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Consequences of the Quasiharmonic Approximation: Tests and Predictions[1] PIERRE CARRIER, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota , JUN TSUCHIYA, Geodynamics Research Center, Ehime University, Matsuyama, Japan, RENATA M. WENTZCOVITCH, Minnesota Supercomputing Institute, Department of Chemical Engineering and Materials Science, University of Minnesota
— The quasiharmonic approximation (QHA) is extremely useful since it allows the computation of thermodynamic properties if one knows the volume dependence of the vibrational density of states. It has an important consequence: the structure and vibrational properties of the solid depend on volume alone. The temperature dependence occurs via extrinsic volumetric effects. We present here a criterion to determine the pressure- temperature range of validity of the QHA, apply it to and test it in MgSiO3-perovskite, and inspect the possibility of a simple volumetric depended of other properties such as acoustic velocities, i.e., "Birch's Law."

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Renta M. Wentzcovitch

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