PEAK PROFILES FROM FAULTING IN SMALL DOMAINS

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The existence of stacking faults in a crystallite is known to influence the x-ray powder diffraction peak profile by systematically shifting, and asymmetrically broadening the peak to different degrees depending on the fault type and probability. In the theory describing the peak profile due to faulting it is common to assume that the crystallite is infinite, and then introduce a separate size effect at a later stage. This approach carries with it the assumption that the truncation of the crystallite stacking sequence at the surface has a negligible influence on the effect of faulting. While this is approximation maybe acceptable for large crystalline domains, it becomes less valid as the domain size decreases.

The present study will then explicitly demonstrate how a nearby surface influences the effect of faulting on the powder diffraction peaks. Relations describing how the resulting peak profile changes with the position of the fault in a finite columnar stack will be given. Also, the profiles from an average fault position will be compared with the profile calculated using current theory which describes the faulting effect neglecting the influence of the surface. This work is important to give insight into how the effects of faulting in nanoscale materials are observed differently by diffraction than that from materials with larger crystallite sizes.