ANISOTROPIC STRAIN-LIKE LINE BROADENING DUE TO INHOMOGENEITIES

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If, in a solid solution, there is a considerable variation of the lattice parameters with composition, inhomogeneities within a sample can exhibit themselves by a broadening of reflection profiles [1]. This has been applied for interdiffusion studies (e.g. [2]), but also for the estimation of homogeneity of powder samples [3]. Until now such studies concerned primarily cubic substances.

In the present paper the broadening due to composition inhomogeneities - but neglecting concentration gradients within coherently scattering domains - is derived for all crystal systems. In general an anisotropic apparent strain-like diffraction line broadening occurs. The extent of anisotropy can be correlated with the anisotropy of the concentration dependence of lattice parameters. For the case of a pseudo-Voigt-like distribution of composition, the broadening ends up as a special case of the more general strain-broadening model derived in Ref. [4]. If only inhomogeneity broadening is present, in the triclinic case the 15 strain parameters S_{HKL} from [4] can be reduced to six parameters. The new model can also be considered to be applicable for broadening caused by gradients of temperature or of hydrostatic pressure.

For a hexagonal ε-iron nitride powder with the average composition ε-$Fe_3N_{1.30}$ produced by gas nitriding (NH_3/H_2 mixture) an anisotropic strain-like broadening was observed, whereas size-broadening was apparently negligible. The well known lattice parameter dependence of the hexagonal lattice parameters *a* and *c* is consistent with the extent of anisotropy observed and the (nearly Gaussian) composition variation can be expressed as $Fe_3N_{1.30\pm0.03}$. A Rietveld refinement (JANA2000 [5]) fitting the three symmetry allowed strain parameters S_{400}, S_{004} and S_{202} of the general model [4], showed, that - as it is expected from the inhomogeneity broadening model - the resulting value for S_{202} can be calculated from the other two values, S_{400} and S_{004}.

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