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Reduced charge transfer in mixed-spin ferropericlase inferred from its high-pressure refractive index

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Abstract

Physical properties of mantle minerals are essential for comprehensive geodynamic modeling. High-pressure experiments allow measurements of physical properties but fundamental insights into their evolution with pressure are often experimentally inaccessible. Here we report the first in situ experimental determination of the optical refractive index, its wavelength-dispersion, and optical absorption coefficient of ferropericlase up to ~140 GPa at room temperature. All these properties change gradually in dominantly high-spin (below ~50 GPa) and low-spin (above ~80 GPa) ferropericlase. However, in the mixed-spin state (i.e., significant presence of both high- and low-spin iron), the index dispersion and the absorption coefficient decrease by a factor of three and ~30%, respectively. These anomalies suggest that charge transport by small polaron is reduced in mixed-spin ferropericlase, providing fundamental insights into the factor-of-three lower electrical conductivity of ferropericlase at ~50–70 GPa.

Keywords: High-pressure, diamond anvil cell, refractive index, ferropericlase, MgO, DFT, spin transition, band gap, electrical conductivity; Physics and Chemistry of Earth's Deep Mantle and Core