理学部セミナー

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題目：Viscosity Model Derived from First Principles Simulations of $MgO\text{-}SiO_2$ Melt System

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Abstract: Knowledge about the viscosity of silicate liquids, which form magmas and partial melts, is crucial to our understanding of chemical and thermal evolution of the Earth. The melt viscosity (η) can vary by several orders of magnitudes over the ranges of temperature (T), pressure (P) and composition (X) that are relevant. We perform equilibrium first-principles molecular dynamics simulations using density functional theory to investigate the viscosity of seven liquids in the $MgO\text{-}SiO_2$ binary system. These simulations show that the melt viscosity for different liquids varies with temperature at zero pressure to different extents: It decreases by five orders of magnitude for silica liquid between 2750 and 8000 K whereas it decreases by one order of magnitude for MgO liquid over a similar temperature interval. Using these results, we derive/evaluate different types of models for accurate description of the viscosity-temperature-composition (η-T-X) relationship. The Arrhenian model requires that the pre-exponential factor and the activation energy to depend on composition as the 4th power of the molar SiO_2 content (X). This means that the degree of polymerization controls the melt viscosity. Other viscosity models each with three adjustable parameters dependent on X used to describe deviation from Arrhenius behavior represent marginal improvement. Since the end members MgO and SiO_2 can perhaps be considered to represent, respectively, the least and most viscous components, the proposed binary models are anticipated to provide meaningful constraint on the viscosity of natural magmatic melts.

上記の通り理学部セミナーを開催します。

Dr. Karki は酸化物やケイ酸塩結晶、メルトの構造、物性の第一原理計算の分野において、これまで、数多くの第一級の研究成果をあげてこられました。現在、日本学術振興会の外国人招へい制度により来日されており、この機会に上記セミナーを企画致しました。奮ってご参加ください。

地球科学分野
松井　正典