Abstract Submitted
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Modeling and measurements of XRD spectra of extended solids under high pressure.[1] I.G. BATYREV, S.P. COLEMAN, US Army Research Laboratory, APG, MD 21005-5069, E. STAVROU, J.M. ZAUG, Lawrence Livermore National Laboratory, 7000 East Ave, Livermore, CA 94550, J.A. CIEZAK-JENKINS, US Army Research Laboratory, APG, MD 21005-5069 — We present results of evolutionary simulations based on density functional calculations of various extended solids: N-Si and N-H using variable and fixed concentration methods of USPEX. Predicted from the evolutionary simulations structures were analyzed in terms of thermo-dynamical stability and agreement with experimental X-ray diffraction spectra. Stability of the predicted system was estimated from convex-hull plots. X-ray diffraction spectra were calculated using a virtual diffraction algorithm which computes kinematic diffraction intensity in three-dimensional reciprocal space before being reduced to a two-theta line profile. Calculations of thousands of XRD spectra were used to search for a structure of extended solids at certain pressures with best fits to experimental data according to experimental XRD peak position, peak intensity and theoretically calculated enthalpy. Comparison of Raman and IR spectra calculated for best fitted structures with available experimental data shows reasonable agreement for certain vibration modes.

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