## In situ powder neutron diffraction of cation partitioning vs. pressure in Mg<sub>0.94</sub>Al<sub>2.04</sub>O<sub>4</sub> synthetic spinel

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## ABSTRACT

Powder neutron diffraction [ISIS Facility (U.K.), POLARIS diffractometer] was used to investigate the effect of elevated pressure on cation partitioning in synthetic  $Mg_{0.94}Al_{2.04}O_4$  spinel. The distributions of Mg, Al, and vacancies were studied as a function of pressure, by refinement of the Tand M-site scattering lengths, and determination of the cation partitioning through numerical minimization methods. The partially disordered Mg/Al distribution, which results from the synthesis process, show an increase in ordering between 6 and 18 kbar, where Mg and Al order to the T- and Msites, respectively. Pressure effectively tends to stabilize MgAl-spinels with a "normal structure," and this behavior is supported by numerical simulations based on classical electrostatic calculations.