Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**Anomalous vibrational effects in non-magnetic and magnetic Heusler alloys** ALEXEY ZAYAK, KARIN RABE, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, PETER ENTEL, Institute of Physics, University of Duisburg-Essen, Duisburg 47048, Germany — First-principles calculations are used to address the problem of phonon anomalies in non-magnetic and magnetic Heusler alloys. Phonon dispersions of the cubic $L2_1$ structure were obtained along the [110] direction. We consider compounds that exhibit phonon instabilities and compare them with their stable counterparts. The analysis of the electronic structure allows us to identify the characteristic features leading to structural instabilities. The phonon dispersions of the unstable structures show that, while the acoustic modes tend to soften, the optical modes disperse in a way that is significantly different from that of the stable structures. In an external field the affected optical modes are Raman active, which is considered as an indication of a stronger covalent interaction in the case of unstable systems. This covalent interaction changes the usual metallic behaviour of some Heusler alloys leading to the possibility of localization of vibrational modes and a possible relationship to similar features observed in perovskites.

Karin Rabe
Department of Physics and Astronomy,// Rutgers University,// Piscataway, New Jersey 08854-8019

Date submitted: 29 Nov 2004 Electronic form version 1.4