Modifying mechanical properties of silicon dioxide using porous graphene: molecular dynamics simulations

Yutao Zhao¹, Guihua Xie¹, Junlin Zhao¹, Chengyuan Wang¹∗ and Chun Tang¹∗

¹ Faculty of Civil Engineering and Mechanics, Jiangsu University, Zhenjiang 212013, People’s Republic of China
² Office of Zhenjiang City Main Street Construction Engineering, Zhenjiang 212004, People’s Republic of China
∗ Authors to whom any correspondence should be addressed.

E-mail: cywang@ujs.edu.cn and tangchun@ujs.edu.cn

Keywords: silicon dioxide, mechanical properties, porous graphene, molecular dynamics

Abstract

Graphene or other 2D materials are often used as agents to reinforce engineering structures because they possess extremely high mechanical strength and structural flexibility. This is however not cost effective and the reported enhancement is often limited although the mechanical properties of graphene are often several orders higher than cements or concretes. Defective graphene is mechanically weaker than pristine graphene but stronger than engineering structures, moreover, it is cheaper because the synthesis condition is low. In this work we perform systematic molecular dynamics simulations to evaluate the effect of porous graphene (PG), a type of defective graphene, on reinforcing mechanical properties of silicon dioxide (SiO₂) which is the key components of engineering structures. Our results show that PG is mechanically weaker than pristine graphene but stronger than SiO₂, therefore, with certain amount of PG encapsulation into SiO₂, the mechanical properties can be improved under tensile, shear and compressive loadings, although not as significant as the effective of pristine graphene. The modification mechanism is found to depend both on the intrinsic mechanical properties of GP and the interface induced surface stress redistribution in SiO₂. The effects of defect concentration, volume fraction, loading methods and interface roughness are found to be influential on the reinforcing effect. Our findings are expected to offer new strategies for rational design of low-cost but high-strength engineering composite structures.

Introduction

Recent years have witnessed the fast development of nanoscience and nanotechnology that lead to exotic applications in our daily lives. For example, wearable devices based on nanotransistors can be used in diagnosis, lithium batteries [1, 2] are widely used in smart phones, and novel energy converting devices [3] have been developed to provide green energy. Applications in mechanical property modification of materials is also growing in recent years, such as the creation of nanotwinned grain boundary to raise the mechanical strength of metals and diamonds [4], the use of twin gradient structures in modification of mechanical properties of metals [5, 6] is also showing its promise. Inspired by the superior mechanical properties of nanomaterials and nanostructures, scientists and engineers have started to fabricate composites that contain both traditional components and high strength nanoagents such that the mechanical properties of these composite structures or materials can be tailored to improve their performance [7–15].

Interestingly, both experimental and theoretical studies have demonstrated the advantages of utilizing nanomaterials for enhancing mechanical properties of infrastructures in civil engineering. Graphene is naturally considered to be the ideal candidate for this purpose [16–18], not for its excellent electronic or chemical properties, but due to its extremely high strength sp² type C–C covalent bonds, which is considered to be the strongest chemical bonds in nature. Several groups show that upon dispersion of graphene or graphene oxide, the mechanical properties of cement composites or concrete can be improved by more than 20% when tested under compression [19, 20]. The flexural strength of cement paste can be increased by 15%–24% after
dispersion of graphene nanoplatelets [21]. Molecular dynamics simulations have been performed by theorists to uncover the underlying mechanism and propose strategies to fully take advantages of nanomaterials such as graphene or graphene oxide [21, 22]. Although positive results on enhancing mechanical properties of such engineering structures, however, it should be noticed that the mechanical strength of graphene is several orders higher than that of the concretes or cements [23, 24]. Unfortunately, the reported enhancement in literature is often below 30%, the reason is rather complex such as the weak interlayer van der Waals interaction between graphene and engineering components, the low weight percentage of graphene dispersed due to the high cost. It indeed on the other hand indicates that the enhancement of engineering structures not necessarily has to rely on perfect graphene, defective or other types of graphene derivatives that have lower strength can also be practical candidates, meanwhile, the synthesis condition could be lowered so as to reduce the costs. Moreover, the defective sites may provide additional interfaces between engineering materials and defective graphene, this has often been an obstacle when constructing graphene-engineering materials contacts [25, 26].

