

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

High PT elasticity within the quasiharmonic approximation with relaxed thermal stresses¹ PIERRE CARRIER, JOAO F. JUSTO, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, 55455. — We describe in detail a method to compute high PT elasticity within the quasiharmonic approximation (QHA). This approach differs from the usual formulation used to compute the statically constrained high PT elastic constants by including corrections due to deviatoric thermal stresses. The formulation is general and valid for crystals with up to triclinic symmetry. We use perovskite and post-perovskite phases of MgSiO₃ to exemplify the use of the method to calculate elasticity and crystal structures at high PT.

¹Research supported by grants NSF/EAR 0635990 and NSF/ITR 0428774 (VLab)

Pierre Carrier
University of Minnesota

Date submitted: 26 Nov 2007

Electronic form version 1.4