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Thermoelasticity of tremolite amphibole: Geophysical implications

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Abstract

We investigated the structure, equation of state, thermodynamics, and elastic properties of tremolite amphibole [$Ca_2Mg_5Si_8O_{22}(OH)_2$] up to 10 GPa and 2000 K, using *first principles* simulations based on density functional perturbation theory. We found that at 300 K, the pressure-volume results can be adequately described by a third-order Birch-Murnaghan equation of state with bulk moduli K_0 of 78.5 and 66.3 GPa based on local density approximation (LDA) and generalized gradient approximation (GGA), respectively. We also derived its coefficients of the elastic tensor based on LDA and GGA and found that the LDA result is in good agreement with the experimental results. At 300 K, the shear modulus G_0 is 58.0 GPa based on LDA. The pressure derivative of the bulk modulus K' is 5.9, while that of the shear modulus G' is 1.3. The second Grüneisen parameter, or $\delta_T = [-1/(\alpha K_T)](\partial K_T/\partial T)_P$, is 3.3 based on LDA. We found that at ambient conditions, tremolite is elastically anisotropic with the compressional wave velocity anisotropy AV_P being 34.6% and the shear wave velocity anisotropy AV_S being 27.5%. At higher pressure corresponding to the thermodynamic stability of tremolite, i.e., ~3 GPa, the AV_P reduces to 29.5%, whereas AV_S increases to 30.8%. To evaluate whether the presence of hydrous phases such as amphibole and phlogopite could account for the observed shear wave velocity (V_S) anomaly at the mid-lithospheric discontinuity (MLD), we used the thermoelasticities of tremolite (as a proxy for other amphiboles), phlogopite, and major mantle minerals to construct synthetic velocity profiles. We noted that at depths corresponding to the mid-lithosphere, the presence of 25 vol% amphibole and 1 vol% phlogopite could account for a V_S reduction of 2.3%. Thus based on our thermoelasticity results on tremolite amphibole, it seems that mantle metasomatism could partly explain the MLD.

Keywords: Tremolite, equation of state, elasticity, Mid-Lithospheric Discontinuity (MLD)