SACADA Database Code: 84

Topology: umk

# of independent nodes (IN): 1
Transitivity: [1452]
Space Group: P63/mcm
Pearson: hP24
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
umk (SACADA #84)		2.663		0.641	301.4	258.0	40.1	SACADA[1]
TA4								doi: 10.1134/s1063776111060173
TA4								link

Elasticity tensor (kBar)[1]

6436.2949	1694.1020	854.7126	3.4619	0.5649	-0.9088
1694.1020	6393.8623	854.9397	9.7839	9.4798	0.6203
854.7126	854.9397	7488.4984	3.6560	-6.2088	0.0981
3.4619	9.7839	3.6560	2350.8770	4.9850	3.1790
0.5649	9.4798	-6.2088	4.9850	2507.8646	0.2513
-0.9088	0.6203	0.0981	3.1790	0.2513	2497.7001

[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].