Effects of Si on the crystal structure andelastic property of Fe at Earth's inner core pressures

Mika Fujibuchi[1]; # Taku Tsuchiya[2]

[1] Earth Sciences, Ehime University; [2] GRC, Ehime Univ

Earth's inner core is generally thought to consist of Fe-Ni alloy. Some amount of light element are also maybe contained in the inner core. Recent high-pressure experiments and theoretical simulations have suggested that Si is a highly possible candidate of impurity elements in the inner core. In this study we investigated the effects of Si on the crystal structure and elastic property of iron at the Earth's inner core pressures by first-principle calculations to clarify the acceptability of Si as an inner core constituent. Calculated results showed Si having large effects to change the elasticity of the hcp phase of iron at the inner core P,T condition. We will report the Si content for several iron phases needed to reproduce the observed inner core elasticity.

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