Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

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.

[1]S. Narasimhan and D. Vanderbilt, Phys. Rev. B, 43, 4541 (1991)
[2]L. Chaput, A. Togo, I. Tanaka and G. Hug, submitted to Phys. Rev. B
[3]R. E. Peierls, Quantum Theory of Solids, Oxford University Press,1964

Laurent Chaput
Institut Jean Lamour, UMR CNRS 7198, Nancy Universite, Bd. des Aiguillettes, BP 23, 54506 Vandoeuvre Les Nancy Cedex, France

Date submitted: 11 Nov 2010 Electronic form version 1.4