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A comparison of interatomic interaction potentials in modeling elastic properties of pseudo-graphene crystals

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Abstract. In this work, we simulate mechanical properties of pseudo-graphene crystals G5-7v1, G5-6-7v2, G4-8v1, G5-6-8v2, G5-6-8v4, G5-8v1, which include dense networks of wedge disclinations of alternate signs. The crystals were studied using the molecular dynamics method. The paper compares the values of elastic properties of graphene and pseudo-graphene obtained through AIREBO, Tersoff, and LCBOP interatomic interaction potentials. It shows that the application of these potentials in modeling pseudo-graphene crystals is limited. The study concludes that it is necessary to update the existing potentials of interatomic interaction in allotropes of carbon or create a new one.

Keywords: molecular dynamics, pseudo-graphene, elastic properties, disclination, defect structure

Introduction

Graphene is a two-dimensional carbon crystal with a variety of promising properties: high conductivity (Novoselov et al. 2005), thermal conductivity (Chen et al. 2010), and a unique set of mechanical properties (Lee et al. 2008). Its successful synthesis (Novoselov et al. 2004) attracted great attention and marked an active growth of interest in the study of two-dimensional crystals.

In graphene, just as in three-dimensional crystals, one can observe crystal lattice defects (Hao et al. 2011; Wei et al. 2012). Among them are two-dimensional (pores and inclusions), one-dimensional (interfaces without misorientation and grain boundaries), and point-like (vacancies, interstitial atoms and impurity atoms, dislocations and disclinations) defects (Romanov et al. 2015; 2018). It is important to study the effects of such defects to predict the properties of graphene samples and to control their characteristics. For example, an interface in graphene can increase its thermal (Jafri et al. 2010) or electrical conductivity (Bagri et al. 2011).

A wide range of research works focuses on two-dimensional carbon crystals, different from graphene (Baughman et al. 1987; Enyashin, Ivanovskii 2011; Gong et al. 2020; Terrones et al. 2000).

They have a high density of carbon atomic rings with defects organized periodically. These crystals are commonly referred to as 'graphene allotropes' (Wang et al. 2015; Zhuo et al. 2020), 'carbon allotropes' (Deb et al. 2020; Zhang et al. 2015), 'pseudo-graphenes' (Abramenko et al. 2020), etc. The majority of these materials are yet to be synthesized (with the exception of biphenylene (Fan et al. 2021) — the only synthesized pseudo-graphene crystal (PGC) so far). However, it is important to predict the properties of such materials to improve the modelling methods and algorithms to a further degree of precision. We hope that in the near future predicted property values of a non-synthesized material will be as close to the actual ones as possible. In addition, the predictions can be used as a roadmap for researchers who aim to synthesize such crystals as, thanks to the prediction algorithms, lots of material suggestions have proven to be unstable (Xie et al. 2020), and, thus, crystals were impossible to synthesize.

The properties of carbon-based materials can be studied theoretically using various methods: atomistic modeling, density functional theory, analytical calculation, etc. One of the most popular calculation methods is molecular dynamics. It is a fast prediction method that allows calculating simple and complex properties on a high-scale crystal lattice. The molecular dynamics method uses a special approximation function — interatomic potential. It displays the dependency of potential energy between each pair of atoms on the distance between the atoms. The function serves as a physical basis of molecular dynamics and each material requires a new function. Given that this function is an approximation, the approaches to its description vary. For example, for calculations on graphene we could use Tersoff, AIREBO, LCBOP (Los, Fasolino 2003; Stuart et al. 2000; Tersoff 1988) and other styles of interatomic potentials.

In this article, we provide a comparison between the three mentioned above interatomic potentials used in molecular dynamics calculations to study the mechanical properties of several PGCs. Our goal is to find out whether the interatomic potentials designed for graphene are applicable to PGCs. We start with the description of the modeling technique and materials models in Section 2. In Section 3, we analyze the mechanical properties of several PGCs using molecular dynamics. In Section 4, we discuss the obtained results and compare the potentials.

