نشریه مهندسی مکانیک امیرکبیر

Amirkabir Journal of Mechanical Engineering

Amirkabir J. Mech. Eng., 55(10) (2024) 253-256
DOI: 10.22060/mej.2024.22431.7617

Investigating of the stability and structural, mechanical and electronic properties of two new superhard conductive carbon structures

S. Ghorbanali[1]*, E. Zaminpayma[2]

[1] Department of Physics, Tafresh University, Tafresh, Iran
[2] Department of Physics, Qazvin Branch, Islamic Azad University, Qazvin, Iran

ABSTRACT: In this research, two new superhard metallic carbon allotropes αC28 and βC32 are predicted using density functional theory (DFT). These stable tetragonal structures belong to the P4/MMM space group. Molecular dynamics simulation performed under canonical ensemble (NVT) to investigate the thermal stability of new αC28 and βC32 carbon crystals at temperatures of 300 and 1000 K, confirms their thermal stability. In addition, we calculated the mechanical coefficients and band gap energy of these two structures to examine their mechanical and electronic stability. These new carbon allotropes are composed of sp2 and sp3 bond hybridization, which shows excellent mechanical properties with Vickers hardness of 45.7 and 47.9 GPa. Other mechanical properties of these crystals such as bulk modulus (265.8, 284.9), shear modulus (254.7, 273.5), and Young's modulus (579.1, 621.6) also confirm the superhardness of these structures. The results related to the electronic band structures indicate that both structures have metallic properties. The width of both conduction and valance bands for both structures is about 20 eV. The results of calculations show that αC28 and βC32 can be synthesized in the laboratory in the future and will have potential applications in mechanical and electronic devices.

Review History:
Received: may, 25, 2023
Revised: Jan. 09, 2024
Accepted: Jan. 13, 2024
Available Online: Jan. 23, 2024

Keywords:
New carbon structures
superhard materials
thermodynamic stability
elastic constants
electronic properties

1- Introduction

Carbon, as one of the most important elements of superhard materials, has a valence electron structure of $2s^2 2p^2$, which can create new allotropes with different properties with sp, sp^2, and sp^3 hybrid bonds. Among them, the most famous and widely used superhard material is diamond, due to its scarcity in the world and complicated conditions for laboratory synthesis, the search for new superhard materials has attracted the attention of many researchers[1, 2]. In this study, we proposed two new superhard tetragonal carbon structures named αC_{28} and βC_{32}, whose electronic and mechanical properties were investigated through density functional theory (DFT). With many searches in SACADA[3], and RCSR[4] carbon databases and articles in this field, the originality of these two structures was confirmed for the authors. The structural, electronic, and elastic properties along with elastic anisotropy properties, and thermal, dynamic, and mechanical stability of these structures have been investigated in this research work.

2- Methodology

In recent years, DFT has been used as an important theoretical tool to predict the physical properties of various new crystals[5]. Here, the calculations were performed using the fixed core PAW method with the help of the SIESTA simulation code, in which the within the general gradient approximation (GGA) with the correlation function of the PBE code was used to parameterize the potential exchange-correlation[6].

3- Results and Discussion

The investigated crystals consist of four, five, and eight-sided irregular carbon rings, whose network parameters at ambient pressure are shown in Table 1.

Table 1. Crystallographic data for αC28 and βC_{32}.

	Diamond	αC_{28}	βC_{32}
Space group	Fd-3M(227)	P4/MMM	P4/MMM
C_1-C_1	1.44	1.44	1.46
C_1-C_2	-	1.48	1.49
C_2-C_3	-	1.52	1.50
C_3-C_3	-	1.56	1.54
C_3-C_4	-	1.53	1.55
C_4-C_4	-	1.50	1.52
a, b	3.57	6.08	6.09
c	-	5.68	7.19
ρ	5.68	7.499	8.345
V	3.517	2.658	2.392

*Corresponding author's email: s.ghorbanali@tafreshu.ac.ir

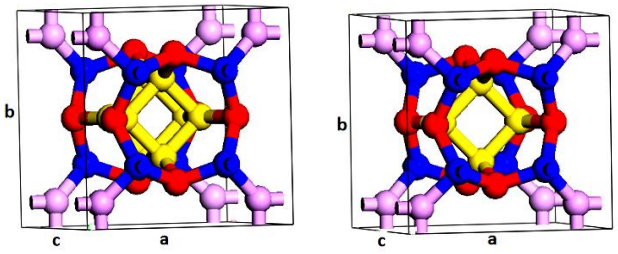

Fig. 1. Crystal structure of αC28 and βC_{32}.

