Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Role of the defect core in energetics of vacancies in aluminum**[1]

VIKRAM GAVINI, Department of Mechanical Engineering — Electronic structure calculations at macroscopic scales are employed to investigate the crucial role of a defect-core in the energetics of vacancies in aluminum. We find that vacancy core-energy is significantly influenced by the state of deformation at the vacancy-core, especially volumetric strains. Insights from the core electronic structure and computed displacement fields show that this dependence on volumetric strains is closely related to the changing nature of the core-structure under volumetric deformations. These results are in sharp contrast to mechanics descriptions based on elastic interactions that often consider defect core-energies as an inconsequential constant. Upon studying the influence of various macroscopic deformations, which include volumetric, uniaxial, biaxial and shear deformations, on the formation energies of vacancies, we show that volumetric deformations play a dominant role in governing the energetics of these defects. Further, by plotting formation energies of vacancies and di-vacancies against the volumetric strain corresponding to any macroscopic deformation, we find that all variations in formation energies collapse on to a *universal* curve. Implications of these results in the context of dynamic failure in metals due to spalling are analyzed.

[1]Air Force Office of Scientific Research, Grant no. FA9550-09-1-0240.

Vikram Gavini
Department of Mechanical Engineering

Date submitted: 16 Nov 2009 Electronic form version 1.4