Motivated by the above scenario, by using molecular dynamics simulations technique in this work, we investigate the modification of mechanical properties of engineering materials using porous graphene (PG) [27–29], a type of defective graphene, as the reinforcement agent. We use silicon dioxide (SiO2) as the model material in this study and show that although PG is weaker than pristine graphene, load tests under tensile, shear and compression indicate its promises in improving mechanical properties of SiO2, the interfaces between PG and SiO2 determine the deformation modes and overall mechanical properties. We also show that with increased surface roughness of SiO2, the enhancement can be improved. Our results may provide new guidelines to effectively enhancing mechanical properties of composite in general by using imperfect nanostructures.

Methods

Molecular dynamics simulations were performed using the LAMMPS [30, 31] package and the OVITO [32] software was used to visualize the structure dynamics. The SiO2 crystal of β-cristobalite phase with size of 57.28 Å × 57.28 Å × 57.28 Å was built as the model system in this study, the system contains 12288 atoms in total. The graphene and porous graphene have the same dimensions in the x-y plane as that of the SiO2 crystal were built for further simulations on the mechanical properties of the composites, the pristine graphene model contains 1268 carbon atoms. The pores were created by removing atoms from circular areas of various diameters in the pristine graphene, different pore sizes/distributions were considered to uncover the size and defect concentration effects. The graphene or porous graphene was then encapsulated in-between two slabs of SiO2 layers that have the same number of atoms as the above mentioned single-crystal SiO2 model. To study how different amount of porous graphene modifies the mechanical properties of the SiO2 structure, the thickness along z direction were then adjusted to different values. Periodic boundary condition was applied in all directions in this study. Energy minimization was firstly applied to the models using the steepest descent algorithm to obtain structurally optimized geometrical model, structural relaxation was then performed via the Nose-Hoover thermostat [33]. To eliminate the thermal effect on the study, the simulations were all conducted at low temperature of 0.1 K. The Vashishta potential [34] developed in 1997 was used to describe the interatomic interactions for the SiO2 crystal and the airebo potential [35] was used to describe interactions for carbon atoms. The L-J potential was used to simulate interactions between SiO2 and carbon, the parameters chosen here are $\varepsilon_{Si-C} = 0.0096 \text{ eV}, \sigma_{Si-C} = 3.0 \text{ Å}, \varepsilon_{O-C} = 0.003256 \text{ eV}, \sigma_{O-C} = 3.19 \text{ Å}$ [36], here Si, C and O denote silicon, carbon and oxygen atoms, respectively. The timestep used in the study is 1 fs. The strain is applied to the system by varying the simulation box at strain rates of $10^{-4} \text{ps}^{-1}$ for tension, shearing and compression. The obtained stress-strain relationships for the models under various loading conditions were then analyzed for evaluating the performance of PG reinforcing SiO2 structures. The structural evolution and the stress states under strain were also analyzed to uncover the atomistic origins of the enhancement.

