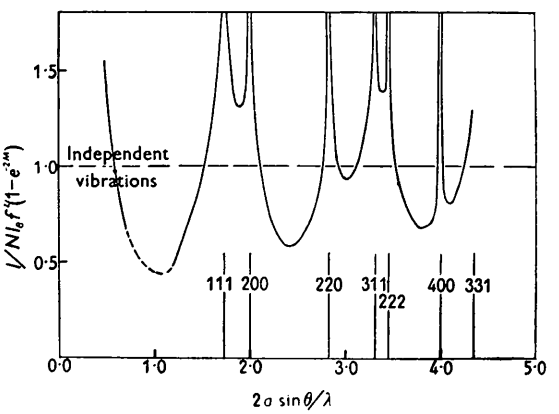

Fig. 1. Approximate temperature diffuse scattering curve for the powder pattern of a face-centered cubic element, expressed in units of the scattering for independent vibrations of the atoms.

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