Geodynamics Seminar

第325回ジオダイナミクスセミナー

Melting the Deep Mantle - Magma Oceans and Ultra-Low Velocity Zones

Dr. Nico De Koker (Assistant Professor, GRC)

主催：愛媛大学地球深部ダイナミクス研究センター
日時：4/13（金）午後 4時30分～
場所：総合研究棟 4F 会議室

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

As the primary medium through which planetary differentiation occurs, silicate melts are a key entity in the study of the thermal and chemical evolution of Earth. Over the past few years we have used first-principles molecular dynamics simulations to investigate the liquid state physics of the magnesio-, calsio- and aluminosilicate melts at pressure and temperature conditions relevant to the entire mantle. First-principles methods characterize bonding directly in terms of the electronic charge density computed via density functional theory, and is equally robust at ambient and extreme pressure and temperature conditions. This allows accurate predictions of the physics of melts at extreme conditions to be made.

Liquid state diffusion and thermodynamics have been investigated in detail, with special attention to dependence on pressure, temperature and composition. Comparison to corresponding changes in liquid structure enables us to understand thermodynamic and diffusive behavior in a detailed atomistic context. Our results provide a rigorous test for a new fundamental thermodynamic relation for melts, which we derived to accurately describe liquid state thermodynamics. The relation is unique in that it accounts for electronic free energy contributions and displays the correct limiting behavior at extreme volume and temperature, capturing the thermodynamics of liquid-vapor coexistence.

Our work has allowed for deeper insight into the evolution of terrestrial planets, including the thermal state and mode of crystallization of magma oceans, the possible presence of melt in the deep earth, and their relative buoyancy. This insight in turn acts as a guide for questions to be addressed in the future, as first-principles simulations of systems of larger numbers of atoms and complex chemical compositions representative of natural systems become feasible.

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
問い合わせ先：桑山 靖弘（TEL:089-927-8408,e-mail:kuwayama@sci.ehime-u.ac.jp）