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Computational search and investigation of structural phases of Aluminum-Carbon alloy

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Abstract
In this study, we employed an evolutionary algorithm and density functional theory (DFT) calculations to identify stable and metastable structural phases of aluminum-carbon compounds. Initially, a variable - composition structure search was conducted at ambient pressure to determine the convex hull of the system. Subsequently, we performed a fixed - composition structure search for alloys located on this convex hull, along with some neighboring alloys to identify their stable and metastable structural phases. Along with the most stable phase, seven metastable phases were chosen from this set, and their phonon, mechanical, and electronic properties were determined using DFT calculations. The phonon dispersion calculations reveal that all eight chosen structures are dynamically stable. A comparison of the mechanical properties of these structures reveals a novel and extremely hard phase in the aluminum-carbon alloy, which can be synthesized in thin-film form or utilized in high-temperature operating conditions. First-principles electronic structure calculations reveal that surface carbon doping in the Al-C system enables tunable metallic conductivity while maintaining an exceptional hardness-to-weight ratio.

Keywords: Aluminum-Carbon Alloy; Evolutionary Algorithm; Density Functional Theory (DFT); Stable and meta stable structures; Mechanical and Electronic Properties

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