Modeling technique and materials

The method of molecular dynamics is effective for in-depth investigation of elastic deformation in graphene crystals and pseudo-graphenes. We used the LAMMPS software package to obtain the elastic properties of the studied crystals and made a comparison between the three potentials of interatomic interaction: AIREBO, Tersoff, and LCBOP. AIREBO and LCBOP potentials were developed for the simulation of carbon systems and successfully tested for the simulation of graphene (Baimova et al. 2014; Hansen-Dörr et al. 2019). The Tersoff potential used in this work was developed for modeling silicon carbide. It also showed good results when modeling two-dimensional allotropes of carbon (Shirazi et al. 2019; Winczewski et al. 2018). In our work, the simulation was performed at room temperature and with periodic boundary conditions applied to the boundaries of the system. Energy minimization was carried out using the Polak-Ribière conjugate gradient algorithm (Polak, Ribiere 1969). To obtain the elastic constants in the simulation, a deformation of 0.5% was applied. We visualized the obtained numerical results with the OVITO software package.

To interpret the obtained data, it is necessary to convert the tensor of elastic constants into elastic moduli, such as Young's modulus and Poisson's ratio. Hooke's law for a two-dimensional anisotropic body has the following format:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ 2\varepsilon_{xy} \end{bmatrix}, \quad (1)$$

where σ_{ij} and ε_{ij} are components of stress and strain, correspondingly; C_{ij} are components of the matrix of elastic constants.

For the matrix of elastic constants, components C_{12} and C_{21} obey the condition $C_{12} = C_{21}$, while components C_{16}, C_{26}, C_{61}, and C_{62} are equal to zero due to the symmetry properties of a two-dimensioal crystal. The labeling of elastic constants corresponds to the labeling of three-dimensional bodies, i. e., index '1' corresponds to the x-direction, '2' to the y-direction, and '6' to the xy-component. Thus, there are 4 independent components — C_{11}, C_{22}, C_{12}, and C_{66}. The conventional elastic moduli of the material are calculated by the following formulas:

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$$\nu_{12} = \frac{C_{12}}{C_{22}}\ ; \nu_{21} = \frac{C_{12}}{C_{11}}\ ; E_1 = \frac{C_{11}C_{22} - C_{12}^2}{C_{22}}\ ; E_2 = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}}\ ; G = C_{66}\ , \tag{2}$$

where E_i is Young's modulus corresponding to the i-direction; ν_{ij} is Poisson's ratio for the longitudinal direction i and the transverse direction j, G is a shear modulus.

For the case of a two-dimensional isotropic crystal, the following conditions are satisfied: $C_{11} = C_{22}$, $C_{12} = C_{21}$, $C_{66} = (C_{11} - C_{12})/2$. Thus, there are only two independent components: C_{11} and C_{12}. The elastic properties of the material are calculated by the following formulas:

$$\nu = \frac{C_{12}}{C_{11}}\ ; E = \frac{C_{11}^2 - C_{12}^2}{C_{11}}\ ; G = \frac{E(1+\nu)}{2}\ . \tag{3}$$

The obtained results for the mechanical properties of graphene and pseudo-graphene crystals are expressed in GPa, similarly to three-dimensional materials. The transition from N/m to Pa is made taking into account the 'thickness' of the two-dimensional crystal, which was taken to be 3.4 Å (Maitra et al. 2012).

In this work, we consider a graphene crystal and a number of low-energy pseudo-graphenes: G5-7v1, G5-6-7v2, G4-8v1, G5-6-8v2, G5-6-8v4, G5-8v1. The nomenclature of these crystals corresponds to the carbon rings that make up this crystal. It is known that graphene consists of hexagonal six-member atomic rings. In the presence of defects in graphene, rings with symmetry different from six-member are formed. Thus, pseudo-graphene G5-7v1 consists of only five- and seven-membered atomic rings. See the review (Abramenko et al. 2020) for more detailed information on the nomenclature. Pseudo-graphenes are the lowest energy 'allotropes' of graphene (Romanov et al. 2018). The crystals under study are shown in Fig. 1. When modeling these two-dimensional crystals, an approximation was used in which the crystal has a flat shape, i. e., they do not bend.

