https://doi.org/10.22226/2410-3535-2021-1-79-83 PACS: 61.48.Gh, 87.64.kp

Molecular dynamics simulation of high-speed loading of 2D boron nitride

I. A. Shepelev[†,1], S. V. Dmitriev[2], E. A. Korznikova[2,3]

[†]igor_sar@li.ru

[1]Saratov State University, Saratov, 410012, Russia
[2]Institute for Metals Superplasticity Problems, RAS, Ufa, 450001, Russia
[3]Ufa State Aviation Technical University, Ufa, 450008, Russia

The purpose of this work is to carry out a thorough analysis of fine structural parameters and energy scattering channels in a hexagonal boron nitride lattice subjected to shock loading. This external influence leads to the formation of a shock wave in the material. It has been shown that shock waves can be initiated by giving an initial pulse to a single atomic row in the direction normal to that row. At the same time, such initial conditions do not correspond to the stable shock wave profile, but it is formed after a sufficiently short transition period of about 0.1 ps. It has been shown that shock waves in the material under study can propagate only in the two crystallographic directions, namely zigzag and armchair directions. In all the cases, the shock waves travel faster than the speed of sound in the studied material. Mechanisms of shock wave propagation have been investigated. We have revealed that propagation of the shock wave in the zigzag direction is associated with smallest energy losses. We discover that the major mechanisms of energy dissipation in the material during shock wave propagation are the bond length and the bond angle oscillations.

Keywords: atomistic simulations, 2D materials, shock waves, energy transfer.

УДК: 539

Молекулярно-динамическое моделирование высокоскоростного нагружения двумерного нитрида бора

Шепелев И. А.[†,1], Дмитриев С. В.[2], Корзникова Е. А.[2,3]

[1]Саратовский государственный университет, Саратов, 410012, Россия
[2]Институт проблем сверхпластичности металлов РАН, Уфа, 450001, Россия
[3]Уфимский государственный авиационный технический университет, Уфа, 450008, Россия

Целью данной работы является проведение детального анализа тонких структурных параметров и каналов рассеяния энергии в гексагональной решетке нитрида бора, подвергнутой ударному нагружению. Это внешнее воздействие приводит к образованию в материале ударной волны. Было показано, что ударные волны могут быть инициированы путем приложения начального импульса в один атомный ряд в направлении, нормальном к этому ряду. В то же время такие начальные условия не соответствуют стабильному профилю ударной волны. Однако она формируется после достаточно короткого переходного периода около 0.1 пс. Показано, что ударные волны в исследуемом материале могут распространяться только в двух кристаллографических направлениях-зигзаге и кресле. Во всех случаях ударные волны движутся быстрее скорости звука в исследуемом материале. Также исследованы механизмы распространения ударной волны. Показано, что движение ударной волны в зигзагообразном направлении связано с наименьшими потерями энергии. Установлено, что основными механизмами диссипации энергии в материале при распространении ударной волны являются колебания длины связи и угла связи.

Ключевые слова: атомистическое моделирование, двумерные материалы, ударные волны, перенос энергии.

1. Introduction

Boron nitride (BN), a widely known material for its excellent thermal and chemical stability has recently been rediscovered in 2D form [1] following the recent tendency of design of various new materials with reduced dimension where crystals of one-atom-thickness comprise a large set of materials, covering a broad range of properties [2,3]. Among them one can recall several large groups, namely X-enes [4–7], MX-enes [8] and transition metal dichalcogenides [9]. BN is related to the first group, being a chemical composite consisting of equal numbers of nitrogen and boron atoms [10]. Several crystallographic variations of BN are known up to date [11,12]. Hexagonal boron nitride is the one similar to graphite [13]. Its layer type structure allows to perform the split of layers and thus to obtain a new 2D material known as 2D hexagonal boron nitride (hBN) with the structure type quite similar to graphene. Due to this similarity heterostructures of graphene and hBN are studied extensively by both experimental methods [14] and computer simulations [7,15]. Mechanical properties of boron nitride have been studied extensively [10,16–19] still being much less discovered than those of graphene [20–28].

