American Mineralogist, Volume 92, pages 433–436, 2007

LETTER

Optical absorption spectra of ferropericlase to 84 GPa

HANS KEPPLER,* INNOKENTY KANTOR, AND LEONID S. DUBROVINSKY

Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany

ABSTRACT

Optical and near infrared absorption spectra of ferropericlase $Mg_{0.88}Fe_{0.12}O$ have been measured to 84 GPa. Under ambient conditions, the spectrum shows two crystal field bands of high-spin Fe^{2+} at 8922 and 12 533 cm^{-1}, which shift to higher frequencies with increasing pressure ($d\nu/dP$ = 50.7 and 85.5 cm^{-1}/GPa). Simultaneously, the intensity of the high-frequency band continuously decreases until it vanishes around 40 GPa, suggesting a quenching of the Jahn-Teller effect. Between 51 and 60 GPa, the absorption spectrum changes drastically. Two new bands appear at 60 GPa at 9728 and 14 592 cm^{-1} with frequency shifts at higher pressures of $d\nu/dP$ = 23.8 and 21.0 cm^{-1}/GPa, respectively. If the change in optical spectra between 51 and 60 GPa were interpreted as being due to spin-pairing, the crystal field parameters of low-spin Fe^{2+} at 60 GPa would be Δ = 10 546 cm^{-1} and B = 377 cm^{-1}. This would imply that the main cause of spin-pairing is not the increase in crystal field splitting Δ, but the stronger covalency of the Fe-O bond as seen in the reduction of the Racah parameter B. Even at 84 GPa, ferropericlase is by no means opaque. In particular, the inferred spin-pairing transition between 51 and 60 GPa reduces radiative thermal conductivity only by about 15%. Spin-pairing in ferropericlase is therefore unlikely to have major consequences for the temperature distribution or the mode of convection in the lower mantle. The absorption edge of the high-pressure phase appears to be deeper in the UV than for the low-pressure phase, which could imply a reduced electrical (polaron) conductivity.

Keywords: Ferropericlase, spin-pairing, low-spin, iron, optical spectra, radiative conductivity, crystal field splitting, Racah parameter, Jahn-Teller effect