First principles study of the lattice thermal conductivity of ferropericlase

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The thermal conductivity of minerals governs heat flux, which partially controls the thermal evolution and dynamics of the Earth's lower mantle. Although much progress has been achieved regarding the lattice thermal conductivity (k_{latt}) of periclase, perovskite (Pv) and post-perovskite (pPv) at high temperature and high pressure, the effects of iron incorporation on k_{latt} have not been elucidated. In this study, we carry out an extensive first principles study to calculate k_{latt} of ferropericlase (Fp) and discuss the mechanisms of variation in k_{latt} by incorporation of ferrous iron. Our calculations show that k_{latt} is significantly reduced by the incorporation of ferrous iron compared to that of iron-free periclase, which is consistent with previous measurements. Three different iron concentrations were considered in this study, and it can be found that a further decrease is predicted for increased ferrous iron content. Moreover, it is worth noting that the high spin (HS) to low spin (LS) transition results in an enhancement of k_{latt}.

Generally, under mantle conditions, C_V approaches the classical value k_B and does not influence k_{latt}. The volumes of HS Fp and LS Fp have slight changes compared to that of MgO. Surely, a weak variation in volume is not sufficient to explain the significant reduction in k_{latt} (~92%). The phonon dispersions indicate that the phonon frequencies and group velocities decrease by approximately 25% for both transversal and longitudinal acoustic modes due to the inclusion of ferrous iron, which then contribute to the reduction in k_{latt}. Stronger scattering rates are obtained for both HS Fp and LS Fp with respect to that of MgO, which also leads to a reduction in k_{latt}. Therefore, group velocities decrease and stronger scattering rates are the major factors for significant decrease in k_{latt}.

The scattering rates of Fp in the LS state are slightly smaller than those in the HS state; meanwhile, the phonon dispersion also indicates that the velocities in the longitudinal acoustic modes increase modestly with the spin transition, and those in the transverse acoustic modes are unaffected. The above mentioned characteristics account for the enhancement in k_{latt} by the spin transition.

k_{latt} of iron-bearing periclase in the mixed spin (MS) state is calculated by scaling relation and exhibits a strong anomaly along the spin transition region. The total k_{latt} of a pyrolitic composition along a geotherm shows a weak anomaly between 750 and 1500 km. Moreover, a reduction in k_{latt} at the CMB is expected due to the MS states.

References:
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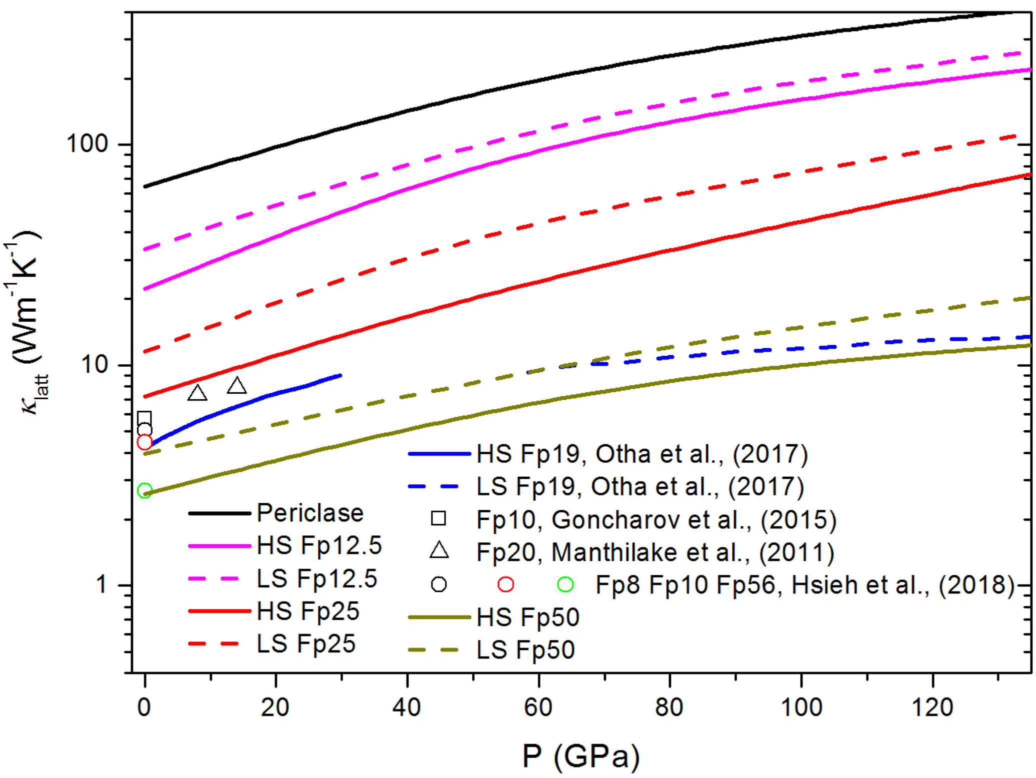

100
10
1
κ_{latt} (Wm^{-1}K^{-1})
0
20
40
60
80
100
120
P (GPa)
Periclase
HS Fp12.5
LS Fp12.5
HS Fp25
LS Fp25
HS Fp19, Otha et al., (2017)
LS Fp19, Otha et al., (2017)
Fp10, Goncharov et al., (2015)
Fp20, Manthilake et al., (2011)
Fp8 Fp10 Fp56, Hsieh et al., (2018)
HS Fp50
LS Fp50