Thermoelastic properties of hcp-Fe-Si-C-S alloys under the Earth's inner core conditions

Yunguo Li*[1], Lidunka Vočadlo[1], and John Brodholt[1]

[1]Department of Earth Sciences [University College London] – Gower Street - London - WC1E 6BT, United Kingdom

Abstract

Geophysical and cosmochemical models constrain the inner core to be composed mainly of iron and few percent light elements including Si, S, C, and H. However, mineral physics results do not agree with the seismological observations of both density and sound wave velocities in the inner core (Vočadlo, 2007; Vočadlo *et al.*, 2009; Belonoshko *et al.*, 2007; Martorell *et al.*, 2013). Recent studies suggest a candidate for the inner core could be *hcp* iron alloyed with light elements (Li. *et al.*, 2001; Antonangeli, *et al.*, 2010; Hirose, *et al.*, 2013). Using *ab initio* molecular dynamics calculations, we have studied the structure and elastic properties of *hcp*-Fe alloys at 360 GPa up to the melting temperature. A ternary *hcp*-Fe30Si1C1 alloy was found to match both the inner-core density and sound velocities. We also found other possible ternary and quaternary candidates based on a solid solution model, where carbon is always a necessary component to be in agreement with the seismic observations. These Fe-C-X compositions provide a new understanding of the Earth's core with important geodynamic implications.

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*Speaker