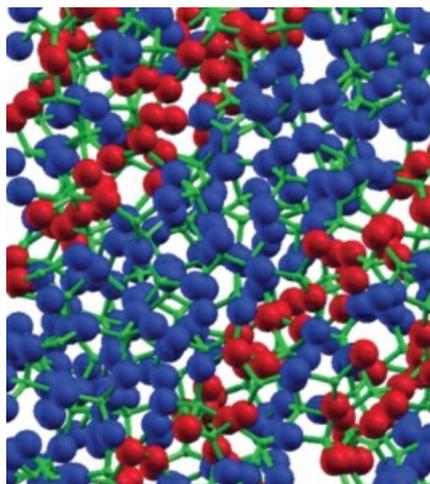


Microscopic mechanisms of the pressure-induced amorphization of SiO₂

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When the low-pressure tetrahedral phases of SiO₂ are compressed at room temperature they retain their structures at pressures well above their stability domain, but they all collapse into denser structures when pressure reaches about 20 GPa. Depending on the experimental conditions, pressure-induced densification can be accompanied by amorphization; by the formation of crystalline, metastable polymorphs; and can be preceded by the appearance of intermediate phase. Based on molecular dynamic simulations, we show that this rich phenomenology can be rationalized through a unified theoretical framework of the atomistic pathways leading to densification. The model emphasizes the role played by the oxygen sublattice, which transforms from a bcc-like order into close-packed arrangements in the denser structures, through a ferroelastic instability of martensitic nature.



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