Short Communications

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Gaussian *versus* Lorentzian distribution for the mosaic spread in single crystals.

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For accurate X-ray or neutron diffraction intensity measurements the mosaic spread of a single crystal should be small. Plots are given from which the quality of the crystal can be checked and from which the scan range can be calculated.

In X-ray and neutron diffraction intensity measurements the required scan range (and counter aperture) depend on the mosaic spread of the crystal. Generally for accurate measurements small mosaic spread values are needed. However, if the peak intensity becomes large the crystal will suffer severely from extinction. To obtain a 1% accuracy in the intensity measurements, one should take the scan range (and the counter aperture) such that 99% of the intensity is observed. The scan range m required to account for the mosaic spread can easily be calculated for a Gaussian and a Lorentzian distribution given by respectively

$$P_G(\omega)=g_G\sqrt{2}\exp\left[-2\pi g_G^2(\omega-\omega_0)^2\right] \quad (1a)$$

and

$$P_L(\omega)=2g_L/[1+4\pi^2(\omega-\omega_0)^2g_L^2]\,. \quad (1b)$$

From (1*a*) and (1*b*) we obtain

$$m_G=2{\cdot}06/P_G(\omega_0)=1{\cdot}46/g_G \quad (2a)$$

and

$$m_L=40{\cdot}52/P_L(\omega_0)=20{\cdot}26/g_L\,. \quad (2b)$$

If, on the one hand, m is equal for the two distributions $P_L(\omega_0)=19{\cdot}67P_G(\omega_0)$. Thus a crystal having a Lorentzian distribution for the mosaic spread will more readily suffer from extinction than a crystal with a Gaussian one. If, on the other hand, $P_L(\omega_0)\simeq P_G(\omega_0)$ m_L will be considerably larger than m_G. From this we see that for accurate measurements a Gaussian distribution of the mosaic spread is preferred.

Experimental

We have determined the angular distribution of the crystallites in KIO_3 and deutero-2,5-dimethyl-3-hexyn-2,5-diol (III-D, H atoms of OH not replaced by D). To this end the profiles of some reflexions were measured by the ω-technique (stationary counter, moving crystal) with a 0·33° counter slit. From (1*a*) and (1*b*) it follows that

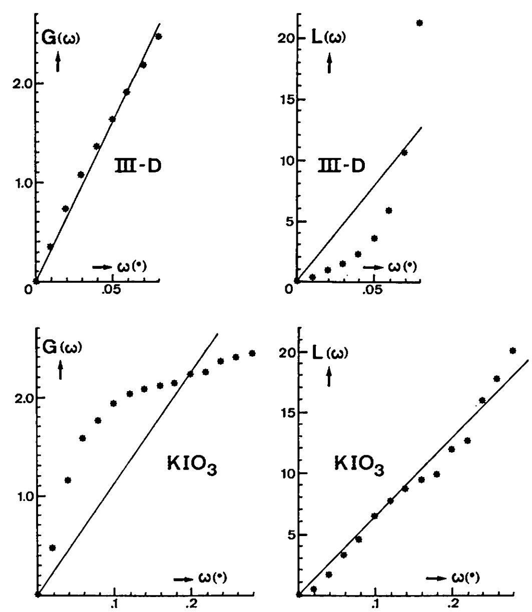

Fig. 1. Plots of $G(\omega)$ and $L(\omega)$ (see text) for III-D and KIO_3.

$$G(\omega)\equiv\sqrt{\ln\,[I(\omega_0)/I(\omega)]}=g_G\sqrt{2\pi}|\omega| \quad (3a)$$

$$L(\omega)\equiv\sqrt{\{[I(\omega_0)/I(\omega)]-1\}}=2\pi g_L|\omega| \quad (3b)$$

with $I(\omega_0)$ the intensity at the profile maximum.

In Fig. 1 observed values for these quantities have been plotted. The experiment shows that for the III-D crystal the mosaic spread can be perfectly described by a Gaussian with $m_G=0{\cdot}11°$ whereas in KIO_3 it satisfies a Lorentzian distribution with $m_L=1{\cdot}99°$.

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