

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Characteristic Picture of Fe-Based Disordered Alloys: *Ab Initio* Study S. J. KANG, MIYOUNG KIM, Seoul National University, YOUNG-KYUN KWON, Kyung Hee University — We use *ab initio* density functional theory to investigate the stability, elastic properties and thermal expansion behaviors of various Fe-based alloys. We focus on systems with cubic unit cell containing between 54 and 128 atoms constructed on underlying body-centered cubic Fe structure with 1 to 20 % of Al, Si, and/or Mn substitutions. We calculate the formation energy of each of the energetically stable disordered structures by performing the geometry relaxation. Physical properties of such alloys are determined by their crystalline structures, and the concentration and atomic configuration of substituted atoms. It is found that their mechanical characters depend on the disorderness of substituted atoms. We study the effect of manganese, which prevents the Fe-based alloy from forming secondary phase exhibiting poor mechanical property. Unusual mechanical properties are found in certain disordered Fe-Si and Fe-Al alloys. Moreover, their thermal expansion behaviors and their effect on structures and atomic configurations are also investigated by molecular dynamics simulations. Most of our results are comparable to experimental data available and their unknown physical reasons will be discussed.

Young-Kyun Kwon
Kyung Hee University

Date submitted: 20 Nov 2009

Electronic form version 1.4