Results and discussions

Figure 1 illustrates the differences in mechanical properties of graphene, PG and SiO2, as mentioned above. Here only tensile responses of the three structures are presented, our simulation tests show that the results on shear deformations exhibit similar trends, while compression of graphene structures along the in-plane directions have been generally demonstrated to be weak, we therefore do not directly discuss this issue here. The stress-strain relationships for graphene, PG and SiO2 under uniaxial tension are shown in figures (a)–(c). It can be clearly seen that when subjected to tensile deformation, the stress-strain relationship for graphene is superior to PG and SiO2, this is not surprising due to the ultra-strong nature of sp$^2$ type C–C bonds. The obtained Young’s modulus for graphene is close to 861 GPa, the breaking stress and strain reaches 93 GPa and 15%, respectively, these results agree well with those reported in literature [37–41]. Upon the introduction of nanopores to the
graphene lattice, the mechanical properties start to deteriorate in that both the Young’s modulus and ultimate stress (strain) decrease substantially, here 3 nanopore sizes are considered, including diameter sizes of 1.5 nm, 2 nm and 3.5 nm. The relationship between the mechanical characteristics and the concentration of the defects, i.e., the pores, are shown in figures 1(d)–(f), where the monotonic decrease of Young’s Modulus and the ultimate stress with the increasing defect concentration are clearly seen. Interestingly, the ultimate strain of the PG show slightly different trends, take the d = 2 nm PG as an example, the ultimate strain decreases from 15% of pristine graphene to 8% when the defect concentration is 7.3%, afterwards, it changes to 8.1% and 7.8% when the defect concentration increases to 14% and 22%, respectively. Similar observations can be found for other simulation results. The stress-strain relationship for crystalline SiO2 is plotted in figure 1(c), the key feature observed here is that, as expected above, its mechanical properties are much weaker than those of pristine graphene and the PGs. Its Young’s modulus is about 39.1 GPa, and the ultimate stress is about 7 GPa at the strain level of 20%. This indicates that the above proposed idea of using PG to improve mechanical properties of SiO2 is well rooted considering their intrinsic mechanical properties.

To evaluate the effects of graphene or PG on mechanical properties of SiO2, we constructed structural models by encapsulating one layer of graphene or PG into the gap of two SiO2 slabs of similar sizes, the x-y plane are the in-plane directions of the graphene systems, the tensile and compressive loadings were applied along the x direction and shear deformation was applied in the x-y plane. This strategy is similar to those applied by Zhang et al [25, 26]. The mechanical responses of the graphene/SiO2 system under tensile deformation is shown in figure 2(a), where it can be seen that the stress-strain relationship differs from those of both graphene and SiO2. The slope of the curve within elastic region is about 62.4 GPa, higher than 39.1 GPa of SiO2. However, multiple local peaks in the curve show up before the system ultimately breaks, the first peak occurs at around 8.9%, meaning that the incorporation of graphene to the composite system does not necessarily improve the yielding strain. Upon further stretching, two major peaks appear at the strain level of 13% and 20%, corresponding to the break of the SiO2 and the entire composite. The appearance of multiple peaks in the stress-strain curves also indicates that the encapsulation of graphene to SiO2 systems raises the plasticity and fatigue resistance of the composite, particularly when subjected to cyclic loadings. Zhang et al have shown that graphene hybrid with silica can improve the mechanical properties of polymer composite materials, similar conclusions were also obtained by Du et al [42, 43]. Similar observations can be found in the PG/SiO2 composite as shown in figure 2(b), where the elastic limit is slightly higher, 13%, but still lower than that of SiO2. The obtained Young’s modulus is 45.8 GPa, also notably higher than that of SiO2. Our calculations for the PG/SiO2 system show that with increasing defect concentration up to 14%, the Young’s moduli are all improved by at least 14 GPa when compared to pristine SiO2. It is therefore encouraging that the encapsulation of defective PG provides efficient reinforcement in raising elastic properties of SiO2 system, partly supporting our original hypothesis. Another feature summarized in figure 2(c) is that with increasing defect concentration, the Young’s modulus gradually decreases, this is easy to understand and consistent with the fact Young’s defective PG decreases with increasing
defect concentration, as shown in figure 1(f). Similar conclusion can be found for the ultimate stress/strain as shown in figure 2(d).

