Stony Brook University
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Doctoral Defense Announcement

Abstract

Structure and Elasticity of NaMgF3 and CaIrO3 at High Pressures and Temperatures—the Perovskite and Post-Perovskite Structure Model of MgSiO3 Investigated with Rietveld Structure Refinement and Ultrasonic Interferometry.

By

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Perovskite-structured $MgSiO_3$ dominates the mineralogy of Earth's lower mantle. As a result, the physical properties and phase transitions of this mineral are key to understanding anomalous seismic observations of the mantle's lowermost 150-300 km—the D" region. Recent literature suggests a post-perovskite phase of $MgSiO_3$, experimentally observed at pressures and temperatures consistent with those expected to exist at D", is at least partially responsible for observed seismic anisotropy. While characterizing the crystal-chemistry, structure, and elastic properties of these two mineral phases *in situ* at high pressure and temperature would immediately shed light on this enigmatic region of the Earth, many conventional experimental apparatus are unable to reproduce these extreme conditions in the laboratory. Thus, measurements of the solubility of trace elements, the elastic changes with pressure and temperature, and the Clapeyron slope between perovskite and post-perovskite phases are in desperate need; however difficult or impossible to perform on $MgSiO_3$ directly. In this dissertation, we address structure changes at high pressure and temperature occurring in materials analogous to $MgSiO_3$ with perovskite and post-perovskite structure, considering that conclusions drawn from this research will prove useful to a subsequent understanding of the elastic, rheological, and crystal-chemical properties of $MgSiO_3$.

Neighborite ($NaMgF_3$) is isostructural to orthorhombic (*Pbnm*) $MgSiO_3$ perovskite. On the basis of X-ray diffraction data, previous research by Yusheng Zhao *et al.* has shown that increasing temperature, or potassium substitution for sodium in the structure, drives an evolution in the average structure (> 100 Å) towards a perovskite with cubic ($Pm\bar{3}m$) symmetry. Through utilization of pair-distribution function analysis and nuclear magnetic resonance spectroscopy, experimental techniques sensitive to short-range structure (< 20 Å), we show that when the average structure appears cubic with X-ray diffraction the local structure remains orthorhombic.

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