Elastic Properties of fcc-Fe under Lunar Core Conditions

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Venue: Zoom

A link will be sent @grc-all within 30 minutes before the beginning of the seminar.

Keywords:

1. High pressure
2. Lunar interior
3. ab initio calculations

From both seismic velocities and selenodetic data it can be seen that the Moon has undergone major differentiation and is composed of a crust, a mantle, and a small core. The composition of the lunar core is expected to be predominantly iron; however, it is likely to contain some proportion of light elements, such as silicon and sulphur. Constraints on the lunar core composition can give insight into the lunar interior structure, the formation of the Moon, and the palaeomagnetic dynamo. Sound velocities are critical to add constraints to the interiors of planetary bodies as they can be compared with seismic velocities from the inversion of seismic data.

Computational methods have been used to investigate the elastic properties of iron under lunar core conditions. At lunar core conditions of ~5–6 GPa and ~1,300–1,900 K the face-centred cubic (fcc) phase is the stable phase of iron and remains magnetic at these pressures. This incorporates an extra layer of complexity when calculating elastic properties as spin polarised calculations must be performed. Spin polarised ab initio calculations have been used to investigate magnetism in fcc-Fe and spin polarised ab initio molecular dynamics simulations have been used to calculate the elastic tensor of fcc-Fe, and therefore the sound velocities in fcc-Fe at lunar core conditions. The calculated sound velocities are compared with those from experimental literature.

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