Under shear deformation, the calculated shear modulus, ultimate stress and strain of pristine SiO$_2$ crystal are 3.335 GPa, 0.643 GPa and 20%, respectively. Upon dispersion of graphene structures, it is observed that both the shear modulus and ultimate stress are notably raised, the former by at least 5 GPa and the later by at least 0.35 GPa. This observation is critical because in many engineering applications, structures carry shear loads more often as compared to the situation of carrying tensile loads. It is thus plausible that using defective graphene structures is effective in reinforcing composite structures. We note here that the variation of shear modulus for the PG/SiO$_2$ composite with respective to defect concentration is not monotonic in this set of simulations, probably due to the numerical errors or the stacking between PG and SiO$_2$ surface because we do observe decreasing trend in other sets of simulations with varied geometrical parameters of PG. Meanwhile, the calculated ultimate stress does show a decreasing trend within the defect concentration range we considered here. The variation of breaking strain is somewhat less influenced.

The compressive responses of the PG/SiO$_2$ system shown in figures 2(g), (h) provide some similar conclusions in the variation of modulus and ultimate stress with increased defect concentration. However, it

Figure 2. (a) and (b) Stress–strain relationships for graphene and PG encapsulated SiO$_2$ composites under tensile loadings, insets show typical failure structures. (c)–(h) show extracted mechanical properties extracted from tensile, shear and compress simulations.
should be noted that the compressive modulus is not enhanced when comparing to SiO₂ single crystal (29.4 GPa), this is apparently attributed to the weak compressive load carrying capability of graphene or PG along the in-plane direction, due to the 2 dimensional structural nature. Similarly, the ultimate stress is decreased comparing to 7.35 GPa of single crystal SiO₂. Interestingly, the ultimate strain show slight enhancement, because it is difficult to break graphene or PG via compression.

The effects of graphene or PG on the mechanical properties SiO₂ can be examined through analyzing the stress distribution dynamics before and after graphene/PG encapsulation. For pristine SiO₂, it is found that although the overall stress is zero at equilibrium state, silicon and oxygen atoms however, experiences distinct stress states, i.e. silicon is under tension and oxygen is under compression, such status is maintained up to the strain level of 7%, as shown in figure 3(a). When elongated to 19.9%, prior to the breaking point, the stress states of all atoms shift towards tensile level. Then, upon breaking, the high tensile stress state is suddenly released and the blue colored compressive states reappear in oxygen atoms, as shown in figure 3(c).

Different from the observations in pristine SiO₂, when a layer of graphene is encapsulated into the gaps of SiO₂ slabs, it is seen in figure 3(d) that a large number of oxygen atoms close to the graphene layer do not exhibit compressive stress states anymore. This observation indicates that the interaction at the SiO₂-graphene interfaces applies tensile states to the SiO₂ surface layer, thus although the overall Young’s modulus is raised, the breaking strain of the SiO₂ layers is substantially reduced, leading to the earlier failure of the graphene/SiO₂ system as observed in figure 2. Upon introduction of pores to the graphene system, although similar tensile stress states are found at the PG/SiO₂ interfaces, however, the reduced contact area between SiO₂ and PG leads to the later failure of the composites, therefore, the breaking strain of PG/SiO₂ does not show monotonic decreasing trend with defects concentration, as has been illustrated above in figure 2. This character also holds true when the system is under shear deformation.

We next proceed to study the effect of PG or graphene concentration on the overall mechanical properties of the PG/SiO₂ composites. To do this, the volume fraction of the PG layer was varied by changing the thickness of the SiO₂ slabs, the corresponding volume fraction obtained here are 5.4%, 5.9% and 6.8%. The summarized results for PG/SiO₂ system with various defect concentrations (here 3 sets of representative results on pristine graphene and PG with 6.16% and 13.85% defect concentrations are presented) are shown in figure 4, and