The analysis of works devoted to the study of the influence of high strain rates on the structure and properties of 2D materials revealed a significant difference from those at conventional strain rates. For example, in an experimental study [29], it was shown that carbon nanotubes are damaged much more when compressed by a shock wave than when static compression occurs at the same pressure level. Graphene has the potential to absorb shock waves without destruction [30] or as an intermediate layer for reflection and attenuation of the shock wave [31]. Potential applications of several 2D materials (including graphene and boron nitride) in ballistic applications are discussed [32,33]. Studies of the structure evolution of various bulk conformations (nanoscrolls, fullerenes, nanotubes) of graphene and boron nitride in collision with an obstacle were conducted in [34], where it was shown that the scenario of structure evolution in a collision strongly depends on the initial velocity and orientation. Amorphization of boron nitride structures begins earlier than carbon structures due to the lower strength of the former [32]. The evolution of a defective graphene structure induced by high-speed loading was studied in [35,36]. It is shown that in contrast to normal deformation rates, where the strain energy is primarily dissipated by the deformation of covalent bonds and the occurrence of bending stresses, the use of high-speed loading can lead to healing of defects and the appearance of shear bands.

Due to the fact that 2D hBN is a material with a wide range of potential applications where a considerable probability of high-speed loading exists, investigation of its mechanical behavior and strain accommodation mechanisms under high rate loadings is an important task addressed in this research.

2. Material and methods of investigation

The simulations are carried out by the method of molecular dynamics using LAMMPS package [37]. This method has earlier been shown to be an effective tool for investigation of various effect in crystals, for instance nonlinear dynamics of lattices [25,38–41], evolution of structure and mechanical properties upon loading [42–44], phase transformations [45] and many other applications. The interaction of nitrogen and boron atoms in the boron nitride lattice is described using a refined Tersoff potential (BN. extep) addressed circumstantially in [46]. The integration step in our calculations is 1 fs. Periodic boundary conditions are applied in both directions. Fig. 1 shows the initial structure and the scheme of the shock wave emergence. The x axis corresponds to the zigzag direction and the y axis — to the armchair direction. In the study of the waves propagating along the armchair direction, boron nitride lattices consisting of 2400×50 atoms with dimensions of 6.13×520.33 nm, are considered. In the case of propagation along the zigzag direction, the size of the computational cell was 50×1200 atoms that corresponds to 150.12×10.7 nm.

Launching of the shock wave in the zigzag direction was performed by applying the initial velocities v_0 to one row of atoms ($n=1,2$) of the armchair profile along the x axis while all other atoms had zero velocities and zero initial displacements. Initiation of a single zigzag atomic row ($m=1,2$) with initial velocity of v_0 along the y axis resulted in the formation of the shock wave propagating along the armchair. The described above initial conditions do not correspond to the shock wave profile that was formed after a transition time period of about 0.1 ps.

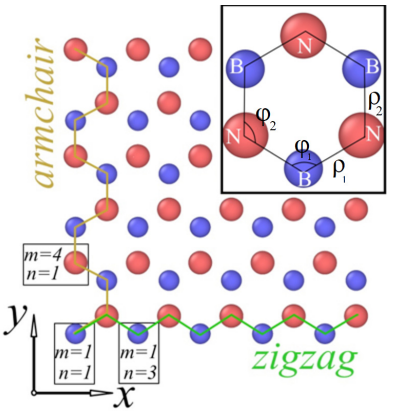

Fig. 1. (Color online) Schematic representation of boron nitride composed of nitrogen (red) and boron (blue) atoms. Cartesian axes x and y are oriented along the zigzag and armchair crystallographic directions, respectively. Numbering of atoms is shown: index m varies along the armchair direction and n along the zigzag direction. The inset represents the elementary cell of BN with the valence angles being equal to $\varphi_1=\varphi_2=120°$ and interatomic distances $\rho_1=\rho_2=1.4457$ Å in the equilibrium state.

3. Results and discussion

Emergence of the shock wave is the result of the application of an impulse to one row of atoms in the direction of the planned propagation. Since the energy of the valence bond is quite high and its braking is associated with an extreme impact not being the case of this study, the accommodation of shock energy is primarily realized via compression of the bond. This moving compression region forms a soliton propagating in the direction of the initial impact. Aim

of our study was to analyze properties of this shock wave, its stability in time and mechanisms of its propagation. The propagation velocity and energy of the shock wave, as well as the level of compression change upon varying the energy of the excitation initiating a shock wave. In the cases under consideration, the shock wave velocity was always higher than the speed of sound (v_s=18.6 km/s for boron nitride [47]). To determine the quantitative characteristics of the shock wave, the dependences of the shock wave energy and its radiation on the shock wave propagation velocity were plotted in Fig. 2 a. It can be noted that for the motion of the compression wave in the direction of the armchair, all other parameters being equal, was associated with higher values of energy than in the direction of the zigzag. In all considered cases, the radiation decreased with decreasing the soliton velocity.

