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Research Article

Keywords: C3N and BC3 nanosheets, C3N-BC3 hybrid, Ballistic properties, Molecular dynamics

Posted Date: December 15th, 2020

DOI: <https://doi.org/10.21203/rs.3.rs-118827/v1>

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Version of Record: A version of this preprint was published at Scientific Reports on April 12th, 2021. See the published version at <https://doi.org/10.1038/s41598-021-86537-z>.

Hypersonic impact properties of pristine and hybrid single and multi-layer C₃N and BC₃ nanosheets

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Abstract

Two-dimensional (2D) materials are competitive candidates replacing or supplementing conventional semiconductors due to their atomically uniform thickness. To observe and exploit the unique properties of two-dimensional (2D) materials, it is therefore vital to obtain clean and repeatable interfaces. Also, carbon, nitrogen, and boron nanostructures are promising ballistic protection materials due to their low density and excellent mechanical properties. In this study, we evaluated the ballistic properties of C₃N and BC₃ nanosheets against the hypersonic bullets with Mach number greater than 6. Besides, we created a hybrid sheet using van der Waals bonds between them based on the hypervelocity impacts of fullerene (C₆₀) molecules utilizing molecular dynamics simulation. In the following, the ballistic properties of different structures were examined, and it was shown that C₃N nanosheets have higher absorption energy than BC₃ after C₆₀ penetration. In contrast, in lower impact speeds and before penetration, single-layers exhibited almost similar behavior. Our findings also reveal that in hybrid

structures, the C_3N layers will improve the ballistic properties of BC_3 . The energy absorption values with a variable number of layers and interlayer distance are investigated, for homogeneous or hybrid configurations (stacking of C_3N and BC_3). In this work, we have discussed two interlayer distances of $X = 3.4\text{\AA}$ and $4X = 13.6\text{\AA}$ for different configurations. These results provide a fundamental understanding of ultra-light multilayered armors' design using nanocomposites based on advanced 2D materials. It can also be used to select and make 2D membranes and allotropes for DNA sequencing and filtration.

Keywords: C_3N and BC_3 nanosheets; C_3N - BC_3 hybrid; Ballistic properties; Molecular dynamics

1 Introduction

Two-dimensional materials have been able to revolutionize the use of materials in various fields shortly after their discovery. The interface mediating the connection between nanomaterials and other materials or between themselves is the most important factor and place for new features to emerge ^{1,2}. Graphene is one of the most significant 2D materials. Utilize a variety of practical problems faced graphene for specific applications. The zero-band characteristic of graphene limits its applications in semiconductors. Two of the known (2D) dielectric materials are polyaniline (C_3N) and BC_3 . The results show that C_3N and BC_3 are semiconductors with a band-gap of 0.39eV and 0.54eV, respectively ^{3,4}. C_3N is a semiconductor that can be tuned to cover the entire visible range by the fabrication of quantum dots with different diameters ⁵. Due to the appearance of new properties and their several applications, 2D hybrid materials have been studied by many researchers ⁶. The mechanical properties of pure BC_3 and C_3N are studied, and details of the results are available under different conditions.

Mechanical results showed that Young's modulus of C_3N is higher than graphene and other 2D materials ⁷⁻⁹. So, we can say that C_3N and BC_3 are excellent candidates for replacement with graphene for different applications. The mechanical properties of C_3N sheets without any defects and containing some defects, such as cracks and cavities, were examined. It has also been shown that as the temperature rises from 200 to 900 Kelvin, Young's modulus decreases by 9% ¹⁰. In 2019, using a simulation of molecular dynamics, Zahedi et al. studied the mechanical properties of BC_3 with a focus on defects at different temperatures. The results of this work are compared with C_3N and show that the mechanical properties of C_3N under the same conditions are higher than BC_3 and the higher values of elastic modulus due to stiffening in C-N bond compared with C-B bond ones ¹¹. The mechanical and thermal properties of the hybrid of 2D materials are available using molecular dynamics simulation ¹²⁻¹⁹. Using the MD technique, in 2013, Zhao et al. examined the mechanical properties of hybrid graphene and hexagonal boron nitride (h-BN) sheet with the concentration of BN, ranging from 0% to 100%. Irrespective of the form and distribution of BN, Young's modulus of the hybrid sheet decreases with increasing concentration of BN. However, adding a small amount of BN to graphene causes a noticeable drop in the strength of the hybrid sheet ¹². The ballistic properties of 2D materials are of great importance. Protecting structures and devices from the impact of high-energy projectiles is still an open issue for theoretical modeling and applied research. It is also relevant in several technology topics, including materials science and engineering, automotive, aerospace, and defense ²⁰. Spacecrafts, for instance, are frequently exposed to micrometeoroids and orbital debris hypervelocity collisions (velocities of up to 7–8 km/s). They result in surface degradation, failures on-board instrumentation up to full perforation, and structural damage during operation. In 2017, Signetti et al. studied the ballistic properties of 2D materials due to the high velocity of the collision of a C_{60} molecule using the DFT and FEM simulation

