SACADA Database Code: 132

Topology: 3,4T157

# of independent nodes (IN): 2
Transitivity: [2465]
Space Group: P6/mmm
Pearson: hP24
Coordination Number (CN): 3, 4 (1:1)

Year: 2002

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T157 (SACADA #132)		2.660		1.007	301.9	244.9	35.3	SACADA[1]
Polymerized carbon (6,0)Nanotub	2-5		1.27					doi: 10.1134/1.1470541

Elasticity tensor (kBar)[1]

5461.3169	1746.1139	983.2960	0.0000	0.0000	-0.0000
1746.1139	5461.3169	983.2960	0.0000	0.0000	0.0000
983.2960	983.2960	9242.4415	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	1857.6015	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	2659.5483	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	2659.5483

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].