Now let us consider how the velocity and energy of a shock wave change over time for all the cases considered above. The graphs in Fig. 2 a show the evolution (for the first row of atoms along the propagation of the soliton) of the shock wave energy in time, and Fig. 2 b shows the evolution of the shock wave velocity in time. Dependence of the soliton energy as a function of its velocity is presented in Fig. 2 c.

The most interesting feature is the propagation of a shock wave in the zigzag direction. If we consider both plots in Fig. 2, we can see that the energy of the shock wave dissipates slower than in the case of the armchair direction. Thus, it is confirmed that the zigzag direction in a hexagonal lattice is the most favorable for the propagation of a shock wave, which can travel long distances with a small change in its characteristics. The question arises, what is the reason for this behavior. To answer this question, we have considered the dynamics of the angles φ and the bond lengths ρ of atoms (shown in the inset of Fig. 1) in time when a shock wave passes through them.

The graphs in Fig. 3 show the dependences of the angles φ and the lengths ρ of the bonds of atoms when being passed through by the shock wave. When the shock wave passes

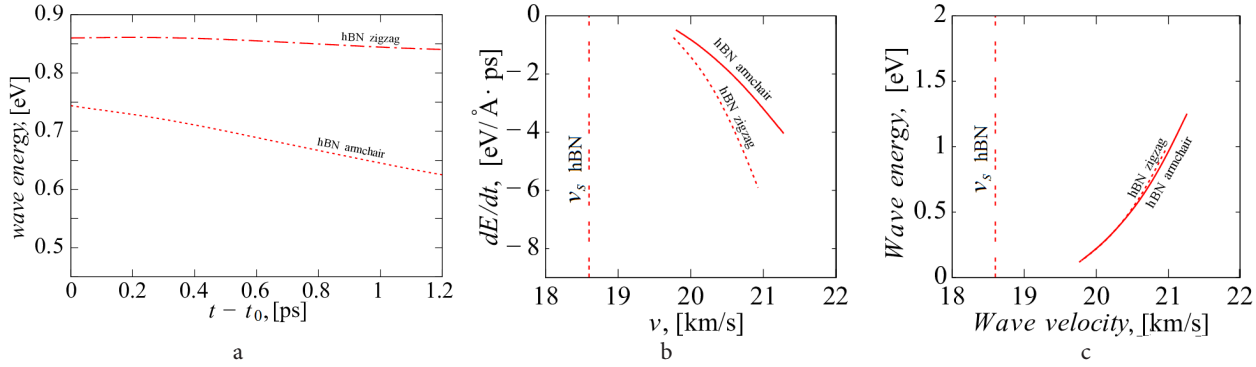

Fig. 2. Evolution of the energy of the shock wave per unit length (a) and its derivative dE/dt as the function of the wave velocity (b), dependence of the wave energy on the velocity of the wave in the steady state (c). The solid and dashed lines show the results for the waves moving along the armchair and zigzag direction respectively. Vertical lines indicate the speed of longitudinal sound for hBN.

