Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First Principles Calculation of Elastic Properties of Early-Late Transition Metal Alloys WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — Amorphous metals are of practical interest in applications requiring high strength materials. We choose to examine the elastic properties of crystalline phases to understand the elastic properties of amorphous solids. In this talk, we discuss our work using first principles methods to calculate elastic properties for crystalline alloys in various chemical families containing transition metals, specifically early (Ta,W) and late (Fe,Co,Rh,Ni,Cu,Zn) due to their good glass forming ability, as well as select borides. Certain Laves phases, which are known to have local chemical ordering similar to amorphous solids, are focused on. We analyze trends in the elastic properties of chemical families based on computed enthalpies of formation, elastic properties of pure elemental phases, and electronic and structural information. In particular, we use effective medium theories and enthalpies of formation to predict trends in bulk moduli. This information can be used to predict future candidate systems for high-strength amorphous metals.

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Date submitted: 08 Nov 2012 Electronic form version 1.4