![Figure 3. Stress distribution patterns at different strain levels during tensile deformation for pristine SiO₂ crystal (a)–(c), graphene/SiO₂ composite (d)–(f) and PG/SiO₂ composite (g)–(i).](image-url)
interesting characters can be observed. Firstly, the Young’s modulus of the composite increases with PG volume fraction, while the ultimate stress/strain show irregular trends. This can be understood from the above analysis that increased PG volume fraction makes PG undertake more proportions of the load and thereby increases Young’s modulus. On the other hand, increased PG volume fraction means increased PG/SiO$_2$ interface-to-volume ratio, while from figure 3 it is understood that such interface introduces extra strain/stress to the SiO$_2$ structure, therefore, the system breaks earlier with lower defect concentration for most cases. When the concentration of defects (pores) is further increased, the true contact area between PG and SiO$_2$ is reduced, as a result, when defect concentration is increased to 13.85%, it is seen from figure 4(c) that the ultimate strain shows positive correlation with volume fraction, the ultimate stress therefore also shows different behavior as compared to the cases with low pore defect concentration, as shown in figure 4(b). Overall, an interplay between Young’s modulus modification and ultimate strength (strain) tuning is observed, i.e. low defect concentration leads to increased Young’s modulus while higher defect concentration leads to improved ultimate strength. This scenario also holds true for the PG/SiO$_2$ composites when subjected to shear deformation and the overall trend is very similar, as results shown in figures 4(d)–(f), where the patterns are very close to those in figure 4(a)–(c).

Secondly, the composite shows distinct variation trend in mechanical responses when subjected to compressive deformation, i.e., the compressive modulus decreases with PG volume fraction in general, so as the ultimate stress, the ultimate strain however shows slight increase with respect to the volume fraction. This observation can be understood from the fact that when graphene or PG is subjected to in-plane compression, out-of-plane deformation is easily induced due to its two-dimensional structure and ultrahigh flexibility, leading to increased gap space between the two SiO$_2$ slabs, in other words, the cross-sectional area along the loading direction is increased. Therefore, although some of the models exhibit improved breaking strain with increasing volume fraction, the increased cross-sectional area leads to reduced modulus and ultimate stress. It can be anticipated that such reducing effect won’t be significant because when larger size graphene or PG is utilized, folding or other types of local deformation modes may occur, the overall change of cross-sectional area is thus minimal.

The above analysis indicates that the interface between SiO$_2$ and PG plays an important role in modifying the mechanical properties of the PG/SiO$_2$ composites, this motivates us to explore whether the variation of surface roughness of SiO$_2$ affects the overall mechanical properties. To evaluate this, we randomly removed some surface atoms from SiO$_2$ to achieve varied roughness level and then performed mechanical property tests.

Figure 4. Effect of PG volume fraction on mechanical properties of PG/SiO$_2$ composites under tensile (a)–(c), shear (d)–(f) and compress loadings (g)–(i).
Results from tensile tests are shown in figure 5. It is seen that within the considered roughness range (from 0.125 nm to 0.225 nm), the Young’s modulus show certain improvement in general when compared to the same system with zero roughness, this is attributed to the improved contact quality between PG and SiO₂. The ultimate stress values extracted from the stress-strain curves, however, do not show monotonic changing trend, probably due to the limited cases and roughness ranges considered in this sets of simulations. For future work, it is necessary to explore the interplay between roughness and pore sizes and the combined effects on the mechanical properties of the PG/ SiO₂ composites.

Conclusion

In conclusion, we have performed systematic molecular dynamics simulations on the mechanical properties of the silicon dioxide/porous graphene composite. The object is to assess whether defective graphene structures could be utilized as effective fillers to reinforce mechanical properties of SiO₂ or other materials used in engineering components. Our results indeed provide evidence that although porous graphene is weaker than pristine graphene, it is stronger than SiO₂, upon simple dispersion of PG into the gap of SiO₂ slabs, certain amount of improvement in mechanical responses to external loadings are achieved. Such effect is modified by several parameters such as the defect concentration, loading methods, volume fraction of PG and interface roughness. The results lend confidence to engineers in that adaption of defective 2D materials could be a feasible and effective approach for fabricating high performance composite structures, and as a result, the cost will be significantly reduced. Further research on this topic is also required to optimize the performance, for example, how to take advantages of out-of-deformation modes of PG such as wrinkles and crumples to better match the surface conformations of SiO₂ or other materials that have larger roughness is an interesting topic for both experimental tests and simulation studies.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (NSFC #12072134) and Jiangsu Province NSF under the grant number BK20191426.
Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Chengyuan Wang  https://orcid.org/0000-0002-9790-4342
Chun Tang  https://orcid.org/0000-0002-7767-2126

