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Title

Phonon density of states of Fe₂O₃ across high-pressure structural and electronic transitions

Source

Physical Review B (Condensed Matter and Materials Physics), vol.84, no.6, 1 Aug. 2011, 064424 (7 pp.). Publisher: American Physical Society, USA.

Abstract:High-pressure phonon density of states (PDOS) of Fe₂O₃ across structural and electronic transitions has been investigated by nuclear resonant inelastic x-ray scattering (NRIXS) and first-principles calculations together with synchrotron Mossbauer, x-ray diffraction, and x-ray emission spectroscopies. Drastic changes in elastic, thermodynamic, and vibrational properties of Fe₂O₃ occur across the Rh₂O₃(II)-type structural transition at 40-50 GPa, whereas the Mott insulator-metal transition occurring after the structural transition only causes nominal changes in the properties of the Fe₂O₃. The observed anomalous mode-softening behavior of the elastic constants is associated with the structural transition at 40-50 GPa, leading to substantial changes in the Debye-like part of the PDOS in the terahertz acoustic phonons. Our experimental and theoretical studies provide new insights into the effects of the structural and electronic transitions in the transition-metal oxide (TMO) compounds. (34 References).