

In situ powder neutron diffraction of cation partitioning vs. pressure in $\text{Mg}_{0.94}\text{Al}_{2.04}\text{O}_4$ synthetic spinel

ALESSANDRO PAVESE,^{1,*} GILBERTO ARTIOLI,¹ AND STEVE HULL²

¹Dipartimento di Scienze della Terra, Università di Milano, I-20133 Milano, Italy

²Rutherford Appleton Laboratory, ISIS Facility, Chilton-Didcot, Oxfordshire, OX11 0QX, U.K.

ABSTRACT

Powder neutron diffraction [ISIS Facility (U.K.), POLARIS diffractometer] was used to investigate the effect of elevated pressure on cation partitioning in synthetic $\text{Mg}_{0.94}\text{Al}_{2.04}\text{O}_4$ spinel. The distributions of Mg, Al, and vacancies were studied as a function of pressure, by refinement of the T- and 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 M-sites, 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.