The 444th Geodynamics Seminar

Ab initio prediction of a possible incongruent melting relation in the MgO-SiO_2 system at multi-megabar

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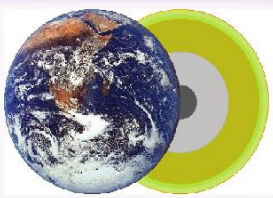

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Abstract

Magnesium silicates are thought to be major components of the mantle of terrestrial planets and the core of gas and ice giants (Guillot, 1999; Seager *et al*., 2007). However, the thermodynamic phase equilibrium in the MgO-SiO_2 system is still not well studied at multi-megabar, including melting relations. A recent laser shock experiment (Spaulding *et al*., 2012) reported two discontinuous phase changes of $MgSiO_3$ at 300-400 GPa, which were interpreted as a liquid-liquid transition, but an *ab initio* molecular dynamics study (Militzer, 2013) identified no clear transition in liquid $MgSiO_3$. On the other hand, Boates and Bonev (2013) examined a decomposition reaction of liquid $MgSiO_3$ into solid MgO and liquid SiO_2 by *ab initio* free energy calculations based on the two-phase thermodynamic model method (Lin *et al*., 2003) and reported that liquid $MgSiO_3$ is dissociated at ~300 GPa, implying a possible incongruent melting. However, the reaction they considered would be too simple and unrealistic. The detailed phase diagram in the MgO-SiO_2 system is therefore required to be clarified at multi-megabar. In this study, we determine the melting phase relations in this binary system by our original approach for free energy based on the thermodynamic integration method (Kirkwood, 1935) combined with *ab initio* molecular dynamics simulations.

Our calculations show a congruent melting in this binary system at 300 GPa, which does not explain the cause of the experimental findings observed by Spaulding *et al*. (2012). The calculated mixing entropy is almost equal to the configurational entropy of an ideal mixing at 300 GPa and 10000 K. In addition, we find that our phase diagram disagrees with the previous result reported by an *ab initio* study (Boates and Bonev, 2013) because the entropy they calculated will include no configurational entropy of mixing.

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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