methods. The critical penetration energy of graphene membranes and 2D allotropes, including h-BN, has been determined as a case study. In addition, the rules of scalability of energy absorption with the variable number of layers and the distance between the layers have been investigated for homogeneous or hybrid configuration ²¹. By combining the finite element method and the molecular dynamics method, Sadeghzadeh and his colleagues were able to model the problem of different particles colliding with graphene plates in a relatively comprehensive way. They showed that the number of layers, aspect ratio, sheet size, interlayer distance, delamination, and projectile shape significantly influence the impact resistance of graphene sheets ²². In another study, Rafael et al. studied the scale effect on the ballistic penetration of graphene sheets. In this work, a combination of numerical and analytical modeling has been employed to address this issue. They used the reactive molecular dynamics method and examined ballistic tests for single, double, and triple-layered graphene sheets. Their results showed that the specific penetration energy decreases as the number of layers (N) increases, from ~ 15 MJ/kg for $N = 1$ to ~ 0.9 MJ/kg for $N = 350$, for an impact velocity of 900 m/s ²³. The ballistic tests on the two-dimensional materials have also been observed in other works ^{24,25}.

So far, there have been no reports of the ballistic properties of BC_3 and C_3N structures. Therefore, due to the unique properties of these two structures and potential applications in various industries, as well as the structural similarity with graphene and the fact that in some properties due to the weakness of graphene can replace graphene in electronic devices, a more detailed study of the ballistic properties of this type of graphene-like structures is essential. Therefore, the ballistic properties of C_3N and BC_3 were examined using an MD simulation technique. In different conditions, the elastic properties of the two structures have been studied and compared. The findings show the outstanding mechanical properties of semiconductors BC_3 and C_3N in full. These features make them

promising designers and also introduce them to the new catalysts for the design of new nanoelectronics and nanoelectromechanical devices.

2 Computational Methods

A large-scale atomic/molecular massively parallel simulator (LAMMPS) was used for simulation ²⁶. Image processing and analysis are carried out by OVITO visualization software ²⁷. The interaction between carbon-nitrogen atoms in C₃N and carbon-boron in BC₃, as well as carbon-carbon in the C₆₀ molecule, has been defined through the Tersoff potential presented by Kinaci et al. ^{28,29}. However, to investigate the ballistic of these two structures, the optimized potential of interatomic bonds has been used in previous reports ³⁰. In this potential, the relationship between the energy and the displacement of atoms concerning each other is expressed as:

$$U_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})] \quad (1)$$

Function $f_R(r_{ij})$ indicates the repulsion potential of two particles, e.g., in a nucleus-nucleus interaction, and $f_A(r_{ij})$ denotes the attraction potential resulting from valence electrons. b_{ij} is a bonding strength term that depends on the local atomic medium surrounding a specific bond, and it is a decreasing function of atoms rearrangement number. b_{ij} contains all the multi-particle effects of potential. These relations express existing functions in these potentials:

$$f_R(r_{ij}) = -A_{ij} e^{-\lambda_{ij}r_{ij}}, \quad f_A(r_{ij}) = -B_{ij} e^{-\mu_{ij}r_{ij}} \quad (2)$$

$$(3)$$

$$f_c(r_{ij}) = \begin{cases} 1 & r_{ij} < R_{ij} \\ \frac{1}{2} + \frac{1}{2} \cos \left[\frac{\pi(r_{ij} - R_{ij})}{S_{ij} - R_{ij}} \right] & R_{ij} \leq r_{ij} \leq S_{ij} \\ 0 & r_{ij} < S_{ij} \end{cases}$$