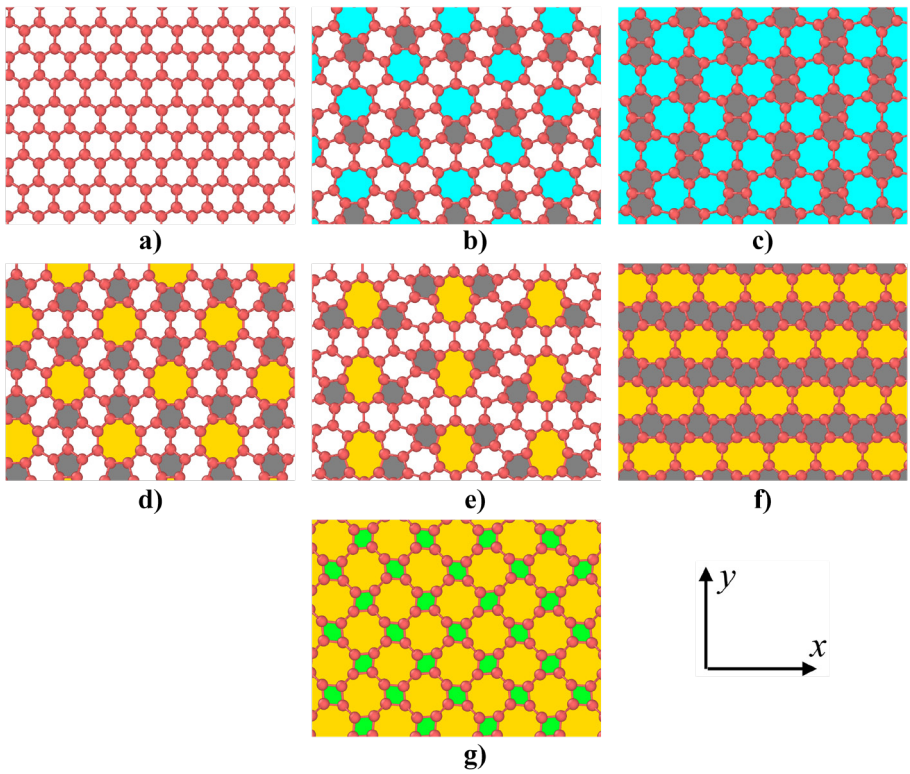

Fig. 1. Structure and primitive lattice of graphene (a) and pseudo-graphenes G5-7v1 (b), G5-6-7v2 (c), G5-6-8v2 (d), G5-6-8v4 (e), G5-8v1 (f) and G4-8v1 (g). The colors indicate defective carbon atomic rings: 7-unit rings — blue, 5-unit rings— gray, 8-unit rings—yellow, 4-unit rings—green

Results of molecular dynamics calculations

Tables 1–3 present a comparison of elastic properties of the studied PGCs and graphene, calculated using the AIREBO, Tersoff, and LCBOP potentials.

Table 1. Elastic constants for graphene and pseudo-graphene crystals calculated via molecular dynamics using AIREBO interatomic potential

	Graphene	**G5-6-7v2**	**G5-7v1**	**G4-8v1**	**G5-6-8v2**	**G5-6-8v4**	**G5-8v1**
C_{11}, GPa	952.4	**1016.03**	**1016.5**	598.2	**1040.3**	923.31	**1195.98**
C_{22}, GPa	952	**950.85**	**1010.7**	596.3	**970.89**	864.64	928.13
C_{12}, GPa	336	180.8	129.2	445	116.61	201.29	**45.78**
C_{66}, GPa	297.5	456.45	391.4	453.5	328.68	414.68	211.34
E_1, GPa	833.81	**981.65**	**999.98**	**266.11**	**1026.29**	876.45	**1193.72**
E_2, GPa	833.46	**918.68**	**994.28**	**265.27**	**957.82**	820.76	926.38
ν_{12}	0.353	0.190	0.128	**0.746**	0.120	0.233	**0.049**
ν_{21}	0.353	0.178	0.127	**0.744**	0.112	0.218	**0.038**
G, GPa	297.5	456.45	391.4	453.5	328.68	414.68	211.34

