Potential Impact of Icosahedral Short Range Ordering on Transport Properties of Liquid Fe-Alloys at the Core Conditions

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Electrical and thermal conductivity of liquid Fe-alloys in the outer core directly modulates the geodynamo power budget and has implications toward the determination of the age the of the inner core. Moreover, the transport properties of liquid Fe-alloys control the convection mechanism in the outer core. However, transport properties of liquid Fe-alloys remain poorly constrained at the core conditions. While the impurities play a role in the transport of heat and charge in the outer core, the presence of icosahedral short range order (ISRO) in liquid Fe-alloys adds an additional layer of complexity and may significantly impact the transport properties of the Fe-alloys at the core conditions.

The presence of ISRO with the fivefold symmetry in melts was first postulated by Frank (1952) to explain the observed large undercooling of pure metals but only demonstrated experimentally in the last decade (Schenk et al. 2002). Typically, ISRO structures consist of 12 atoms with fivefold symmetry on the outside, surrounding the additional atom in the center of the structure. The ISRO favor dilute alloys where the atomic radius of the host alloy (Fe) is bigger than solute (e.g. Si) as in the case of Fe-Si (Holland-Moritz et al. 2006) and an icosahedron structure with a smaller atom in the center is energetically favorable. Moreover, the concentration of ISRO increases with pressure but only in a limited temperature range above the melting boundary (Li et al. 2017).

It has been suggested recently that at high pressure, the presence of ISRO in liquid Fe-alloy affects the electronic component of heat and charge transport. ISRO structures also increase the viscosity of the melt by dynamically slowing down of atomic motion within the liquid required for momentum transfer (Lü et al. 2017; Hu et al. 2015). Additionally, ISRO polyhedron tends to increase the interfacial energy between the liquid and crystal, leading to the suppression of nucleation in liquids (Li et al., 2017). Here we discuss the potential implications and the impact of the ISRO structures on the transport properties of liquid Fe-alloys in the outer core.

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