American Mineralogist, Volume 107, pages 421–431, 2022

Measurements of the Lamb-Mössbauer factor at simultaneous high-pressure-temperature conditions and estimates of the equilibrium isotopic fractionation of iron

Dongzhou Zhang[1,4,*], Jennifer M. Jackson[2], Wolfgang Sturhahn[2], Jiyong Zhao[3], E. Ercan Alp[3], and Michael Y. Hu[3]

[1]Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, Hawaii 96822, U.S.A.
[2]Seismological Laboratory, California Institute of Technology, Pasadena, California 91125, U.S.A.
[3]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.
[4]GSECARS, University of Chicago, Argonne, Illinois 60439, U.S.A.

Abstract

Isotopic fractionation has been linked to the lattice vibrations of materials through their phonon spectra. The Lamb-Mössbauer factor (f_{LM}) has the potential to provide information about the lattice vibrations in materials. We constrain the temperature evolution of the f_{LM} of γ- and ε-Fe at in situ high-*P*-*T* conditions between 1650 K and the melting point. We find that the vibrations of γ- and ε-Fe can be described using a quasiharmonic model with a pressure- and temperature-dependent Debye temperature computed from the measured f_{LM}. From the Debye temperature, we derive the equilibrium isotopic fractionation β-factor of iron. Our results show that the quasiharmonic behavior of metallic iron would lower the value of $\ln\beta_{Fe}^{57/54}$ by 0.1‰ at 1600–2800 K and 50 GPa when compared to the extrapolation of room temperature nuclear resonant inelastic X-ray scattering data. Our study suggests that anharmonicity may be more prevalent in Fe metal than in lower mantle minerals at 2800 K and 50 GPa, a relevant condition for the core formation, and the silicate mantle may be isotopically heavy in iron.

Keywords: Iron isotope fractionation, high pressure-temperature, Mossbauer spectroscopy, anharmonicity