Anomalies in thermal properties and equations of state of ferromagnesite (Mg,Fe)CO_3 across spin transition

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Ferromagneiste (Mg,Fe)CO_3 is considered as a major carbon carrier in the Earth's lower mantle; this mineral may play a significant role in the Earth's deep carbon cycle. Thorough knowledge of the thermal properites (e.g. heat capacity, thermal conductivity) of ferromagnesite can thus provide valuable insights to its role in the deep carbon cycle. With Fe^{2+} substituting Mg^{2+} in the octahedral site, ferromagnesite undergoes a spin transition from the high-spin (HS, $S = 2$) to the low-spin (LS, $S = 0$) state at around 45–50 GPa. Previous first-principles calculations [1] using the local density approximation + self-consistent Hubbard U (LDA+U_{sc}) method have succesfully explained the spin transition and accompanying volume/elastic anomlies in ferromagnesite observed in room-temperature experiments. Here, we combine LDA+U_{sc} method with lattice dynamics to compute the full thermal equations of state and thermal properties of ferromagnesite at high pressure and high temperature. Our calculaions show that spin transition in ferromagnesite is accompanied by anomlies in nearly all thermal properties, including thermal expansion, Gruneisen parameter, heat capacity, and thus thermal conductivity. We also discuss the potential geophysical and geochemical consequence of spin transition in ferromagnesite.

[1] Hsu and Huang (2016) *Phys. Rev. B* **94**, 060404(R).