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Comparison of LiF and NiO crystallographic structure using XRD JAIME MOYA, NUWANJULA SAMARASINGHA, STEFAN ZOLLNER, New Mexico State University — Using x-ray diffraction (XRD), the crystallographic structures of LiF and NiO powders and single crystals were compared. Two types of scans were taken: ω -2 θ scans were taken for both the powders and single crystals, and ω (rocking) scans were taken for the single crystals. LiF is of the face-centered cubic rock salt structure, whereas NiO contracts along the [111] direction producing a rhombohedral (hexagonal) crystal structure. Therefore, the cubic (222) peak splits in bulk NiO into hexagonal (006) and (202) peaks. From the ω -2 θ NiO powder scans, no splitting of the c(222) peak is observed because the NiO is a nano-powder, preferring high symmetry orientations. The ω -2 θ peaks are broader in NiO because the grain size is smaller in the NiO than in LiF powders. The rocking curve scans of the c(222) peaks show that the crystals have multiple domains.

Jaime Moya New Mexico State University

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