References

[1] Zhang W X, Wang H, Zhao P and He C 2021 Preparation of cluster-like SnS/SnO2/C nanoparticle with enhanced electrochemical performance for lithium-ion batteries Ionics 27 1919
[2] Haro M et al 2021 Nano-vault architecture mitigates stress in silicon-based anodes for lithium-ion batteries Commun. Mater. 2 16
[3] Centi G and Perathoner S 2011 Nanostructured Electrodes and devices for converting carbon dioxide back to fuels: advances and perspectives. ed I. Zang Energy Efficiency and Renewable Energy Through Nanotechnology (London: Springer London)
[4] Li B, Sun H and Chen C 2016 Extreme mechanics of probing the ultimate strength of nanotwinned diamond Phys. Rev. Lett. 117 116103
[5] Lu L, Chen X, Huang X and Lu K 2009 Revealing the maximum strength in nanotwinned copper Science 323 607
[6] Fang T H, Li W L, Tao N R and Lu K 2011 Revealing extraordinary intrinsic tensile plasticity in gradient Nano-Grained copper Science 331 1587
[7] Lv S et al 2018 Investigation of the field characteristics and collective mechanical properties of defective graphene Nanomaterials 8 164
[8] Fang Q, Shen Y and Chen B 2015 Synthesis, decoration and properties of three-dimensional graphene-based microstructures: a review Chem. Eng. J. 264 753
[9] Ma B, Li H, Li X, Mei J and Lv Y 2016 Influence of nano-TiO2 on physical and hydration characteristics of fly ash–cement systems Constr. Build. Mater. 122 242
[10] Lu L, Ouyang D and Xu W 2016 Mechanical properties and durability of ultra high strength concrete incorporating multi-walled carbon Nanotubes Materials 9 419
[11] Tamin M, Hassan N M, Fattah K and Talachi A 2016 Performance of cementitious materials produced by incorporating surface treated multiwall carbon nanotubes and silica fume Constr. Build. Mater. 114 934
[12] Eftekhar M and Mohammadi S 2016 Multiscale dynamic fracture behavior of the carbon nanotube reinforced concrete under impact loading Int. J. Impact Eng. 85 55–64
[13] Song X, Zhang J and Shang S 2017 Mechanical properties of early-age concrete reinforced with multi-walled carbon nanotubes Mag. Concr. Res. 69 683
[14] Ghabari S A, Ghafari E and Assi L 2018 Pore structure of cementitious material enhanced by graphitic nanomaterial: a critical review Front. Struct. Civ. Eng. 12 137
[15] Park S, Lee K-S, Boozoku G, Cai W, Nguyen S T and Rusoff R S 2008 Graphene oxide papers modified by divalent ions—enhancing mechanical properties via chemical cross-linking ACS Nano 2 572
[16] Jang S-H, Kawashima S and Yin H 2016 Influence of carbon nanotube clustering on mechanical and electrical properties of cement pastes Materials 9 220
[17] Du H, Gao H J and Pang S D 2016 Improvement in concrete resistance against water and chloride ingress by adding graphene nanoplatelet Cem. Concr. Res. 83 114
[18] Bai S, Jiang L, Xu N, Jin M and Jiang S 2018 Enhancement of mechanical and electrical properties of graphene/cement composite due to improved dispersion of graphene by addition of silica fume Constr. Build. Mater. 164 433
[19] Kashif Ur Rehman S et al 2018 Influence of graphene nanosheets on rheology, microstructure, strength development and self-sensing properties of cement based composites Sustainability 10 822
[20] Xu G, Du S, He J and Shi X 2019 The role of admixed graphene oxide in a cement hydration system Carbon 148 141
[21] Belli A, Mobillo A, Bellezze T, Tittarelli F and Cachim P 2018 Evaluating the self-sensing ability of cement mortars manufactured with graphene nanoplatelets, virgin or recycled carbon fibers through piezoresistivity tests Sustainability 10 4013
