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Stress Concentration Factor of Single-Layered Graphene Sheets Containing Elliptical Vacancies

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ABSTRACT

In the present study, potential of finite element based molecular structural mechanics (MSM) for evaluating stress concentration factor of single-layered graphene sheets (SLGSs) with elliptical vacancies is successfully addressed. The MSM approach mimics the interatomic forces of the nanostructure by defining an equivalent frame structure containing beam elements. To obtain the mechanical and cross sectional properties of the equivalent beam, the potential energies of chemical bonds between carbon atoms in the hexagonal lattice of SLGSs are equaled to the strain energies of the beams. This novel proposed approach accurately predicts the stress concentration in graphene sheets with significantly less computational effort in comparison to computational physics methods. Both armchair and zigzag configurations are considered. Furthermore, a comparison between the results obtained by presented MSM approach and theory of elasticity for thin infinite panels having elliptical holes is presented. Influence of chirality, and geometry of elliptical vacancies are investigated in details. Results reveal that MSM approach can successfully predicts stress concentration factor phenomena in nano structures, especially SLGSs. It is seen that chirality has a significant effect on the stress concentration factor so that armchair SLGSs show a larger value of stress concentration.

Keywords: Defected grapheme; Elliptical vacancies; Molecular structural mechanics; Stress concentration factor; Finite element method.

1 INTRODUCTION

2D nanostructures are expected to have an important role in a huge variety of applications, extending from high performance sensors, gas separation, nanoelectromechanical systems devices, flexible electronics, and nanocomposites [1,2]. Over the last decade, carbon allotropes have been the leading material in the field of nanotechnology. After the discovery of fullerene (zero-dimensional) and carbon nanotube (one-dimensional), researchers have attempted to isolate 2D carbon nanostructure, called single layer graphene sheets (SLGSs). Graphene as a one-atom-thickness material has attracted notable excitement due to its extraordinary mechanical, electrical and thermal properties which open an opportunity to construct future nano-sized devices made of it. Because of its wide potential in nanotechnology, evaluation of unique mechanical properties of graphene has been of

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great interest [3–5] and the response of graphene against various loading conditions e.g. bending, buckling, and vibration has been extensively studied [6–9].

Due to the discrete nature of nanostructures, application of classical continuum mechanics is questionable. To conquer this, an atomistic point-view needs to be adopted. Computational physics methods, i.e. ab initio [10], Monte Carlo simulations [11], and molecular dynamics (MD) simulation [12], have been successfully implemented by the researchers in order to investigate nanostructures and especially graphene sheets. However, the computational expenses persuade researchers to find semi-atomistic methods which contain not only suppleness of the continuum view, but also the realistic standpoint of atomistic approaches.

A semi-atomistic approach first introduced by Li and Chu named molecular structural mechanics (MSM) used in order to analyze the behavior of the nanotubes [13]. Base of this method is to mimic the nanostructure like SLGSs to the macro frame-like structure contain usual mechanical element as beam or bar. These mechanical elements are coequvalent the chemical bonds between atoms in the nanostructure. By introducing this method, many research were used it to simulate the mechanical behavior of the nanostructure such as carbon nanotubes or SLGSs [14–16].

By using MSM, the mechanical properties of perfect SLGSs were evaluated by Sakhaee-Pour [17] and the Young's and shear modules were obtained as well as Poisson's ratio. The results demonstrated that the MSM approach could predict the mechanical properties like the atomistic method. In addition, the mechanical properties of SLGSs were obtained using truss elements instead of beam ones by Scarpa et.al [18]. Also, Lu et.al [19] studied the pure bending condition of the monolayer graphene analytically and compare their results with ab initio potential energy. Furthermore, Firouz-Abadi et.al modified the MSM approach for analyzing the SLGSs buckling [20]. By comparing the molecular dynamic method and MSM, they modified the cross section of the beam element of the MSM approach so that the MSM results were getting closer to the molecular dynamics ones. Finally, they showed that by using the modified MSM, the buckling load of the SLGSs were considerably lower than what the classical MSM predicted.

