The 402th Geodynamics Seminar

Ab initio free energy calculations of liquids and crystalline solids based on the thermodynamic integration method: Melting of the rocky core in Jupiter

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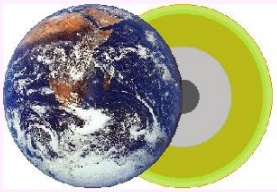
Date: 11.21.2014 (Fri) 16:30 ~
Venu: Meeting Room #486, Science Research Bldg 1, Ehime Univ.

日時：2014年11月21日(金)16:30～
場所：愛媛大学 総合研究棟Ⅰ 4階共通会議室



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Abstract

Phase boundaries can be determined by comparing Gibbs fee energies of each phase. However, it is difficult to evaluate free energies of liquids due to difficulty on calculating entropy in disordered structures. The thermodynamic integration (TI) method (Meijer +, 1990) based on statistical mechanics is a powerful technique to estimate the free energies since it can directly accesses free energy without calculating entropy. In our study, free energy calculation methods for not only liquids but also crystalline solids have been developed based on a combination of the TI method and the *ab initio* molecular dynamics (AIMD) method and applied to evaluation of the melting points of MgO and SiO_2. These minerals are major candidates of constituent materials of the rocky core in gas giants such as Jupiter and Saturn. The knowledge of the nature of the rocky core gives understanding of the internal structure and planetary evolution. If they melt in deep planet, it may influence the diffusion of heavy elements into the surrounding fluid layer. However, it has not been clarified even whether these minerals melt or not in the center of the gas giants.

In previous study (Wilson & Militzer, 2012), free energies of liquids and crystalline solids were calculated by two-step TI, where the first step is integration from an ideal system to a classical system, and the second step is integration from a classical system to an *ab initio* system. In contrast, in our technique, free energies of each phase have been switched directly from an ideal system to an *ab initio* system. The ideal systems for the cases of liquids and crystalline solids are an ideal gas and Einstein solids, respectively.

AIMD simulations have been carried out at 4 TPa, which corresponds to pressure condition of the Jovian core (Nettelmann +, 2012), and then the melting points of MgO and SiO_2 have been estimated. In addition, we have studied the melting relation in the MgO-SiO_2 system based on the ideal solution approximation. This result suggests that the Jovian core can melt partially. Therefore, the internal structure and planetary evolution models may need to take a liquid state of the core into account.

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