Contribution of symmetrized projections in HREM analysis for the characterization of $Ca_{1-x}Cd_xWO_4$ crystal microstructures

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To understand the role of crystal structures and local ordering states in the photonic properties of a system (1-x)$CaWO_4$ - x$CdWO_4$ with $0 < x < 1$, two phases with specific compositions x=0.5 (tetragonal scheelite) and 0.8 (monoclinic wolframite) were studied. Associated with microdiffraction and selected-area-electron-diffraction experiments (SAED), we show here an additional method in crystallographic image processing (CIP) based on the analysis of the symmetrized experimental HREM maps.

The powder samples, obtained by co-precipitation method, were at first analyzed and refined by XRD then by electron microscopy using a LaB6 Tecnai G20 (super-twin objective lens) with 0.25 nm point-to-point resolution at 200kV.

For the composition x = 0.5, the microdiffraction and SAED results converged to three possible space groups: Pc, P2/c and $P2_1/c$. A way to find the right one consisted in identifying the symmetry projections of HREM images in the main zone axes. From an experimental map recorded along [001], three images were processed by imposing the relative symmetry projections p11m (Pc), p2mm (P2/c) and p2gm ($P2_1/c$) to the amplitudes and phases of diffracted waves in the FFT. The projection p2mm clearly showed the best agreement with the experimental data.

The HREM features were compatible with the existence of average atoms Ca_{1-x}/Cd_x and argue in favor of total disorder of these sites, as suggested by XRD data. Also, no extra-reflection was observed in electron diffraction meaning both compounds can be considered as crystallized disordered solid solutions.