

Abstract Submitted
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Modeling of amorphous poly-CO structure with N and He I.G. BATYREV, W.D. MATTSON, US Army Research Laboratory — Density functional theory simulations of amorphous poly-CO structure were performed with addition of N or He atoms to crystalline delta phase of CO. For the CO-N mixtures the concentration of N was varied in the range from 6.25 % to 50% with different distribution of N atoms in the unit cell. For all studied concentrations and initial configurations, isotropic compression led to polymerization beginning at a pressure of 11 GPa. For the CO-He mixtures, the concentration of He atoms in delta phase of CO was 6.25%. Formation of random networks begins at 9 GPa and at 11 GPa all CO molecules have formed a combination of closed rings and chain type structures without isolated CO molecules with a density of 2.40 g/cm³. He atoms facilitate complete formation of the random structure at lower pressure than that for pure poly-CO, which isn't completely polymerized until compressed to a pressure of 18 GPa. He atoms also help stabilize the structure while lowering the pressure down to 100 Bar with only few CO molecules detaching in the process. Without He atoms at the same pressure there are approximately ten times the number CO molecules occupying voids in the random network.

Janathan Mullin
US Army Research Laboratory

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