The proposed αC_{28} and βC_{32} superhard carbon structures have tetragonal symmetry and P4/MMM group, which are shown in Fig.1. These structures consist of four types of non-equivalent carbon atoms, which are marked with different colors in the figure.

To investigate the thermal stability of αC_{28} and βC_{32} carbon crystals at temperatures above zero such as 300 and 1000 K, molecular dynamics simulation was performed under canonical ensemble (NVT).

In Fig. 2 and Fig. 3, throughout the simulation, the total energy fluctuates around a constant value at 300 K and 1000 K, so these new crystalline phases have good thermal stability in the mentioned temperature range. To determine the mechanical stability, the values of independent elastic constants C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66} related to carbon crystals αC_{28} and βC_{32} are calculated and the results are listed in Table (2). The elastic constant components αC_{28} and βC_{32} are consistent with the mentioned Born equations (Eq. 1), which can be concluded that the predicted structures are mechanically stable at ambient pressure.

Table 2. Calculated elastic constants, elastic modulus (GPa), and hardness (GPa) of αC28 and βC_{32}.

	diamond	αC_{28}	βC_{32}
C_{11}	1056.2	672	697
C_{33}	-	535	627
C_{44}	566.7	281	286
C_{66}	-	193	223
C_{12}	120.1	162	125
C_{13}	-	56	75
B	431	265.8	284.9
G	522	254.7	273.5
E	1116	579.1	621.6
v	0.07	0.136	0.135
B/G	0.825	1.044	1.042
H_v	89	45.7	47.9

$$C_{44}\rangle 0, C_{66}\rangle 0, C_{11}\rangle C_{12}$$
$$2C_{13}{}^{2}\rangle C_{33}\left(C_{11}+C_{12}\right) \quad (1)$$

To check the electrical properties, the band structure of these crystals was calculated at the symmetrical points shown in Fig. 4 and Fig. 5 (the Fermi level is at zero).

As can be seen in the figure, both structures are these new carbon allotropes are metallic and there is no energy gap between valence and conduction bands.

In the end, to ensure the establishment of bonds and the formation of hybridization between carbon atoms, the density of electrons in the inner space of the unit cell was investigated and calculated, and the results of the calculations are shown

