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A new tetragonal superhard metallic carbon allotrope

Qun Wei[a,*], Quan Zhang[b], Haiyan Yan[c], Meiguang Zhang[d,**], Bing Wei[a]

[a] *School of Physics and Optoelectronic Engineering, Xidian University, Xi'an 710071, PR China*

[b] *School of Microelectronics, Xidian University, Xi'an 710071, PR China*

[c] *College of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, 721013 Baoji, PR China*

[d] *College of Physics and Optoelectronic Technology, Baoji University of Arts and Sciences, Baoji 721016, PR China*

Abstract

A new metallic superhard carbon allotrope C_5 with five carbon atoms per unit cell is theoretically predicted to be stable at ambient pressure through first-principles calculations combined with unbiased swarm structure searching techniques. This novel carbon allotrope consisting of a mixture of sp^2 and sp^3 carbon network exhibits excellent mechanical properties with claimed hardness of 58.5 GPa. Results from our calculated strain-stress relationship reveals that the failure mode of crystal lattice for C_5 is dominated by shear type in the (010)[101] direction with shear stress magnitude of 74.3 GPa. The calculated electronic band structure of C_5 suggests its metallic nature. Detailed analyses of band decomposed charge density show that the metallic nature is contributed by the sp^2 carbon atoms, which form conducting pathways along the *a*- and *b*-axes.

Keywords: superhard metallic carbon; first-principles calculations; mechanical and electronic properties