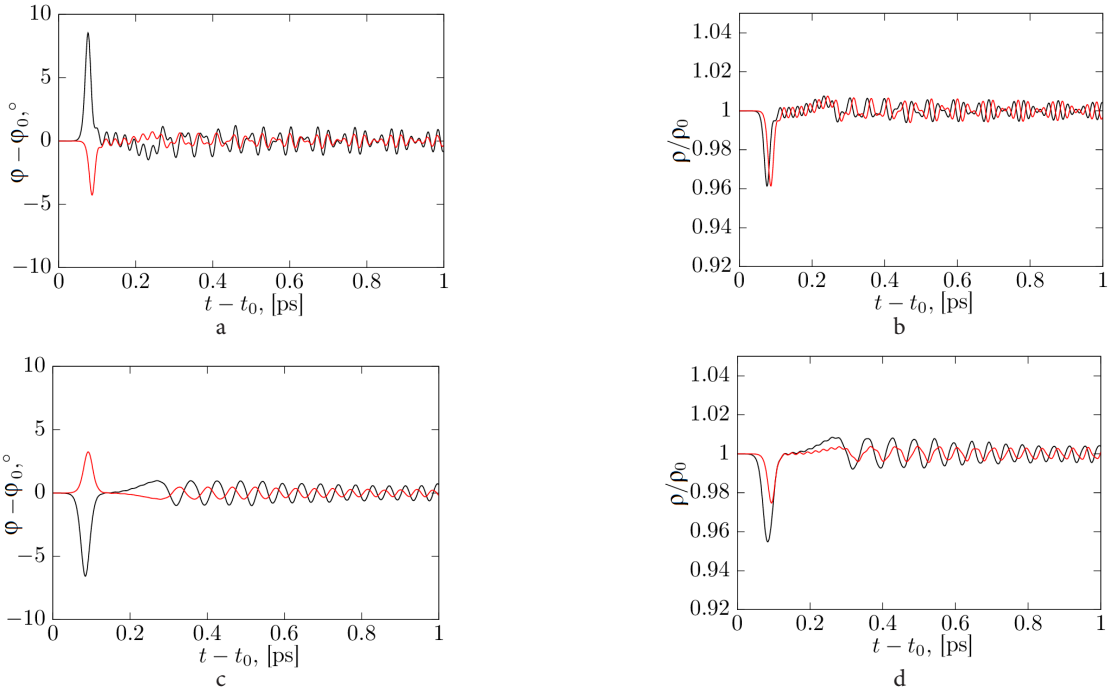

Fig. 3. (Color online) Shock wave induced oscillations of the valence angles (a, c) and valence bond lengths (b, d). The black (red) color corresponds to the valence bond angle and length φ_1 and ρ_1 (φ_2 and ρ_2). (a, b) corresponds to the case of the shock wave propagation in the armchair direction, (c, d) - in the zigzag direction. The insets in the panel in (a) and (c) show the power spectrum of shock wave induced oscillations in the armchair and zigzag direction, respectevely, details of the spectrum calculations are given in [6].

through the lattice, one can see that one of the coupling angles φ_1 is stretched, and the other angle φ_2 is compressed. This is clearly seen in the graphs in Fig. 3 a, c. In this case, all bond lengths, both ρ_1 and ρ_2, are compressed. At the initial stage, immediately after passing through the shock wave atoms, a vibrational mode with a high degree of regularity arises. If we consider the intensity of these vibrations, we can see that the vibrations in the zigzag direction are higher in frequency than for the armchair direction. After the 15 – 20 periods of oscillations, the regular mode is destroyed and chaotic phonon oscillations are established, the intensity of which for the chair direction is much higher than for the zigzag direction, while it can be noted that chaotic oscillations in the zigzag direction have lower frequency.

In this case, the energy dissipated by atoms after passing through the soliton is proportional to the square of the vibration frequency of the bond length (angle). This is probably the reason why, during the propagation of a shock wave in a hexagonal lattice in the zigzag direction, lower energy losses are observed and a less intense deceleration of the shock wave propagation occurs (see Fig. 3).

4. Conclusion

Molecular dynamics analysis of plane compressive shock waves in boron nitride propagating along the armchair and zigzag directions is carried out. It was shown that shock waves can be initiated by imparting an initial impulse to one atomic row in the direction normal to this row. These initial conditions do not correspond to the shock wave profile that forms after a transition period of about 0.1 ps. Shock waves travel at speeds exceeding the speed of sound. To reveal the mechanism of energy dissipation, we analyzed the vibrations of bond angles and bond lengths caused by a shock wave. It is found that the shock wave excites a highly symmetric vibrational mode with a frequency close to the upper edge of the spectrum of small amplitude vibrations. The mode is unstable and after 5 to 20 periods of oscillations, depending on the direction of propagation, it breaks down and turns into irregular oscillations. The largest vibration amplitudes were initiated by a shock wave moving in the boron nitride in the direction of the armchair, which corresponds to the maximum energy emission intensity. In this case, the triggering of a compression soliton in the zigzag direction is associated with lower amplitudes and frequencies of atomic vibrations, which, in turn, leads to less intense scattering and the retention of stable parameters of the shock wave motion. It should be nothed that the shock waves induced in graphene are characterized by a larger degree of energy dissipation than in the boron nitride. For this reason, their lifetime is noticeably shorter. Besides, the anisotropy, which is observed in the boron nitride, is almost absent in the graphene, namely the shock wave features are very similar in the both crystallographic directions.

