American Mineralogist, Volume 106, pages 1586–1595, 2021

A Grüneisen tensor for rutile and its application to host-inclusion systems

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Abstract

Rutile is often found as inclusions in garnet, quartz, and several other rock-forming minerals, and it is also a common accessory phase in high-pressure metamorphic rocks. Its relatively simple structure, chemistry, broad *P-T* stability field, and its wide occurrence in nature makes it a candidate for the application of elastic geobarometry. However, thermodynamic studies coupled with observations on natural samples predict that rutile inclusions in garnets should exhibit zero residual pressure. This implies that the rutile inclusions are detached from the inclusion walls in the host garnet after entrapment. We determined the elastic and vibrational properties of rutile via ab initio hybrid Hartree-Fock/Density Functional Theory simulations under different strain states. Our results confirmed the thermodynamic behavior of rutile in garnet and allowed us to determine for the first time the components of the phonon-mode Grüneisen tensors of rutile. We demonstrated that pure rutile inclusions in garnets from metamorphic rocks exhibit no residual strain or stress, consistent with thermodynamic modeling. Nevertheless, there are rutile inclusions in garnet surrounded by optical birefringence haloes, which are indicative of residual inclusion pressures. Careful examination of these show that they contain significant amounts of amphibole, which reduce the elastic moduli of the composite inclusion to less than that of the garnet hosts. A calculation method for the residual pressures of multi-phase inclusions is described.

Keywords: Rutile, Grüneisen tensor, HF/DFT, elastic geobarometry