The 438th Geodynamics Seminar

Some thermodynamic properties of larnite (β-Ca_2SiO_4) constrained by high T/P experiment and/or theoretical simulation

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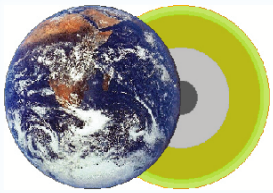

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Pure larnite (β-Ca_2SiO_4; Lrn) was synthesized at 6 GPa and 1473 K for 6 hours by using a cubic press, its thermal expansivity was investigated up to 923 K by using an X-ray powder diffraction technique (ambient P), and its compressibility was investigated up to ~16 GPa by using a diamond-anvil cell coupled with synchrotron X-ray radiation (ambient T). Its volumetric thermal expansion coefficient (α_V) and isothermal bulk modulus (K_T) were constrained as α_V = $4.24(4)\times10^{-5}$/K and K_T = 103(2) GPa (the first pressure derivative obtained as 5.4(4)), respectively. Its compressibility was further studied with the CASTEP code using density functional theory and planewave pseudopotential technique. We obtained the K_T values as 123(3) GPa (LDA; high boundary) and 92(2) GPa (GGA; low boundary), with the values of the as 4.4(9) and 4.9(5), respectively. The phonon dispersions and vibrational density of states (VDoS) of Lrn were simulated using density functional perturbation theory, and the VDoS was combined with a quasi-harmonic approximation to compute the isobaric heat capacity (C_P) and vibrational entropy (S^0_{298}), yielding $C_P = 212.1(1) - 9.69(5)\times10^2T^{-0.5} - 4.1(3)\times10^6T^{-2} + 5.20(7)\times10^8T^{-3}$ J mol^{-1} K^{-1} for the T range of ~298-1000 K and S^0_{298} = 129.8(13) J mol^{-1} K^{-1}.

詳細は当センターホームページ：http://www.grc.ehime-u.ac.jp/ をご覧ください
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