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Face-Centred Cubic Iron: Ab Initio Calculations of Sound Velocities in the Lunar Core

Marisa C. Wood (1), Lidunka Vočadlo (1), Ian G. Wood (1), and Oliver T. Lord (2)

(1) Department of Earth Sciences, University College London, London, United Kingdom, (2) School of Earth Sciences, University of Bristol, Bristol, United Kingdom

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 and small telluric planets such as Mars and Mercury, including formation, the interior dynamics, and the evolution of dynamos.

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 ∼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. In addition to this, the melting curve of ternary systems have been investigated with the use of diamond anvil cell experiments.

[1] Weber et al. (2011) Science 331, 309-312. [2] Dasgupta et al. (2009) Geochim. Cosmochim. Acta 73, 6678-6692. [3] Antonangeli et al. (2015) Proc. Natl. Acad. Sci. U.S.A. 112, 3916-3919. [4] Righter et al. (2017) Earth Planet. Sci. Lett. 463, 323-332. [5] Wieczorek & Zuber (2002) Lunar Planet. Sci. 33, abstract 1384.