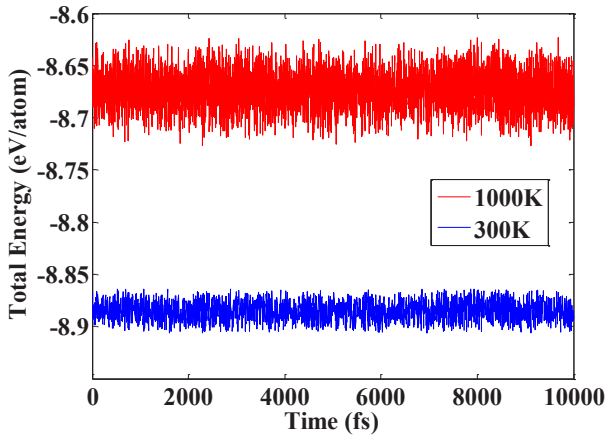

Fig. 2. Total energy fluctuations versus time for αC_{32}

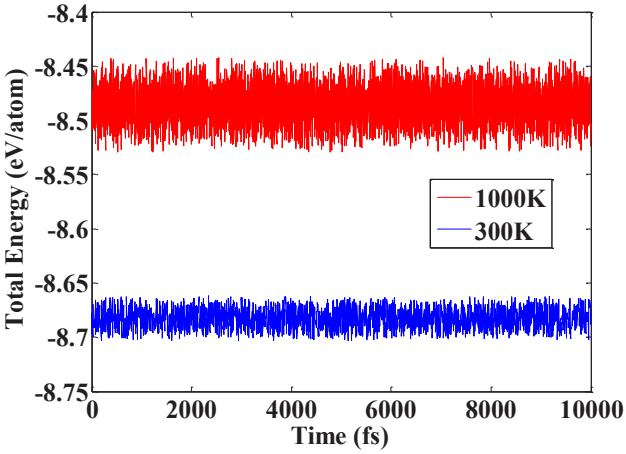

Fig. 3. Total energy fluctuations versus time for αC_{28}

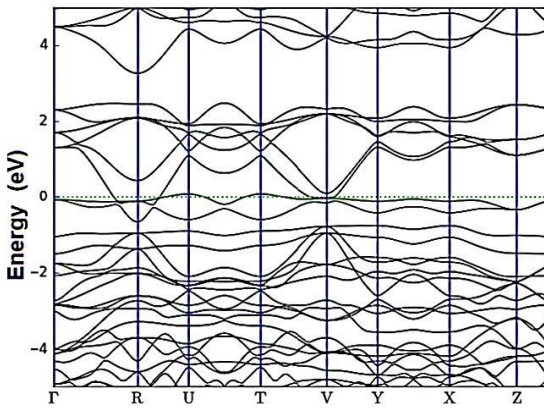

Fig. 4. Total energy fluctuations versus time for αC_{28}

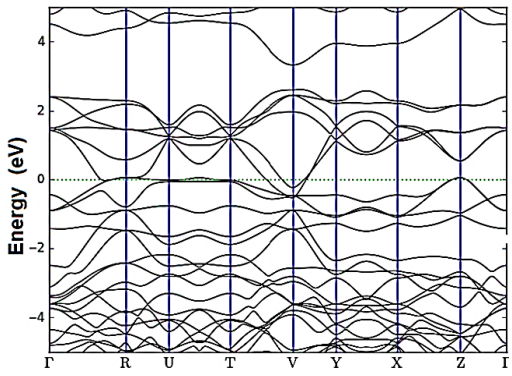

Fig. 5. Electronic band structure for αC_{28}

in Fig. 6. As the figure shows, the corresponding bonds are formed and the electrons are spread around the atomic bonds.

4- Conclusions

In this study, based on DFT method, two new superhard carbon structures that have metallic properties were predicted. It was found that the structures of αC_{28} and βC_{32} are mechanically and thermodynamically stable, which was done by elastic constants and checking the energy calculation, respectively.

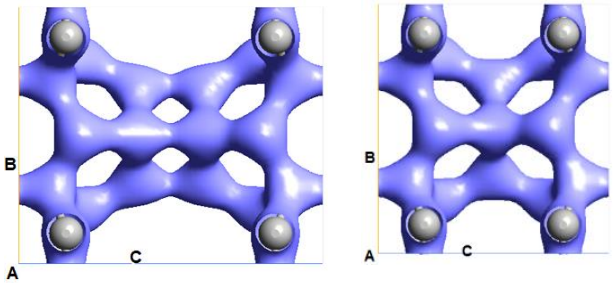

Fig. 6. Electron charge density of αC28 and βC_{32}.

References

[1] M. Xing, X. Li, An orthorhombic carbon allotrope with a quasi-direct band gap and superhard, Diamond and Related Materials, 131 (2023) 109592.

[2] Q. Fan, C. Li, R. Yang, X. Yu, S. Yun, A larger-cell tetragonal carbon allotrope tP176 carbon with superhardness, Materials Letters, 326 (2022) 132925.

[3] R. Hoffmann, A.A. Kabanov, A.A. Golov, D.M. Proserpio, Homo citans and carbon allotropes: For an ethics of citation, Angewandte Chemie International Edition, 55(37) (2016) 10962-10976.

[4] M. O'Keeffe, M.A. Peskov, S.J. Ramsden, O.M. Yaghi, The reticular chemistry structure resource (RCSR) database of, and symbols for, crystal nets, Accounts of chemical research, 41(12) (2008) 1782-1789.

[5] W. Kohn, L.J. Sham, Statistical Mechanics of an Assembly of Quasiparticles, Phys. Rev, 140(4) (1965) A1133.

[6] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Physical review letters, 77(18) (1996) 3865.

HOW TO CITE THIS ARTICLE

S. Ghorbanali, E. Zaminpayma, Investigating of the stability and structural, mechanical and electronic properties of two new superhard conductive carbon structures, Amirkabir J. Mech Eng., 55(10) (2024) 253-256.

DOI: 10.22060/mej.2024.22431.7617