The vibrational attributes of zigzag and armchair configurations of the carbon nanotubes and single layered graphene sheets were illustrated by Hashemnia et.al adopting MSM [21]. They studied different boundary condition and varied aspect ratio for both carbon nanotubes and single layered graphene sheets. The results were demonstrated that the fundamental frequencies of the single layered graphene sheets were lower than those of the carbon nanotubes. Finally, they reported and compared their results with molecular dynamic approach.

Investigating the mechanical behavior of the wrinkled SLGSs were reported by Wang et.al [22]. They derived the continuum mechnics formulation for simulating the characteristic the SLGSs wrinkle. Then, the SLGSs wrinkles effects on the vibrational behavior were studied by simulating the SLGSs as the 3-node beam elements according to the MSM technique. Finally, they concluded that slight wrinkle in the SLGSs did not make considerable effect on the vibrational behavior compare the unwrinkled SLGSs. On the other side, highly wrinkled SLGSs natural frequencies and mode shape were completely different with the unwrinkled ones.

In graphene, carbon atoms are arranged on a perfect honeycomb lattice of sp^2 chemical bonds. However, both experimental and theoretical investigations reveal that graphene structure has inevitable defects during its fabrication process which make significant drastic changes in its mechanical properties. Vacancies which means missing carbon atoms is the most reported defect in graphene sheets. The influence of shapes and distributions of vacancies on mechanical characterization of graphene sheets are studied in the literature [23–25].

One of the inevitable defects of the SLGSs is the Stone-Wales defect which was investigated by researchers [26–28]. The graphene nanofilms which containing the Stone-Wales defect were analyzed by Wand et.al [29]. They obtained the mechanical properties of mentioned SLGSs by studying the position of defects, types of Stone-Wales defects and number of them. The SLGSs defects can be useful for some applications such as desalinations and filtrations due to mechanical and chemical flexibility and stability [30,31]. The stress concentration factor of the defected SLGSs with a circular hole was investigated by Jalali et.al [32]. They used MSM approach in order to find a description for the stress concentration of graphene sheets of both armchair and zigzag configurations. Finally, the MSM method results are compared to those obtained by molecular dynamic simulations to validate the accuracy.

There are many works in the literature that address the fracture behavior and stress concentration of defected graphene sheets based on well-known computational physics approaches like molecular dynamics, Monte Carlo simulations and even DFT calculations. However, the novelty of the present work is introducing finite element based MSM approach for evaluation of stress concentration factor in nanostructures, as a semi-atomic point of view. Hence, this paper aimed to predict the stress concentration factor of the SLGSs having elliptical defects and correlate the classical stress concentration factor concept to the nanostructure by use of MSM approach.

2 MATERIALS AND MODEL

2.1 Stress concentration factor

In mechanical engineering, the effect of geometrical discontinuities like holes, cavities and cracks is taken into account by introducing the concept of stress concentration [33,34]. Based on theory of elasticity, sudden changes in cross sections of structural members causes an increasing effect in the expected stresses at the zone around. This high local stress can be explained by defining an increasing factor called the stress concentration factor, *K*. This factor is calculated by dividing the peak stress, σ_{max} , to a reference stress in the body, σ_{ref} :

$$K = \frac{\sigma_{max}}{\sigma_{ref}} \tag{1}$$

For a thin panel of infinite dimension having an elliptical hole of diameters 2*a* and 2*b* which is loaded by a unidirectional stress of σ_{ref} along *y* direction (See Fig. 1), the expression for the stress concentration factor based on analytical elasticity solution is [33]:

$$K = \frac{\sigma_{max}}{\sigma_{ref}} = 1 + 2\alpha \tag{2}$$

where $\alpha = a / b$ is the aspect ratio of the elliptical hole.

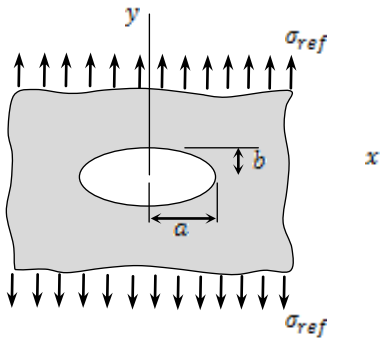

Fig.1
An infinite thin panel having an elliptical hole under unidirectional tension.

