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Structure and stability of Al_2Fe and Al_5Fe_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_2Fe and Al_5Fe_2. The observed structure of Al_2Fe, 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 explai ns why the triclinic structure is stable at high temperatures. Finally, we note that orthorhombic Al_5Fe_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.

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