[22] Hou D, Lu Z, Li X, Ma H and Li Z 2017 Reactive molecular dynamics and experimental study of graphene–cement composites: Structure, dynamics and reinforcement mechanisms Carbon 115 188–208
[23] Malakouti M M and Montazeri A 2016 Nanomechanics analysis of graphene via development of an MD–based AFEM Modares Mech. Eng. 16 1–9 https://mme.modares.ac.ir/article-13-4198-en.html
[24] Wang B, Jiang K and Wu Z 2016 Investigation of the mechanical properties and microstructure of graphene Nanoplatelet-Cement composite Nanomaterials 6 200
[25] Zhao S, Zhang Y, Yang J and Kitipornchai S 2020 Improving interfacial shear strength between graphene sheets by strain-induced wrinkles Carbon 168 135
[26] Liu J, Zhang Y, Zhang H and Yang J 2020 Mechanical properties of graphene-reinforced aluminium composite with modified substrate surface: a molecular dynamics study Nanotechnology 32 085712
[27] Luong D X et al 2020 Gram-scale bottom-up flash graphene synthesis Nature 577 647
[28] Zhou D, Cui Y, Xiao P-W, Jiang M-Y and Han B-H 2014 A general and scalable synthesis approach to porous graphene Nat. Commun. 5 4716
[29] Zheng B and Gu G X 2020 Stress field characteristics and collective mechanical properties of defective graphene J. Phys. Chem. C 124 7421
[30] Plimpton S 1995 Fast parallel algorithms for short-range molecular dynamics J. Comput. Phys. 117 1
[31] Plimpton S, Crozier P and Thompson A 2007 LAMMPS-large-scale atomic/molecular massively parallel simulator Sandia National Lab. 18 43
[32] Stukowski A 2010 Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool Model. Simul. Mater. Sci. Eng. 18 015012
[33] Bosch H A, Hoover W G and Vesely F J 1986 Canonical dynamics of the Nosé oscillator: stability, order, and chaos Phys. Rev. B 33 4253
[34] Broughton J Q, Meli C A, Vashishta P and Kalia R K 1997 Direct atomistic simulation of quartz crystal oscillators: bulk properties and nanoscale devices Phys. Rev. B 56 611
[35] Stuart S J, Tutein A B and Harrison J A 2000 A reactive potential for hydrocarbons with intermolecular interactions J. Chem. Phys. 112 6472
[36] Walther J, Jaffe R, Halicioglu T and Koumoutsakos P 2000 Molecular dynamics simulations of carbon nanotubes in water. Center for turbulence research Proc. of the Summer Program
[37] Lee C, Wei X, Kysar J W and Hone J 2008 Measurement of the elastic properties and intrinsic strength of monolayer graphene Science 321 385
[38] Reddy C D, Rajendran S and Liew K M 2006 Equilibrium configuration and continuum elastic properties of finite sized graphene Nanotechnology 17 864
[39] Lu Q, Gao W and Huang R 2011 Atomistic simulation and continuum modeling of graphene nanoribbons under uniaxial tension Model. Simul. Mat. Sci. Eng. 19 054006
[40] Tang C, Guo W and Chen C 2011 Structural and mechanical properties of partially unzipped carbon nanotubes Phys. Rev. B 83 075410
[41] Akinwande D et al 2017 A review on mechanics and mechanical properties of 2D materials—Graphene and beyond Extreme Mech. Lett. 13 42
[42] Zhang S et al 2017 Improved mechanical and fatigue properties of graphene oxide/silica/SBR composites RSC Adv. 7 40813
[43] Du W, Jin Y, Lai S, Shi L, Shen Y and Pan J 2019 Urethane-silica functionalized graphene oxide for enhancing mechanical property and fire safety of waterborne polyurethane composites Appl. Surf. Sci. 492 298