Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Structure and stability of Al$_2$Fe and Al$_5$Fe$_2$ MICHAEL WIDOM, Carnegie Mellon University, MAREK MIHALKOVIC, Slovakian Academy of Sciences — We employ first principles total energy and phonon calculations to address the structure and stability of Al$_2$Fe and Al$_5$Fe$_2$. The observed structure of Al$_2$Fe, which is reported as stable in the assessed Al-Fe phase diagram, is distinguished by an unusually low triclinic symmetry. The initial crystallographic structure determination additionally featured an unusual hole large enough to accommodate an additional atom. Our calculations indicate the hole must be filled, but predict the triclinic structure is unstable relative to a simpler tetragonal structure based on the prototype Mo Si$_2$. This tetragonal structure is interesting because it is predicted to be nonmagnetic, electrically insulating and high density, while the triclinic structure is magnetic, metallic and low density. We reconcile this seeming contradiction by demonstrating a high vibrational entropy that explains why the triclinic structure is stable at high temperatures. Finally, we note that orthorhombic Al$_5$Fe$_2$ is also destabilized by the tetragonal structure but may be stabilized at high temperatures, again by vibrational entropy and partial occupancy associated with the diffusion of Al atoms along channels.

Michael Widom
Carnegie Mellon University

Date submitted: 10 Nov 2011
Electronic form version 1.4