
Face-centred cubic iron: *ab initio* calculations of sound velocities in the lunar core

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Abstract

Studies, such as the reanalysis of the Apollo lunar seismograms [1], have shown that the Moon has undergone differentiation and possesses a small core. The composition of the lunar core is not well constrained, and many compositional models have been suggested including combinations of iron, nickel, and light elements such as sulphur and carbon [e.g. 1, 2, 3, 4], and other more exotic compositions [5]. Additional constraints are crucial to our understanding of the Moon, including its formation, the dynamics of its interior, and a lunar dynamo.

We use *ab initio* molecular dynamics simulations to calculate elastic constants of face-centred cubic (fcc) iron and iron alloys and hence sound velocities at lunar core conditions, at ~ 5 -6 GPa and $\sim 1,300$ -1,900 K [3]. The results from these simulations will then be compared with the data from the Apollo seismograms and experimental data to help form a description of the lunar interior.

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