The next step in research in this direction can be the analysis of shock waves in other 2D materials with different types of lattices (multilayer or corrugated, such as, for example, in phosphorene, bismuthene and other variations of elements of the V subgroup), to determine the role of the geometry of the lattice in the dynamics of shock waves.

Acknowledgements. This work was supported by the grant of the Council of the President of the Russian Federation for state support of young Russian scientists (project № MK-815.2020.2).

References

1. H. Mei, Y. Zhong, D. He, X. Du, C. Li. Sci. Rep. 10, 7873 (2020). Crossref
2. M. Xu, T. Liang, M. Shi, H. Chen. Chem. Rev. 113, 3766 (2013). Crossref
3. K. S. Novoselov, A. Mishchenko, A. Carvalho, A. H. Castro Neto. Science. 353, 9439 (2016). Crossref
4. A. A. Kistanov, S. K. Khadiullin, K. Zhou, S. V. Dmitriev, E. A. Korznikova. J. Mater. Chem. C. 7, 9195 (2019). Crossref
5. A. A. Kistanov, S. K. Khadiullin, S. V. Dmitriev, E. A. Korznikova. ChemPhysChem. 20, 575 (2019). Crossref
6. I. A. Shepelev, A. P. Chetverikov, S. V. Dmitriev, E. A. Korznikova. Comput. Mater. Sci. 177, 109549 (2020). Crossref
7. A. R. Davletshin, S. V. Ustiuzhanina, A. A. Kistanov, D. Saadatmand, S. V. Dmitriev, K. Zhou, E. A. Korznikova. Phys. B Condens. Matter. 534, 63 (2018). Crossref
8. M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum. Adv. Mater. 23, 4248 (2011). Crossref
9. K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz. Phys. Rev. Lett. 105, 136805 (2010). Crossref
10. A. Pakdel, C. Zhi, Y. Bando, D. Golberg. Mater. Today. 15, 256 (2012). Crossref
11. L. Bourgeois, Y. Bando, T. Sato. J. Phys. Appl. Phys. 33, 1902 (2000). Crossref
12. A. Nagakubo, H. Ogi, H. Sumiya, K. Kusakabe, M. Hirao. Appl. Phys. Lett. 102, 241909 (2013). Crossref
13. C. R. Dean, A. F. Young, I. Meric, C. Lee, L. Wang, S. Sorgenfrei, K. Watanabe, T. Taniguchi, P. Kim, K. L. Shepard, J. Hone. Nat. Nanotechnol. 5, 722 (2010). Crossref
14. J. Xue, J. Sanchez-Yamagishi, D. Bulmash, P. Jacquod, A. Deshpande, K. Watanabe, T. Taniguchi, P. Jarillo-Herrero, B. J. Leroy. Nat. Mater. 10, 282 (2011). Crossref
15. G. Giovannetti, P. A. Khomyakov, G. Brocks, P. J. Kelly, J. Van Den Brink. Phys. Rev. B. 76, 073103 (2007). Crossref
16. P. B. Mirkarimi, K. F. McCarty, D. L. Medlin. Mater. Sci. Eng. R Rep. 21, 47 (1997). Crossref
17. J. C. Meyer, A. Chuvilin, G. Algara-Siller, J. Biskupek, U. Kaiser. Nano Lett. 9, 2683 (2009). Crossref
18. A. Gupta, T. Sakthivel, S. Seal. Prog. Mater. Sci. 73, 44 (2015). Crossref
19. Q. Peng, W. Ji, S. De. Comput. Mater. Sci. 56, 11 (2012). Crossref
20. X. Huang, Z. Yin, S. Wu, X. Qi, Q. He, Q. Zhang, Q. Yan, F. Boey, H. Zhang. Small. 7, 1876 (2011). Crossref
21. V. Singh, D. Joung, L. Zhai, S. Das, S. I. Khondaker, S. Seal. Prog. Mater. Sci. 56, 1178 (2011). Crossref
22. K. S. Novoselov, V. I. Fal'Ko, L. Colombo, P. R. Gellert, M. G. Schwab, K. Kim. Nature. 490, 192 (2012). Crossref
23. L. K. Rysaeva, E. A. Korznikova, R. T. Murzaev, D. U. Abdullina, A. A. Kudreyko, J. A. Baimova,