And the required constants are defined as follows:

$$\begin{aligned} b_{ij} &= X_{ij}(1 + B_i^{n_i} \xi_{ij}^{n_i})^{-0.5n_i}, \xi_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) \omega_{ik} g(\theta_{ijk}) \\ g(\theta_{ijk}) &= 1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{d_i^2 + (h_i + \cos \theta_{ijk})^2}, \omega_{ik} = e^{\left[\mu_{ik}^3 (r_{ij} - r_{ik})^3 \right]} \\ \lambda_{ij} &= \frac{(\lambda_i + \lambda_j)}{2}, \mu_{ij} = \frac{(\mu_i + \mu_j)}{2}, A_{ij} = \sqrt{A_i A_j} \\ B_{ij} &= \sqrt{B_i B_j}, R_{ij} = \sqrt{R_i R_j}, S_{ij} = \sqrt{S_i S_j} \end{aligned} \quad (4)$$

Indices i, j, and k specify the existing atoms in the ijk bond. rij and rik indicate the lengths of ij and ik bonds, respectively, with θ_{ijk} being the angle between them. These coefficients have been used concerning the coefficients presented above. In the study of ballistic properties, multilayered configurations, which is a non-bonded van der Waals interaction, the Lennard-Jones potential is used. The values of ϵ and σ can be seen using the following formulas in Table 1.

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}, \epsilon_{ij} = \sqrt{\epsilon_i \times \epsilon_j} \quad (5)$$

Table 1. Lennard-Jones potential coefficients between different atoms in this study

Pair	σ (Å)	ϵ (eV)
C – N ³¹	3.34577013	0.00369113
C – B ³¹	3.53419521	0.00596172
N – B ²¹	3.409	0.005084
C – C ³²	3.431	0.00455
B – B ²¹	3.453	0.004117
N – N ²¹	3.365	0.006283

In the present work, the dimensions of the structures 6×6 nm² are considered. The total number of atoms present in the simulation is 1404, the share of carbon atoms is 1068 (Contains 60 carbon atoms for the fullerene molecule), and the total share of boron and nitrogen atoms in BC₃ and C₃N structures is 336 (Figure 1). Periodic

boundary conditions were applied in all three directions. After generating the ensemble of random velocity at 300 K, the system runs to reach out to equilibrium at 300 K under the isothermal-isobaric (NPT) ensemble with the Nose-Hoover thermostat. The time step is 0.25 fs for 50 ps, and the velocity Verlet algorithm was used to integrate the Hamiltonian equations of the determined motion. After equilibrium, the ballistic properties are investigated by throwing a fixed-speed fullerene molecule toward C_3N and BC_3 . One row of atoms at the boundary of the structure was fixed in both x and y directions. Consequently, the nanosheets maintained their equilibrium when they collided with the fullerene molecule. The distance between the C_{60} molecule and the surface of the nanosheets is considered to be 5 nm.

Figure 1. The C_3N (left) and BC_3 (right) atomic configuration with a honeycomb structure includes carbon-nitrogen and carbon-boron atoms, respectively. The red bonds show the structure of the fullerene molecule. In their ideal structures, each boron and nitrogen atom is surrounded by three carbon atoms. Carbon, nitrogen, and boron atoms are presented respectively in purple, green, and yellow.

To better understand the stress distribution in the present work, after computing the stress tensor on each atom, the equivalent stress of a sheet is calculated based on Von Mises stress.

$$\sigma_{V-M} = \sqrt{\frac{1}{2}[(\sigma_{11} - \sigma_{22}) + (\sigma_{11} - \sigma_{33}) + (\sigma_{22} - \sigma_{33}) + 6(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2)]} \quad (6)$$

That $\sigma_{1,2,3}$ represents the stress in three directions x, y, and z.

