Electronic and Elastic Properties of Iron-Containing Minerals in Earth’s Interior

Jung-Fu Lin

Department of Geological Sciences, Jackson School of Geosciences, The University of Texas at Austin, TX 78712, USA

As the most abundant 3d transition metal in the Earth’s interior, iron’s existence in the lower-mantle and core phases affects a broad range of physical and chemical properties in these regions. Thus, comprehension of the electronic and elastic properties of Fe-containing compounds under relevant pressure-temperature conditions is essential for interpreting seismological, geochemical, geodynamic, and geomagnetic observations deep in the Earth’s interior. Herein, I will discuss the electronic spin and valence states of iron in the lower-mantle minerals, and the elasticity of candidate iron alloys in the Earth’s core. Specifically, recent studies have shown that lower-mantle minerals such as ferropericlase \([(Mg,Fe)O]\), silicate perovskite \([(Mg,Fe)SiO_3]\), post-perovskite, and ferromagnesite \([(Mg,Fe)CO_3]\) can contain iron in very distinct electronic spin and valence states at high pressure-temperature \((P-T)\) conditions. The electronic spin and valence states of iron in these minerals have been investigated using synchrotron Mössbauer, X-ray diffraction, and emission spectroscopies in high-pressure diamond anvil cells. In particular, I will address the spin states of ferric and ferrous iron in perovskite and post-perovskite as a function of \(P-T\)-composition in the lower mantle, focusing on the use of the hyperfine parameters, quadrupole splittings (QS), and chemical shifts (CS), seen in Mössbauer spectroscopic analyses. Furthermore, precise measurements on the elasticity of candidate iron alloys at simultaneously high \(P-T\) conditions are needed to provide reliable constraints on the composition and seismic features of the Earth’s core. The \(V_p\)-density relation of Fe and its alloys have been recently measured at extremely high \(P-T\) using \textit{in situ} high-energy resolution inelastic X-ray scattering and X-ray diffraction in external heated diamond anvil cells at the Advanced Photon Source. Combining these results with theoretical calculations and thermodynamic modeling, I will discuss how the existence of iron affects the elastic and thermodynamic properties of iron-containing minerals, and our understanding of the geochemistry, geophysics, and geodynamics of the deep Earth.