Spin transition at ultrahigh pressure of exoplanet interiors

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Iron-bearing magnesium oxide [$(Mg_{1-x}Fe_x)O$], which constitutes ~20 vol% of the Earth's lower mantle (depth 660–2890 km, pressure range 23–135 GPa), is also considered a major constituent of terrestrial exoplanets. In the Earth's lower mantle, $(Mg_{1-x}Fe_x)O$ ($0.1 < x < 0.2$) crystalizes in the B1 (NaCl-type) structure. In this (B1) phase, Fe^{2+} undergoes a pressure-induced spin transition from the high-spin (HS, $S = 2$) to the low-spin (LS, $S = 0$) state at ~45 GPa [1], while the intermediate-spin (IS, $S = 1$) state has never been observed [2]. Extensive studies on the B1 phase have indicated that the HS–LS transition is accompanied by anomalous changes of the structural, electronic, optical, magnetic, elastic, thermodynamic, and transport properties of the host mineral and may greatly affect the Earth's mantle properties [3,4]. By contrast, effects of Fe and spin transition at ultrahigh pressure relevant to exoplanet interiors remain unknown. In this talk, I will discuss our recent computational study on $(Mg_{1-x}Fe_x)O$ ($x \leq 0.25$) up to 1.8 TPa [5]. Our calculations indicate that $(Mg_{1-x}Fe_x)O$ undergoes a simultaneous structural and spin transition at ~0.6 TPa, from the B1 phase LS state to the B2 (CsCl-type) phase IS state. Remarkably, Fe's total electron spin (S) re-emerges from 0 to 1 at ultrahigh pressure (along with the B1–B2 transition), against the perception that spin/magnetization is suppressed by pressure. Upon further compression, an IS–LS transition occurs in the B2 phase. Depending on the Fe concentration (x), metal–insulator transition and rhombohedral distortions can also occur in the B2 phase. These results suggest that Fe and spin transition may affect planetary interiors over a vast pressure range.

References

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