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**Modeling of formation of extended NH solids under high pressure.** ISKANDER G. BATYREV, US Army Research Laboratory — Structure of N-H extended network under high pressure was modelled using the evolutionary algorithm program USPEX based on plane wave DFT calculations (VASP). Concentration ratio of $N_2$ to $H_2$ gases was 3:1, 4:1, and 9:1. Range of the studied pressures was 10 – 50 GPa on compression, and from 50 to 1 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 covalent bonds are predicted: with P-1(CI-1) 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. Calculations of the mixtures of $N_2$ and $H_2$ gases at pressures in the range of 10-20 GPa resulted in a variety of structures without a covalent network, but consisting of nitrogen-containing molecules. For example, the lowest energy structure for a 3:1 ratio of N to H atoms consists of tetrazene and $N_2$ molecules. At 10 GPa the lowest energy structure appears to be a combination of protonated ammonia and $N_2$ molecules.

Iskander G. Batyrev
US Army Research Laboratory

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