As a structural planar member, an engineering point of view to graphene sheets may be valuable. Consequently, the defected graphene sheets having vacancies can be considered as a planar structural member containing holes. In this work, the classical concept of stress concentration factor is developed for elliptical vacancies on single-layered graphene sheets (SLGSs) under unidirectional tensile loading condition. The molecular structural mechanics (MSM) approach is adopted to evaluate the stress concentration factor of SLGSs. Despite the accuracy and simplicity of MSM, based on the authors knowledge, this approach is not addressed for evaluation of stress concentration factor in nanostructures. Finally, the results in the nano scale is compared with classical elasticity of thin panels having elliptical holes (Eq. (2)).

2.2 MSM approach

MSM approach is applied to evaluate the stress concentration factor for the SLGSs with elliptical vacancies in atomistic point of view. This approach mimics the interatomic forces of carbon lattice by defining an equivalent macro frame structure containing beam elements. To obtain the mechanical and cross sectional properties of the equivalent beam, the potential energies of chemical bonds between carbon atoms, called covalent bond, are equaled to the strain energies of the beams. The main chemical and strain energies are shown in Fig. 2 and Fig. 3.

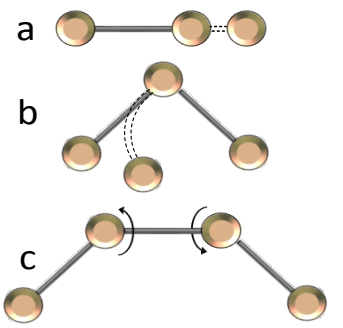

Fig.2
Main chemical energies a) Stretching b) Bending c) Dihedral torsional.

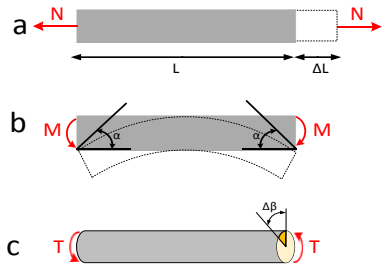

Fig.3
Main strain energies a) Stretching b) Bending c) Torsional.

Applying equivalency between chemical and strain energies, properties of equivalent beam can be obtained. The common deformation energies i.e. stretching energy, bending energy and torsional energy of a beam denoted respectively by U_r, U_θ, and, U_φ are defined as follows [13]:

$$U_r = \frac{EA}{2L}(\Delta r)^2, U_\theta = \frac{EI}{2L}(\Delta\theta)^2, U_\varphi = \frac{GJ}{2L}(\Delta\varphi)^2 \tag{3}$$

where E is the elastic and G is the shearing modulus. A, I, and J are the geometric parameters of the cross section of the beam i.e. the area, the moment of inertia, and the polar moment of inertia, respectively, while L denotes the length of beam. The potential energy of covalent bond in the nanostructure of SLGSs between carbon atoms can be determined as follows [13]:

$$U_r = \frac{k_r}{2}(\Delta r)^2, U_\theta = \frac{k_\theta}{2}(\Delta\theta)^2, U_\varphi = \frac{k_\varphi}{2}(\Delta\varphi)^2 \tag{4}$$

In Eqs. (3) and (4), Δr , $\Delta\theta$, and $\Delta\varphi$ are the stretching displacement, bending rotation, and torsional rotation, respectively. By equaling Eq. (3) and Eq. (4), one may simply obtain the tensile rigidity, $EA = k_r L$, the flexural rigidity, $EI = k_\theta L$, and the torsional rigidity, $GJ = k_\varphi L$, of the equivalent beam.