3 Results and discussion

3.1 Ballistic properties

For vertical stacks of two-dimensional materials, the layers are placed side-by-side with the van der Waals interaction. At the nanoscale, a synergistic interaction occurs between the layers, which is not observed at the micro and macro scales. Several desirable layers, between 5 and 10 layers, indicate that a multilayer two-dimensional material has an impact force even higher than its single-layer counterparts. These results provide a basic insight into the design of ultra-light multi-layered armor using nanocomposites based on advanced 2D materials. In a variety of other applications in the electronics field, impact assessment is of significant importance, which can cause unintended and severe shocks during use. Protection with a massive shield is undoubtedly obvious, but it is often impossible because lightness, flexibility, or ergonomics are of particular importance in all of these applications. Therefore, more and more attention has been paid to the development of unconventional nanocomposites with specific toughness and low weight ²¹.

Thus, in this section, the single-layer and multilayer ballistic properties of C_3N and BC_3 , including a hybrid of both nanosheets, have been investigated. A C_{60} molecule is thrown at different speeds towards the two-dimensional nanosheets studied in the present work. Drawing the residual velocity curve of the projectile (V_{res}) against the initial velocity value of impact (V_0) is a common method for ballistic analysis to compare the response of different thin armor due to impact

(Figure 2). This diagram is known as the ballistic curve, which easily enables us to differentiate between projectile and penetration regimes so that critical penetration energy can be detected.

Figure 2. Left panel: Ballistic curves of single layer C_3N and BC_3 . The residual velocity V_{res} is referred to the average velocity of the C_{60} atoms in the Z direction. Right panel: Configurations of C_3N and BC_3 at the 8.8 km/s initial velocity of C_{60} with MD simulation. The color of each atom indicates its displacement. For visual clarity, the color bar is limited up to 8 Å, and the same color shows all displacements beyond this point.

In this work, we have considered the initial velocity of the C_{60} molecule from 2.45 to 64.27 km/s in fifteen different values. The projectile's initial and secondary velocity and kinetic energy values can be seen accurately in Table 2. It is clear that C_3N provides higher penetration velocity and impact energy than single layer BC_3 . As a result, C_3N has a lower residual velocity after perforation but shows an almost equal restitution coefficient in the ricochet regime compared to BC_3 .

Table 2. Comparison of Residual Kinetic Energy (K_{res}) and Velocity (V_{res}) of monolayer C₃N, BC₃ using molecular dynamics simulations (present study) and K_{res} and V_{res} of graphene, h-BN using DFT and FEM (Previous Reports).

C ₃ N				BC ₃		
Present Study	K ₀ (eV)	V ₀ (km/s)	K _{res} (eV)	V _{res} (km/s)	K _{res} (eV)	V _{res} (km/s)
	23.3	2.45	0	0	-0.17	-0.21
	61.12	4.05	-0.24	-0.25	-0.54	-0.38
	96.82	5.1	-0.36	-0.31	-1.21	-0.57
	155.51	6.46	-0.94	-0.5	-3.09	-0.91
	196.63	7.27	-1.99	-0.73	-4.43	-1.09
	242.39	8.07	-5.19	-1.18	-3.96	-1.03
	293.2	8.87	-5.37	-1.2	-10.15	-1.65
	348.75	9.68	5.64	1.23	68.27	4.28
	543.8	12.08	133.27	5.98	154.08	6.43
	835.13	14.97	228	7.822	273.76	8.571
	955.2	16.1	269.25	8.5	320.24	9.27
	1207.41	18	349.2	9.68	411.63	10.51
	2169.83	24.13	640.5	13.11	769.53	14.37
	3851.88	32.15	1156.98	17.62	1370.92	19.18
	15393.18	64.27	5190.34	37.32	5962.55	40
Graphene ²¹				h-BN ²¹		
Previous Reports	33.63	3.0	-1.30	-0.059	-0.03	-0.09
	59.78	4.0	-2.47	-0.81	-0.14	-0.19
	93.41	5.0	-4.30	-1.07	-2.00	-0.73
	134.51	6.0	-6.43	-1.31	-4.83	-1.14
	183.09	7.0	-8.41	-1.50	-5.37	-1.20
	209.88	7.5	-8.07	-1.47	0.00	0.00
	239.13	8.0	-7.52	-1.42	9.42	1.59
	302.65	9.0	-4.60	-1.11	51.15	3.70
	336.73	9.5	0.00 0.00	0.00	79.06	4.60
	373.64	10.0	11.15	1.73	113.85	5.52

The restitution coefficient was calculated and plotted in figure 3 versus impact velocity. As could be observed, increasing the impact velocity, the restitution coefficient increases gradually. The variation of the restitution coefficient of BC₃ is more limited concerning the coefficient of C₃N sheets.

