Poster Presentation

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Visualizing Structural Modulation in Melilite Electrolytes by X-ray and Electron

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Nowadays novel melilite-type oxides are of growing interest as promising new oxide-ion conductors with potential use in clean energy devices such as solid oxide fuel cells (SOFCs).[1] These oxides have a general formula of A2BC2O7, where A = large divalent alkali earth metals like Ca, Sr, Ba or trivalent rare earth metals like La, Nd, Gd; B and C = small cations like Mg, Si, Ga. In addition to the conventional tetragonal symmetry with space group P^{-}421m, these melilites also show a five-dimensional superspace symmetry P^{-}421m(α, α, 0)00s($^{-}$α, α, 0)000 with modulation vectors q1=α(a*+b*) and q2=α(-a*+b*). Both displacive (cation and anion) and occupational (cation) modulations have been found.[2-3] Here a series of melilite single crystals, such as Ca2MgSi2O7, SrLaGa3O7, SrGdGa3O7, BaLaGa3O7 and CaNdGa3O7 have been successfully obtained using the optical floating zone and Czochralski method. Further investigations were made by a combination of temperature-variant X-ray diffraction and electron microscopy. The mechanism between substitutions in A- and B- sites and structural modulations in melilites is clarified, which paves the way for future crystallographic optimization of electrolyte performances via tailoring interstitial oxygen concentration and enhancing ion mobility.

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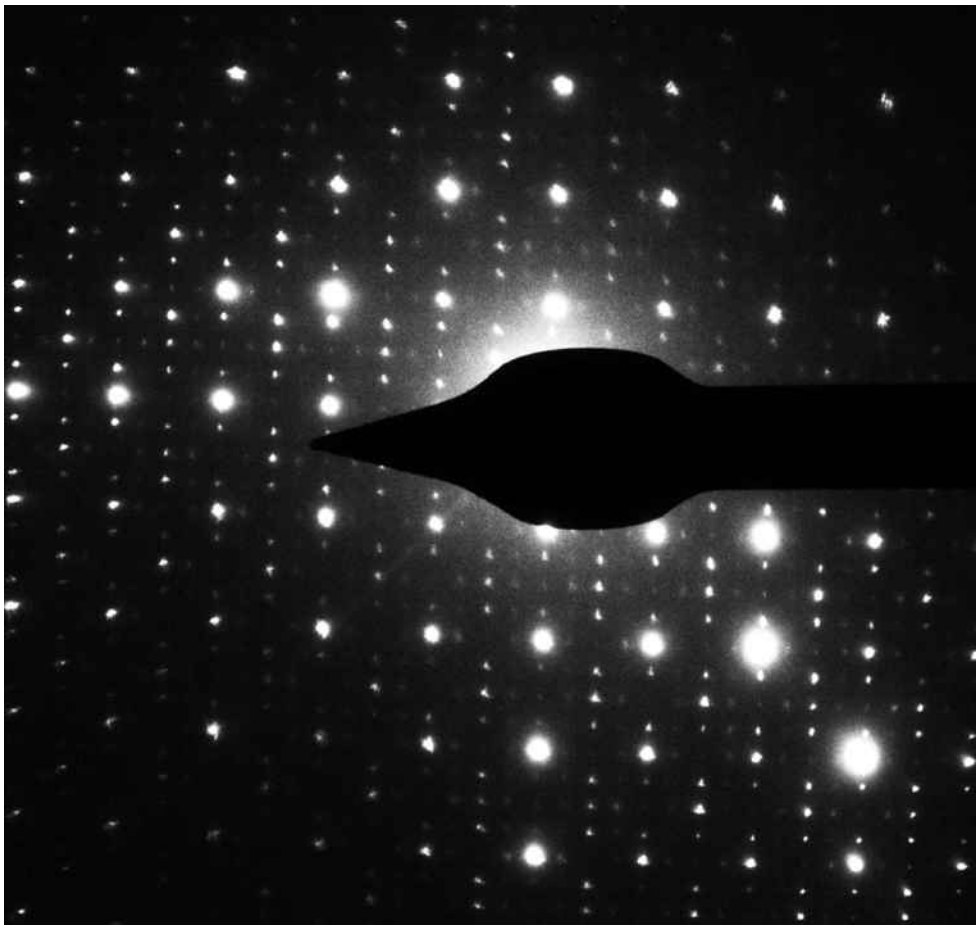

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