

COMPARISON OF SIMULATED AND EXPERIMENTAL XRPD PATTERNS OF Ag WITH TWIN FAULTS USING MAUD AND DIFFAX

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X-ray powder diffraction patterns of face-centered cubic Ag with twin faults were simulated using the DIFFaX¹ program and the Maud² Rietveld refinement program. Maud was used to refine the DIFFaX-generated patterns to determine systematic differences between these computation methods. Comparison of Maud and DIFFaX indicated the Warren³ model of twin faults was appropriate for relatively low fault probabilities. Experimental patterns of nanocrystalline silver with stacking faults were characterized with DIFFaX and Maud. The intensity relationship of the Bragg intensity and diffuse scattering was consistent with a heterogeneous distribution of twin-fault probabilities. A method of estimating the relative twin-fault abundance from the relative peak intensity of diffuse and Bragg scattering was developed.

¹ M. M. J. Treacy, J. M. Newsam and M. W. Deem, A General Recursion Method for Calculating Diffracted Intensities from Crystals Containing Planar Faults, *Proc. R. Soc Lond.* **A433**, 499–520 (1991).

² L. Lutterotti, S. Matthies and H- R. Wenk, MAUD (Material Analysis Using Diffraction): a user friendly {Java} program for {Rietveld} Texture Analysis and more, Proceeding of the Twelfth International Conference on Textures of Materials (ICOTOM-12), **1**, 1599 (1999).

³ B. E. Warren, X-Ray Diffraction, Addison-Wesley, Menlo Park, CA (1969, 1990).