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First Principles Investigation of Structure and Electronic Properties of $a-$ Si_3N_4 RAVI PRAMOD VEDULA, NATHAN L. ANDERSON, ALEJANDRO STRACHAN, Purdue University — We use a combination of molecular dynamics with empirical inter-atomic potentials and density functional theory (DFT) calculations to generate an ensemble of statistically independent, well relaxed a-Si_3N_4 structures. Variations in the annealing conditions used to generate the structures lead to zero-stress structures spanning a wide range of densities ($2.6 g/cm^3$ to $3.1 g/cm^3$) but exhibiting very similar cohesive energies. The bulk modulus was found to be varying between 110-180 GPa depending on the density. The predicted density variation agrees well with the range in experimentally observed density, resulting from different fabrication conditions. The radial distribution functions and angle distributions for different densities are in good agreement with diffraction experiments; further validating our models. The slow annealing procedure used to generate the structures leads to well equilibrated structures with relatively small density of coordination defects and several defect free structures. We also compute the formation energy and charge transition levels for the defects found.

Ravi Pramod Vedula
Purdue University

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