**Structure and properties of inter-granular glassy film in β-Si3N4**

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Based on a previously constructed intergranular glassy film (IGF) model for bulk silicon nitride, a large periodic model of 3864 atoms containing two grains of different orientations and two IGFs was fully relaxed using the *ab initio* density-functional theory. The electronic structure, density of states, and interatomic bonding are obtained and analyzed focusing on the interfacial regions between bulk β-Si3N4 and the Si-O-N glass layer with different orientations. The total bond order density (TBOD), a quantum mechanical metric, is evaluated in different interfacial and bulk regions to reveal the subtle differences in the internal cohesion between crystalline grains of different facets. Moreover, the mechanical properties of this IGF model are calculated using a stress vs strain approach showing the effect of a less rigid glassy layer is the reason for its structural flexibility. These results are compared with parallel calculations on crystalline α-Si3N4, β-Si3N4 and Si2N2O. The insights obtained from these detailed DFT calculation and analysis are discussed in the broader context of implications on the strength, fracture toughness, and processing methods for nanoscale materials.