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First–Principles Thermoelasticity of Beryllium PHILIPPE LEGRAND, GREGORY ROBERT, CEA/DAM/DIF F91297 Arpajon, France — For a few years, we have been working to propose fully ab initio based models to the response of Beryllium to dynamic loading. Ab initio quantum mechanics, based on pseudopotentials, was used including Quantum Molecular Dynamics and phonon calculations. We have already constructed a thermodynamically complete and rigorous equation of state for Beryllium in the hexagonal and body-centred structures, obtained the melting curve and predicted elastic constants as a function of compression. The dependence of the elastic constants and shear modulus function of temperature was also taken into account under the hypothesis that the evolution of the Poisson ratio is independent of the temperature. To rise this hypothesis in our full ab initio scheme, we propose to proceed as follow: the crystal free energy is calculated by adding a static contribution which is accessible to standard DFT calculations to a dynamical contribution which is approximated by the free energy of a system of harmonic oscillators corresponding to the crystal vibrational modes (phonons) calculated within density-functional perturbation theory (DFPT). Then, the second derivatives of the free energy with respect to deformation give the full ab initio elastic constants dependence on temperature.

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