Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Structural Transitions in IrV and RhV[1] MICHAEL MEHL, Naval Research Laboratory, Washington DC, STEFANO CURTAROLO, Duke University, Durham NC and Weizmann Institute of Science, Rehovot, Israel, GUS HART, Brigham Young University, Provo UT — The orthorhombic αIrV phase is only observed in the intermetallics IrV and RhV, where it appears in an apparently second-order phase transition from the tetragonal $L1_0$ phase upon cooling below 500°C.[2] It has been suggested that this transition is driven by an unstable phonon at the R point of the $L1_0$ Brillouin zone.[3] First principles calculations show that all of the phonon modes at R are stable in both materials. We do find a region of unstable phonons near and along the line $(\frac{1}{4}y\frac{1}{2})$. None of these modes relaxes directly into the αIrV structure. The lowest, at $y = \frac{1}{4}$, relaxes the system into the Ga_3Pt_5 structure, which is itself vibrationally unstable at the Γ point, relaxing into a structure with symmetry Amm2 which has not been seen in any intermetallic. We follow this pathway of phonon instabilities to lower energy structures. We also discuss the possibility that the structural transition might be first-order, rather than second-order as indicated.

[1]Parital support from US Office of Naval Research and US DoD High Performance Computing program.
[2]B. Chen and H. F. Franzen, J Less-Common Metals **159** 343-7 (1990).
[3]H. F. Franzen, Chem. Mater. **2**, 486-491 (1990).

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Date submitted: 18 Nov 2009 Electronic form version 1.4