Table 2. Elastic constants for graphene and pseudo-graphene crystals calculated via molecular dynamics using Tersoff interatomic potential

	Graphene	**G5-6-7v2**	**G5-7v1**	**G4-8v1**	**G5-6-8v2**	**G5-6-8v4**	**G5-8v1**
C_{11}, GPa	1050.2	881.2	762.9	734.7	815.29	798.27	726.65
C_{22}, GPa	1050.2	914.1	808.5	734.7	798.81	827.28	724.97
C_{12}, GPa	**68.7**	133.4	221.1	146.69	179.95	163.63	247.16
C_{66}, GPa	490.8	393.6	376.5	**14.92**	327.87	306.53	229.43
E_1, GPa	1045.71	861.73	702.44	705.41	774.75	765.91	642.39
E_2, GPa	1045.71	893.91	744.42	705.41	759.09	793.74	640.91
ν_{12}	**0.065**	0.146	0.273	0.200	0.225	0.198	0.341
ν_{21}	**0.065**	0.151	0.290	0.200	0.221	0.205	0.340
G, GPa	490.8	393.6	376.5	**14.92**	327.87	306.53	229.43

Table 3. Elastic constants for graphene and pseudo-graphene crystals calculated via molecular dynamics using LCBOP interatomic potential

	Graphene	**G5-6-7v2**	**G5-7v1**	**G4-8v1**	**G5-6-8v2**	**G5-6-8v4**	**G5-8v1**
C_{11}, GPa	976.2	958.8	835.2	513.99	933.86	883.71	**1017.86**
C_{22}, GPa	976.3	900.4	854.2	514.69	870.97	827.76	765.06
C_{12}, GPa	216.4	154.9	230.2	367.14	134.63	168.54	159.63
C_{66}, GPa	379.9	378.2	333.7	571.24	297.31	357.51	212.48
E_1, GPa	928.23	**932.15**	773.16	**252.10**	913.05	849.39	**984.55**
E_2, GPa	928.33	875.38	790.75	**252.44**	851.56	795.62	740.03
ν_{12}	0.222	0.172	0.269	**0.713**	0.155	0.204	0.209
ν_{21}	0.222	0.162	0.276	**0.714**	0.144	0.191	0.157
G, GPa	379.9	378.2	333.7	571.24	297.31	357.51	212.48

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Discussion

As can be seen from the results presented in Table 1, the AIREBO potential shows the values for graphene that are comparable with the experimental (Lee et al. 2008) and simulation data obtained using density functional theory (Wei et al. 2009). This potential is quite often used in various studies of graphene and has proven to be effective (Akhunova et al. 2022; Kochnev et al. 2014). However, if graphene is taken as an ideal crystal, then pseudo-graphenes will be graphene crystals with a dense distribution of disclination defects. Thus, it can be assumed that the mechanical performance may be degraded. This is supported by DFT calculations (Fthenakis et al. 2015; Pereira et al. 2016; Sun et al. 2016): the elastic properties of graphene and pseudo-graphenes were compared, and a decrease in the value of Young's modulus for pseudo-graphenes compared to defect-free graphene was observed. This can be considered as one of the criteria to support the fact that the potential of interatomic interaction gives incorrect data for the selected material. One can observe this pattern for almost all pseudo-graphene crystals, excluding only PGC G5-8v1 and G4-8v1. However, for the G4-8v1 crystal, not only underestimated values of Young's modulus were found, but also the formally calculated values of Poisson's ratio greater than 0.5 were observed, which has no physical meaning. This indicates the low suitability of the AIREBO potential for studying the mechanical properties of pseudo-graphenes, despite the fact that it can be used to model the structure of the undeformed crystals (Kolesnikova et al. 2020; Romanov et al. 2018; Rozhkov et al. 2018).

