SACADA Database Code: 203

Topology: $3^2,4^2$T202

# of independent nodes (IN): 4
Transitivity: [4423]
Space Group: F23
Pearson: cF84
Coordination Number (CN): 3, 4 (16:5)

Year: 2003

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^2$T202 (SACADA #203)		2.492		1.461	121.9	97.4	13.7	SACADA[1]
C21 crystal			Metal					doi: 10.1140/epjb/e2003-00060-4

Elasticity tensor (kBar)[1]

2284.1868	687.3980	687.3980	0.0000	-0.0000	-0.0000
687.3980	2284.1868	687.3980	-0.0000	0.0000	0.0000
687.3980	687.3980	2284.1868	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	1112.0938	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	1112.0938	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	1112.0938

[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].