SACADA Database Code: 226

Topology: fer

# of independent nodes (IN): 4
Transitivity: [4874]
Space Group: Immm
Pearson: oI36
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
fer (SACADA #226)		2.940		1.059	332.5	312.1	53.6	SACADA[1]
C-FER			2.5					doi: 10.1002/anie.199307011

Elasticity tensor (kBar)[1]

6839.0559	464.1122	630.1951	33.2898	-0.9174	1.6266
464.1122	10836.9804	26.9832	-13.6266	-1.2317	0.1135
630.1951	26.9832	10493.6537	-4.8664	1.0033	0.8143
33.2898	-13.6266	-4.8664	1833.1307	0.2295	2.1271
-0.9174	-1.2317	1.0033	0.2295	3792.0499	-2.4650
1.6266	0.1135	0.8143	2.1271	-2.4650	2176.1872

[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].