The Tersoff potential is poorly suited for describing the elastic properties of graphene (Lebedeva et al. 2019), but it is often used to study various two-dimensional carbon allotropes (Shirazi et al. 2019; Winczewski et al. 2018). We can observe the same picture in our research (see Table 2), where almost all the results for pseudo-graphenes have acceptable values, with the exception of G4-8v1 PGC. In G4-8v1, an anomalously small value for C_{66} constant is observed. This indicates that the potential is unsuitable for studying this material. It may be necessary to carry out additional refinements in the parameters of the potential, which would make it possible to produce a correct description of the behavior of atoms in the crystal lattice of PGC G4-8v1.

For the results obtained using the LCBOP potential, we can see that it is well suited for studying graphene and for studying parts of pseudo-graphenes. For G5-6-7v2 and G5-8v1, we can see slightly overestimated values when compared with the values for defect-free graphene.

We can take DFT calculations for graphene from (Pereira et al. 2016) as a baseline, where Young's modulus E = 960 GPa. Young's modulus, calculated with Tersoff, is equal to E_1 = 1046 GPa. This value, calculated with AIREBO, is equal to 833 GPa, and with LCBOP to 928 GPa. Comparing to DFT, the deviation for all potentials is more than 10%. This relates not only to Young's modulus, but to other elastic constants as well.

For PGC G4-8v1, all three potentials display unsatisfactory results for elastic constants. The AIREBO and LCBOP potentials result in Poisson's ratio of about 0.7 (this is again unphysical) and Young's modulus of less than 300 GPa. In addition, for all considered potentials, one can notice a very wide scatter when comparing the values of Poisson's ratio with each other, both for PGCs and graphene. This can be justified by the fact that one cannot make a direct comparison between pseudo-graphene and graphene, since they have a completely different crystal structure with a different order of symmetry. The difference in symmetry is true for most PGCs.

The results obtained for elastic constants show that all the crystals studied in this article meet the Born stability criterion (Haastrup et al. 2018). The stability of the studied crystals is also supported by our DFT calculations (Abramenko, Rozhkov 2021) and prior research (Pereira et al. 2016; Sun et al. 2016).

The MD calculations of elastic constants that we have performed on graphene display a wide deviation in comparison not only to DFT, but also to the calculations themselves — elastic constants evaluated with the use of one interatomic potential differ a lot to ones calculated with the use of another interatomic potential.

Current works focusing on modeling elastic properties for defect-free graphene still exhibit strong differences in the reported values. See (Lebedeva et al. 2019) for an in-depth analysis of the scatter in Young's modulus and Poisson's ratio obtained using different potentials. Thus, Young's modulus is reported to be from 800 to 1200 GPa, while Poisson's ratio for graphene can vary from 0.15 to 0.22.

Conclusions

Calculated elastic constant values for pseudo-graphene crystal (PGC) with the use of molecular dynamics differ significantly in comparison with the values calculated with density functional theory (DFT). Even for graphene with the results much closer to DFT calculations, molecular dynamics values vary in an overly wide spectrum.

As of now, it is difficult to make a precise enough prediction of properties of pseudo-graphene crystals as no similarities on predicted values have been found between several interatomic potentials used in calculations. Thus, we cannot use interatomic potentials designed for graphene to calculate the properties of pseudo-graphene.

Among the studied potentials, the LCBOP and Tersoff potentials can be used with limitations to study certain PGCs. However, their results for G4-8v1 PGC and other pseudo-graphene crystals indicate the need to upgrade the obtained potentials or to develop a new interatomic interaction potential adapted for the study of two-dimensional allotropes of carbon.

Conflict of Interest

The authors declare that there is no conflict of interest, either existing or potential.

Author Contributions

All the authors discussed the final work and took part in writing the article.

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