Figure 3. Coefficient of restitution for the collision of a C_{60} molecule along the z-direction

From these results, it is clear that BC_3 sheets absorb more energy from carbon projectiles than C_3N sheets. From another point of view, perhaps this difference can be related to the natural frequency of oscillations of these two sheets. The natural frequency of the BC_3 sheet is higher than that of the C_3N sheet due to its higher flexural strength and therefore better absorbs high-velocity bullets. Because when a bullet or projectile approaches its surface, the atoms of these sheets show the possibility of faster displacements due to the higher frequency in response to the presence of the bullet. This issue can be investigated in future studies by studying the free vibrations of these sheets.

The increasing number of layers for the two interlayer distance modes, including $d=X = 0.34$ nm and $d=4X=1.36$ nm on ballistic properties, has been discussed. Therefore, the C_3N and BC_3 multilayer structures and the hybrid of these two sheets are constructed in the form of van der Waals bonds. The C_{60} molecule is thrown towards desired structures with $V_0 = 64.27$ km/s and $K_0 = 24.66 \times 10^{-16}$ J.

The simulation process in this section for the 4-layer model is delineated in both $d=X$ and $d=4X$ interlayer distances in Figure 4.

Figure 4. Image of configurations created after the C_{60} impact on four-layer stacks of the C_3N , BC_3 , and C_3N - BC_3 hybrid nanosheets with $K_0=15393.19$ eV for different layer spacing including $d=X=0.34$ and $d=4X=1.36$ nm.

The kinetic energy of all states after impact is shown in Figure 5. It is entirely evident that C_3N nanosheets absorb more energy from the C_{60} molecule due to their strong C-N bond, and even when it combines with the BC_3 sheet, they can increase its ballistic properties and reduce the kinetic energy of fullerenes further. It is important to note that as the interlayer distance increases from $d=X$ to $d=4X$,

the amount of kinetic energy decreases significantly. For example, when the interlayer distance is $d=4X$, the kinetic energy of C_{60} is 27 percent lower than when the interlayer distance is $d=X$. As the distance between layers increases, the removed carbon and nitrogen atoms (for example, in C_3N) from the first sheet have more space and do not extend along with the C_{60} molecule's motion. When the surface separation from the first layer hits the sides of the second layer, it does not smooth the path of the C_{60} molecule and only causes more damage to the next layers in the whole sheet. However, this does not happen for shorter interlayer distances. As soon as the atoms separate from the first layer, they quickly hit the second layer, and the path of the projectile molecule will be smoother. Therefore, it can be concluded that although increasing the interlayer distance between 2D materials improves the ballistic properties, on the other hand, it causes irreparable damage to the next layers. So, it is not able to withstand excessive pressures for use and application in two-dimensional membranes and purification applications.

Figure 5. The number of layers effect on the residual kinetic energy K_{res} in the C_3N , BC_3 , and C_3N - BC_3 hybrid nanosheets with $K_0=24.66 \times 10^{-16}$ J for different layer spacing including $d=X=0.34$ and $d=4X=1.36$ nm.

Due to the thin nature of the two-dimensional material, these materials may easily

deform out-of-plane by arc or wrinkle automatically on the substrates. Although these out-of-plane alterations are very small in size (below the Angstrom scale), nevertheless, they significantly change the effective properties. For example, out-of-plane wrinkles may reduce Young's modulus of the single-layer, but increase toughness or chemical activity³³. In the present study, an attempt has been made to remove wrinkles. However, just in the case of C_3N and BC_3 combination with a $d=4X$ layered distance and due to strong van der Waals interaction and prevailing physical and chemical interactions between these two layers, BC_3 structure towards one layer C_3Ns is stretched from top to bottom and causes buckling in the system. This stretch can ultimately have little effect on the results. In many studies, the single-layer thickness of graphene is assumed to be 0.334nm, while measurements using an atomic force microscope (AFM) report this value from 0.4 to 1.7nm³⁴. Another important parameter in elastic properties is the amount of energy absorbed by two-dimensional materials, which is obtained by calculating $|V_0^2 - V_{res}^2|/V_0^2$. Therefore, Figure 6 shows absorbed energy changes by increasing impact velocity and increasing the number of layers for C_3N , BC_3 , and hybrid structures.