D.S. Lisovenko, S.V. Dmitriev. Facta Univ. Ser. Mech. Eng. 18, 1 (2020). Crossref
24. A.V. Savin, E.A. Korznikova, S.V. Dmitriev. Phys. Rev. B. 99, 235411 (2019). Crossref
25. I. Evazzade, I.P. Lobzenko, D. Saadatmand, E.A. Korznikova, K. Zhou, B. Liu, S.V. Dmitriev. Nanotechnology. 29, 215704 (2018). Crossref
26. L. Bai, N. Srikanth, E.A. Korznikova, J.A. Baimova, S.V. Dmitriev, K. Zhou. Wear. 372–373, 12 (2017). Crossref
27. A.V. Savin, E.A. Korznikova, A.M. Krivtsov, S.V. Dmitriev. Eur. J. Mech. A/Solids. 80, 103920 (2020). Crossref
28. A.V. Savin, E.A. Korznikova, S.V. Dmitriev. Mech. Mater. 137, 103123 (2019). Crossref
29. O.B. Naimark, Yu.V. Bayandin, M.A. Zocher. Phys. Mesomech. 20, 10 (2017). Crossref
30. D. Lahiri, S. Das, W. Choi, A. Agarwal. ACS Nano. 6, 3992 (2012). Crossref
31. X. Liu, F. Wang, H. Wu, W. Wang. Appl. Phys. Lett. 104, 231901 (2014). Crossref
32. C.F. Woellner, L.D. Machado, P.A.S. Autreto, J.M. de Sousa, D.S. Galvao. Phys. Chem. Chem. Phys. 20, 4911 (2018). Crossref
33. Z. Meng, A. Singh, X. Qin, S. Keten. Extreme Mech. Lett. 15, 70 (2017). Crossref
34. S. Hosseini-Hashemi, A. Sepahi-Boroujeni, S. Sepahi-Boroujeni. Appl. Surf. Sci. 437, 366 (2018). Crossref
35. X.J. Long, F.P. Zhao, H.K. Liu, J.Y. Huang, Y. Lin, J. Zhu, S.N. Luo. J. Phys. Chem. C. 119, 7453 (2015). Crossref
36. W.R. Jian, X.J. Long, M.X. Tang, Y. Cai, X.H. Yao, S.N. Luo. Carbon. 132, 520 (2018). Crossref
37. S. Plimpton. J. Comput. Phys. 117, 1 (1995). Crossref
38. E.A. Korznikova, S.A. Shcherbinin, D.S. Ryabov, G.M. Chechin, E.G. Ekomasov, E. Barani, K. Zhou, S.V. Dmitriev. Phys. Status Solidi B Basic Res. 256, 1800061 (2019). Crossref
39. R.T. Murzaev, D.V. Bachurin, E.A. Korznikova, S.V. Dmitriev. Phys. Lett. Sect. Gen. At. Solid State Phys. 381, 1003 (2017). Crossref
40. E. Barani, E.A. Korznikova, A.P. Chetverikov, K. Zhou, S.V. Dmitriev. Phys. Lett. Sect. Gen. At. Solid State Phys. 381, 3553 (2017). Crossref
41. E.A. Korznikova, S.Y. Fomin, E.G. Soboleva, S.V. Dmitriev. JETP Lett. 103, 277 (2016). Crossref
42. A. Tsukanov, S. Psakhie. Facta Univ. Ser. Mech. Eng. 14, 269 (2016). Crossref
43. A.S. Bhui, G. Singh, S.S. Sidhu, P.S. Bains. Facta Univ. Ser. Mech. Eng. 16, 337 (2018). Crossref
44. W.-J. Lee, Y.-C. Lo, A. Yang, K. Chen, N.-Y. Chen. Comput. Model. Eng. Sci. 120, 293 (2019). Crossref
45. H.-Y. Chen, N.-T. Tsou. Comput. Model. Eng. Sci. 120, 319 (2019). Crossref
46. J.H. Los, J.M. H. Kroes, K. Albe, R.M. Gordillo, M.I. Katsnelson, A. Fasolino. Phys. Rev. B. 96, 184108 (2017). Crossref
47. R.J. Jiménez-Riobóo, L. Artús, R. Cuscó, T. Taniguchi, G. Cassabois, B. Gil. Appl. Phys. Lett. 112, 051905 (2018). Crossref