Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

High-stress phases of SiC, GaN, InN, ZnO, and CdSe KANOKNAN SARASAMAK[1], AMBARISH J. KULKARNI, MIN ZHOU, SUKIT LIMPIJUMNONG, Suranaree University of Technology, Thailand — Phase transformations of SiC, GaN, InN, ZnO, and CdSe from wurtzite (WZ) to three other different crystalline structures under loading of different stress tensors are studied using first-principle calculations. The first transformation studied is well known and occurs under hydrostatic compression and leads to a six-fold coordinated *rocksalt* (RS) structure. The equilibrium pressures for this transformation of the materials are calculated and found to be proportional to the energy difference between the phases at zero stress and vary monotonically with the materials' ionicity. The second and third transformations studied occur under uniaxial stresses and lead to two new crystal structures previously unknown for these materials. Specifically, uniaxial compression along the [0001] direction or uniaxial tension along the $[01\bar{1}0]$ direction, causes a transformation to a five-fold coordinated *unbuckled wurtzite* structure which we named HX. On the other hand, uniaxial tension along the [0001] direction causes the materials to transform into a body-centered-tetragonal structure which we named BCT-4. The critical equilibrium transformation stresses for these transformations are obtained and their correlation with the ionicity of the materials is analyzed.

[1]currently at CWRU, Cleveland, OH 44106

Kanoknan Sarasamak
Suranaree University of Technology, Thailand

Date submitted: 22 Nov 2007 Electronic form version 1.4