Phonon self energy in transition metals LAURENT CHAPUT, IJL, UMR CNRS 7198, Nancy Universite, France, ATSUSHI TOGO, ISAO TANAKA, Department of Materials Science and Engineering, Kyoto University, Japan, GILLES HUG, LEM, UMR 104 ONERA-CNRS, ONERA, France — We present ab initio calculations of the phonon self energy of transition metals obtained using second order many body perturbation theory.\(^1\) The code we have implemented\(^2\) use the symmetry properties of the phonon-phonon interactions to express the self energy as a sum over irreducible triplets. It is analogous to the reduction of integration to the irreducible part of the Brillouin zone for one particle properties. The self energy of transition metals is then calculated. We show that the Peierls approximation\(^3\) is in fact reasonable for bcc and fcc metals, but fails for the hcp. The decays paths of phonons producing the self energy is finally analyzed using surfaces of reciprocal space defined by conservation law.

\(^3\)R. E. Peierls, Quantum Theory of Solids, Oxford University Press, 1964

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