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Modeling thermoelastic properties of minerals using interatomic potentials derived from first principles

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The knowledge of thermoelastic properties of minerals under extreme conditions of pressure and temperature is an important requirement for physical models of the Earth's interior. Both experimental and atomistic modeling techniques have recently been considerably improved to study these properties in the relevant p/T-range. While experimentally *in situ* measurements of sound wave velocities at high pressure can now be performed, the development of high-level computer simulation techniques has increased the predictive power of atomistic models substantially.

While first-principles modeling techniques based on electronic structure calculations have proven the most powerful and precise tool for theoretical prediction of mineral properties as a function of pressure, their application to the high temperature regime and to (partially) disordered structures is still limited due to the huge computational requirements. A promising alternative is the use of advanced interatomic potentials. To achieve a similar precision and reliability as first-principles methods over a wide range of p/T, for different coordination environments and compositions, the potential model has to include all relevant interactions explicitly.

Here we use an ionic model that allows for ion polarization and shape deformations up to the quadrupolar level [1] to study thermoelastic properties of simple oxides (periclase, corundum, spinel) and silicates ($MgSiO_3$). The parameters of the potential are optimized by fitting forces and multipoles of individual ions, and stress tensors of atomic configurations to reference planewave-DFT calculations. We demonstrate the transferability of the model between different structures and in a wide p/T range by comparison with experimental data obtained by *in situ* GHz-ultrasonic interferometry

in diamond anvil cells [2], and with results from first-principles DFT calculations. Finally, the application of our model to more complex systems is discussed.

References

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