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Atomic structure and elastic properties at high pressure of aluminum oxynitride in cubic phase I.G. BATYREV, J.W. MCCAULEY, B.M. RICE, G.A. GAZONAS, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, A.R. OGANOV, Department of Geosciences and Department of Physics and Astronomy, State University of New York, Stony Brook, NY 11794-2100 — The atomic structure and elastic properties of aluminum oxynitride spinel (AlON) at high pressure (up to 40 GPa) have been calculated from first principles. We have assumed an "ideal" stoichiometry of cubic AlON with 35.7 mole % AlN using the constant anion model. The elastic constants were calculated from independent strains that were applied to a unit cell, parameterizing the total energy as a function of the strain and from a stress-strain relationship. At ambient conditions a clustered distribution of N atoms has $\sim$ 1 eV per 55 atoms higher total energy than for a random distribution and slightly, but systematically lower elastic constants. The pressure dependence of C_{11}, C_{12} and C_{44} for random and cluster distributions of N atoms was calculated in the range of 0-40 GPa by performing six finite distortions of the lattice and deriving the elastic constants from the strain-stress relationship. The calculated values of dC_{11}/dP are in the range of 4.0-6.2 and for dC_{44}/dP $\sim$0.8-1.5. The estimates are in reasonable agreement with experimental measurements of polycrystalline AlON. The minimum energy structure of AlON was found using the evolutionary algorithm USPEX (Oganov & Glass, 2006)

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