Thermodynamics stability and elastic properties of Earth's Mantle minerals from the Decoupled Anharmonic Mode Approximation

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Temperature and pressures induced phase transitions result in substantial changes in mechanical properties of materials and thus are important for interpretation of geophysical data and geodynamic modeling. Accordingly many efforts have been made for the development of theoretical methods for *ab initio* prediction of mineral phase stability and their thermo-elastic properties[1, 2] in the *pT*-chemistry-space.

Temperature often leads to structures with high symmetry and negative curvature of the potential energy surface at $T=0$ (e.g. cubic $CaSiO_3$). For the *ab initio* calculations of mineral properties (quasi)harmonic schemes (SCAILD [3], SSCHA [4] and [5]) are most popular. At high T the validity of the approximation cannot always be justied.

Therefore we have developed the DAMA [6] which allows to calculate the vibrational free energy for materials with dynamical instabilities, their *pT*-stability field and to derive properties of the material at $T>0$, e.g. temperature dependent elastic constant. - We will present applications to Earth's mantle minerals (e.g. $CaSiO_3$), and in particular will discuss physical properties of a new type of perovskite structures with *dynamical* tilting of the AX_3 octahedra. **We have compiled a table of all possible configurations and their space groups in order to help structure refinement of high temperature perovskite structures.**

From these successful tests and comparisons we conclude, that the DAMA formalism can give insight into the mechanism of temperature-driven structural phase transitions and allows to calculate many structural properties at $T > 0$.

[1] Weidner *et al.*, Phys. Earth Planet. Int. **155**, 249 (2006). [2] Vocadlo *et al.*, Nature **423**, 235 (2003). [3] Souvatzis *et al.*, PRL **100**, 095901 (2008). [4] Errea *et al.*, PRB **89**, 064302 (2014). [5] Karki *et al.*, PRB **61**, 8793 (2000). [6] Adams and Passerone, J Phys Cond Matt **28**, 305401 (2016).