American Mineralogist, Volume 103, pages 1959–1965, 2018

Electronic properties and compressional behavior of Fe–Si alloys at high pressure

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Abstract

Planetary cores are composed mainly of Fe with minor elements such as Ni, Si, O, and S. The physical properties of Fe alloys depend on their composition. Changes in *c*/*a* ratio, center shifts, and elastic properties of Fe and Fe–Ni alloys were reported previously. However, such properties of Fe light-element alloys have not yet been extensively studied. Si is a plausible candidate as a light element in planetary cores. Therefore, we studied the electronic properties and compressional behavior of Fe-Si alloys with a hexagonal-close-packed (hcp) structure under high pressure using synchrotron Mössbauer spectroscopy (SMS) and X-ray diffraction (XRD). Center shifts (CS) were observed at pressures of 21.4–45.3 GPa for Fe-2.8wt%Si and of 30.9–62.2 GPa for Fe-6.1wt%Si. Some of SMS and XRD measurements were performed under the same conditions using a newly developed system at the BL10XU beamline of SPring-8, which allowed simultaneous characterization of the electron information and crystal structure. Changes in the CS values were observed at 36.9 GPa in Fe-2.8wt%Si and 54.3 GPa in Fe-6.1wt%Si. The ratios of *c*/*a* in the hcp structure were measured at pressures of 21.2–49.6 GPa in Fe-2.8wt%Si and 32.9–61.4 GPa in Fe-6.1wt%Si. The *c*/*a* ratio changed at pressures of 30–45 GPa in Fe-2.8wt%Si and at 50 GPa in Fe-6.1wt%Si. Changes in the CS and *c*/*a* ratio were explained according to the electronic isostructural transition in Fe–Si alloys. In addition, the transition pressure increased with increasing Si content in metallic iron. This finding is significant as changes in seismic wave velocities due to the change in *c*/*a* ratio of Fe–Si alloys with an hcp structure might be observed if Venus has a solid inner core.

Keywords: Synchrotron Mössbauer spectroscopy, diamond-anvil cell, electronic topological transition, compressional behavior, Fe-Si alloy