Different aspects of microstrain broadening

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Microstrain broadening is – besides crystallite-size broadening – one of the most frequently observed and discussed line-broadening contributions exhibited by polycrystalline materials. Microstrain broadening is, for a certain direction of the diffraction vector, characterised by a d^*-dependent increase of the reflection width on the d^* scale, whereas for crystallite-size broadening the reflection width is constant. If it is sufficient to regard the reflection *hkl* as generated by incoherent superposition of the diffraction effects of crystals having parallel sets of lattice planes *hkl*, the Fourier coefficients A^D (D: distortion as an alternative expression for strain) of the line-broadening contribution due to microstrain are

$$A^{D,hkl}\left(L\right)=\int_{-\infty}^{\infty}p\left(\varepsilon_{hkl}\left(L\right)\right)\cos\left(2\pi L\left\langle d_{hkl}^{*}\right\rangle\varepsilon_{hkl}\left(L\right)\right)d\varepsilon_{hkl}\left(L\right), \qquad (1)$$

where L is the a length perpendicular to the lattice planes and $\varepsilon_{hkl}(L)$ is the strain averaged over this length and $\left\langle d_{hkl}^{*}\right\rangle$ is the inverse (specimen) average *d*-spacing of the reflection *hkl*, and $p(\varepsilon_{hkl}(L))$ is the probability density function of $\varepsilon_{hkl}(L)$. There are various sources for microstrain distributions: occurrence of dislocations, elastic incompatibility stresses as occurring after plastic deformation but also due to anisotropic thermal expansion, inhomogeneities in various physical “fields” like composition, temperature etc.

In this presentation the current state of treatment of microstrain broadening is reviewed with special emphasis on the authors’ contributions:

(i) The special role and the problem of validity of the Stokes-Wilson approximation will be discussed, i.e. that $p(\varepsilon_{hkl}(L))$ is independent of L. In this case it follows directly from Eq. (1) that for a certain direction of the diffraction vector the line-width of the microstrain contribution to a Bragg peak it proportional to $\left\langle d_{hkl}^{*}\right\rangle$ on the d^* scale, or proportional to $\tan\langle\theta_{hkl}\rangle$ on the 2θ scale.

(ii) Within the Stokes-Wilson approximation various approaches exist to deal with the *hkl*-dependence of the line-broadening effects, either phenomenologically or in relation with specific physical models. In the latter case, it is often possible to trace back the microstrain broadening and its anisotropy to a microstrain distribution, which originates from the (local) variation of a “field tensor” (e.g. stress, composition, temperature) connected with strain via a property tensor (compliance, compositional-strain tensor).

(iii) In general, $p(\varepsilon_{hkl}(L))$ may have a more or less arbitrary functional shape, whereas it is often simply taken as a Gaussian (Warren-Averbach approach). Possibilities to deal with more complex $p(\varepsilon_{hkl}(L))$ will be reviewed. Special cases, where (apparently) Lorentzian-shaped microstrain broadening occurs, will be discussed.