Summit to: Computational Materials Science

Simulations of iron under the Earth's core conditions

Yang Sun[1,2]

[1] Applied Physics and Applied Mathematics, Columbia University, USA

[2] Department of Physics, Iowa State University, USA

EXTENDED ABSTRACT: Iron is the primary element in the Earth's core. The properties of iron under extremely high pressure/temperature conditions are fundamental to understanding the Earth's internal structure and evolution. *Ab initio* simulations provide important iron information that is hard to access from laboratory or seismic measurements. In this talk, I will show our recent work using first-principle calculations coupled with a genetic algorithm, Monte-Carlo, and molecular dynamics simulations to understand the formation of the Earth's inner core and to discover iron-rich Fe_nO (n>1) compounds possibly existing in the present inner core. First, I will discuss the nucleation process of the Earth's inner core. Recent attempts to explain how the inner core solidified were surprisingly unsuccessful, which led to the so-called "inner core nucleation paradox". To address the paradox, we developed potentials from *ab initio* data to simulate the iron's crystallization process under core conditions. We demonstrate molten iron could crystallize into the hcp phase via a two-step nucleation process with an intermediate bcc phase under the Earth's core conditions [1]. This provides a key factor in understanding the initial formation of the inner core and its present crystal structures. Next, I will show how we identify iron-rich Fe-O compounds and use it to solve the complex XRD data from high PT experiments. It has been thought only oxygen-rich Fe-O compounds exist. Using crystal structure prediction and DFT calculations, we discovered a new family of iron-rich Fe_nO compounds at Earth's core conditions. This challenges the traditional view and suggests oxygen should be a possible light element in the solid inner core. The existence of these oxygen-bearing Fe phases could extend the deep oxygen cycling to the solid inner core, as part of an entire global oxygen cycle [2].

Keywords: Earth's inner core; Atomistic simulations; Nucleation

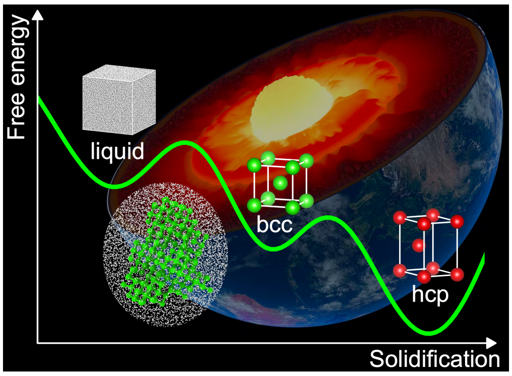

Figure 1. Schematics of liquid-bcc-hcp two-step nucleation process in the Earth inner core [1]. The insert shows a bcc nucleus spontaneously formed in the liquid during molecular dynamics simulations.

REFERENCES

[1] Y. Sun *et al.* PNAS 119, e2113059119 (2022)

[2] J. Liu, Y. Sun, *et al.* arXiv:2110.00524 (2021)

BIOGRAPHY

Yang Sun completed his Ph.D. in 2016 from the University of Science and Technology of China and Postdoctoral Studies at Ames National Laboratory, US DOE in 2016-2019, and Columbia University in 2019-2020. He currently works as Associate Research Scientist at Columbia University and Research Scientist at Iowa State University. He has published more than 60 papers in reputed journals, including PRL, ACS Nano, and PNAS.