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Hexagonal $Na_{0.41}[Na_{0.125}Mg_{0.79}Al_{0.085}]_2[Al_{0.79}Si_{0.21}]_6O_{12}$ (NAL phase): Crystal structure refinement and elasticity†

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Abstract

At lower mantle conditions, subducted mid oceanic ridge basalts (MORB) will crystallize more than 20 vol% of an aluminum-rich phase, which is referred to generally as the new aluminum (NAL) phase. Given that a significant proportion of the lower mantle may be comprised of subducted crust, the NAL phase may contribute to the bulk elastic properties of the lower mantle. In this study we report for the first time the structure, Raman spectrum and elasticity of single crystals of $Na_{0.41}[Na_{0.125}Mg_{0.79}Al_{0.085}]_2[Al_{0.79}Si_{0.21}]_6O_{12}$ NAL phase, synthesized at 2260 °C and 20 GPa. The single-crystal structure refinement of NAL, which is consistent with the space group $P6_3/m$, reveals dynamic disorder of Na atoms along channels within the structure. The elastic tensor was experimentally determined at ambient conditions by Brillouin scattering spectroscopy. The elastic modulii obtained from the Voigt-Reuss-Hill approximation using the elastic constants determined in this study are K_S = 206 GPa and μ = 129 GPa, whereas the isotropic compressional and shear sound velocities are v_P = 9.9 km/s and v_S = 5.8 km/s. The NAL phase is elastically anisotropic, displaying 13.9% compressional and shear wave anisotropy. Elastic constants as well as Raman active modes of NAL have also been calculated using density-functional theory and density-functional perturbation theory.

Keywords: NAL phase, Brillouin spectroscopy, single-crystal X-ray diffraction, lower mantle, elasticity