Figure 6. The energy changes adsorbed by the left sheet: increasing impact velocity and right panel: the increasing number of layers for C_3N , BC_3 , and their hybrid structures.

To better understand the behavior of stress distribution in different systems after the C_{60} penetration, we obtained the von Mises stress of single-layer and three samples of four-layer structure for $d=X$ and $d=4X$ layered spacing, which is depicted in Figure 7. The results show that the stress distribution is different in several modes. The nitrogen and boron atoms do not have the same behavior at different interlayer distances, and this is related to the distribution of stress in the structures. It has been observed that C_3N has better performance in stress distribution and distributed maximum stresses uniformly throughout the monolayer sheet. Thus, the stress concentration in this structure has been lower than the others; it will have better mechanical and ballistic properties.

Figure 7. Von Mises stress distribution on a single layer and four-layer stacks of the C_3N , BC_3 , and C_3N - BC_3 hybrid nanosheets after the C_{60} impact with $V_0=64.27$ km/s for different layer spacing including $X=0.34$ and $4X=1.36$ nm.

4 Conclusions

In this work, we studied the ballistic behavior of single and multi-layered armor C_3N and BC_3 and their hybrid, which is exposed to the impact of a high-speed C_{60} molecule by using molecular dynamics simulation techniques. Our results indicated that the speed and energy of the C_{60} molecule dropped sharply after hitting the single layers, which shows the high absorption energy of these two structures. Meanwhile, the absorption energy of C_3N is higher than BC_3 and is enhanced the absorption power of BC_3 , even in hybrid systems. In this work, we have introduced the interlayer distance as one of the effective parameters in ballistic properties and showed that when this distance changes from $d=X = 0.34$ nm to $d=4X = 1.36$ nm: for example, in two-layer C_3N , the kinetic energy of the C_{60} for the $4X$ interlayer After the collision is calculated to be 27% less than the $d=X$ distance. However, the damage caused by the increase in the interlayer distance for the single layers is also predictable after the C_{60} molecule hits the first sheet. To this end, in the present study, the von Mises stress distribution behavior has been analyzed to create two-dimensional nanoparticles composed of C_3N and BC_3 . Therefore, the C_3N structure has a better stress distribution than BC_3 .

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Figures

Figure 1

The C_3N (left) and BC_3 (right) atomic configuration with a honeycomb structure includes carbon-nitrogen and carbon-boron atoms, respectively. The red bonds show the structure of the fullerene molecule. In their ideal structures, each boron and nitrogen atom is surrounded by three carbon atoms. Carbon, nitrogen, and boron atoms are presented respectively in purple, green, and yellow.

Figure 2

Left panel: Ballistic curves of single layer C₃N and BC₃. The residual velocity V_{res} is referred to the average velocity of the C₆₀ atoms in the Z direction. Right panel: Configurations of C₃N and BC₃ at the 8.8 km/s initial velocity of C₆₀ with MD simulation. The color of each atom indicates its displacement. For visual clarity, the color bar is limited up to 8 Å, and the same color shows all displacements beyond this point.

Figure 3

Coefficient of restitution for the collision of a C₆₀ molecule along the zdirection

Figure 4

Image of configurations created after the C60 impact on four-layer stacks of the C3N, BC3, and C3N-BC3 hybrid nanosheets with $K_0=15393.19$ eV for different layer spacing including $d=X=0.34$ and $d=4X=1.36$ nm.

Figure 5

The number of layers effect on the residual kinetic energy K_{res} in the C_3N , BC_3 , and C_3N - BC_3 hybrid nanosheets with $K_0=24.66 \times 10^{-16}$ J for different layer spacing including $d=X=0.34$ and $d=4X=1.36$ nm.

Figure 6

The energy changes adsorbed by the left sheet: increasing impact velocity and right panel: the increasing number of layers for C_3N , BC_3 , and their hybrid structures.

Figure 7

Von Mises stress distribution on a single layer and four-layer stacks of the C₃N, BC₃, and C₃N-BC₃ hybrid nanosheets after the C₆₀ impact with $V_0=64.27$ km/s for different layer spacing including $X=0.34$ and $4X=1.36$ nm.