Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Modeling of extended solids using DFT and evolutionary algorithms. ISKANDER G BATYREV, US Army Research Lab. — We present overview of our recent results on simulation of poly-CO, mixtures of N2 and H2, and mixtures of N2 and CO gases in amorphous and crystalline phases under high pressure using density functional theory (DFT) and evolutionary algorithms. Structure of N-H extended network under high pressure was modelled using the evolutionary program USPEX based on plane wave DFT calculations with norm-conserving pseudopotentials. Range of the studied pressures was 10 – 50 GPa on compression, and from 50 to 10 GPa on isotropic decompression of the extended network. Formation of an extended network with covalent bonds occurs between 30-50 GPa. Higher concentration of N requires higher pressure to form a covalent bond network. New structure of NH extended solids with high symmetry and covalent bonds are predicted: with C2M(C2H-3) symmetry group for 9:1 ratio, with PBAM (D2H+9) symmetry group for 4:1 ratio, and with P-1(CI-1) for 3:1 ratio of N_2 to H_2 gas. Modeling structure of N2-CO crystals using the same methods resulted in formation of crystals with covalent bonds and high symmetry: P41212 (D4+4) for 50% of N2 and CO, CM (CS-3) for 80 N2 and 20% CO, and R3 (C3-4) for 90% N2 and 10% CO at pressure of 50 GPa. We show that some of the structures, obtained at high pressures, may exist upon lowering of the pressures.

Iskander G Batyrev
US Army Research Lab.

Date submitted: 09 Nov 2016 Electronic form version 1.4