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The effect of the hedenbergitic substitution on the compressibility of jadeite

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Abstract

Four synthetic crystals belonging to the jadeite (Jd, $NaAlSi_2O_6$)-hedenbergite (Hd, $CaFeSi_2O_6$) solid solution were investigated by X-ray diffraction in situ at high pressure using a diamond anvil cell to P_{max} = 10.6 GPa. The samples exhibited space group symmetry $C2/c$ throughout the investigated pressure range and did not show any phase transformations. V_0, K_{T0}, and K' were simultaneously refined by fitting a third-order Birch-Murnaghan equation of state to pressure-volume data for all samples. The following relationship between bulk modulus and molar fraction of jadeite is observed:

$$K_{T0} = 108.7(2)\ (\text{GPa}) + 0.191(9) \times [\%\ \text{molar Jd}] + 0.0006(1) \times [\%\ \text{molar Jd}]^2$$

The bulk modulus of hedenbergite is 19% lower than jadeite with a strong axial anisotropy that increases with increasing the Hd content. In particular, the compressibility along the **b** axis (the most compressible in pyroxenes) increases by about 35% going from Jd to Hd while along the **c** axis the increase in compressibility is about 24%. The **a** axis does not show any variation in the deformation rate along the join. The analysis of the crystal structure behavior with pressure for all samples clearly indicates that the main cause of the strong anisotropy on the **b-c** plane is related to the narrowing of the M1 octahedral chain and to anion-anion interactions increasing the packing efficiency of the anion skeletons of the crystals going from Jd to Hd.

Keywords: High pressure, solid solution, crystal structure, X-ray