In the present study, finite element method (FEM), as the most popular computational solution in the field of structural analysis, is applied. Geometrical 2D modeling is performed by constructing an end-to-end connecting beam network on the pattern of honeycomb lattice of graphene, while the length of beams is selected equal to carbon-carbon bond. To create the desired vacancy, an elliptic of diameters $2a$ and $2b$ whose center is coincident with a vertex of honeycomb lattice is plotted and all the beams which are completely inside the elliptic are removed. It means that dangling bonds have been remained in the model. It is noted that due to the discrete nature of the SLGSs, the edge of the elliptical vacancy is not exactly smooth and the diameters of the vacancy will be changed stepwise. It is impossible to model an infinite SLGS in FEM, hence, a square honeycomb lattice area containing an elliptical vacancy is modelled and its dimension is defined large enough so that the stress distribution around the vacancy not to be noticeably influenced by the edge effect. The center of square area is coincident with the center of elliptical vacancy. For nodes located at the lower edges, the movements along y direction and rotations are fixed, while, left and right edges are allowed to be free. The unidirectional tensile loading is applied in the form of concentrated nodal force, F, which is dispersed at the nodes of the upper edge along y direction (See Fig. 4). One

can conclude that the value of applied force does not affect the evaluation of stress concentration factor, as the solution is linear and both the maximum and the reference stresses are proportionally related to the applied force.

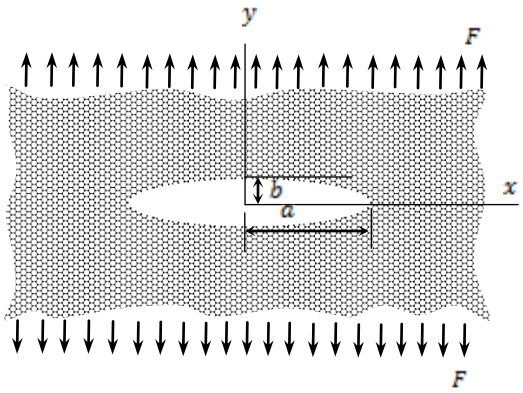

Fig.4
Frame-like MSM model of SLGS having elliptical vacancies.

Assuming [*K*] as the global stiffness matrix, {*u*} as the global nodal displacement vector, and {*f*} as the nodal external force vector, the governing differential equations for whole system of frame-like beam structure can be construct as follows:

$$[K]\{u\} = \{f\} \tag{5}$$

By solving Eq. (5), the displacements, strains and stresses in the beam lattice is obtained. Then, based on Eq. (1) one can calculate the stress concentration factor, *K*, by dividing the maximum axial stress of beams, which occurs around the vacancy edges, to the axial stress of beams far enough from the vacancy as the σ_{ref} . A sample axial stress contour plot of beams is represented in Fig. 5.

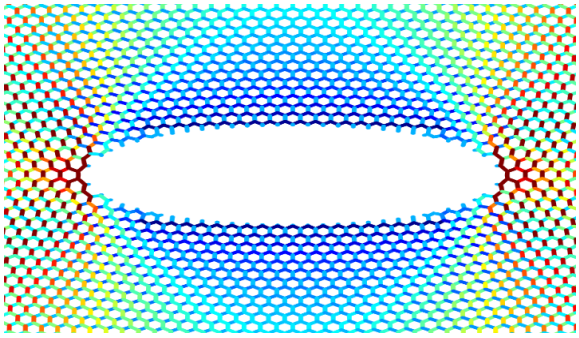

Fig.5
A sample axial stress contour plot of beams.

3 RESULTS AND DISCUSSION

In this section evaluation of stress concentration factor, *K*, based on MSM approach is performed and the numerical results are presented. In order to find rigidities of the equivalent beam, the force constants of carbon-carbon bond in the hexagonal lattice of SLGS are considered as: $k_r = 6.52\times10^{-7} N/nm$, $k_\theta = 8.76\times10^{-10} N.nm$, $k_\varphi = 2.78\times10^{-10} N.nm$ from molecular mechanics [13]. The length of equivalent beams, L , is considered equals to the carbon-carbon covalent bond as $1.421\mathring{A}$ [13]. Besides, SLGSs with either armchair or zigzag configurations are considered.

At first step, the MSM approach needs to be validated. Therefore, the MSM present results for the case of circular holes (*a*=*b*) is compared by reported results by Pugno and Ruoff [35] introducing Quantized Fracture Mechanics (QFM). As an energy-based theory, QFM modifies continuum-based fracture mechanics by substituting the differentials in Griffith's criterion with finite differences. The stress concentration, *K*, versus the number of

omitted atoms is depicted in the Fig. 6. One can see a conformity in the results. This confirms that the application of MSM in present work is reliable for a study on stress concentration factor of defected graphene sheets.

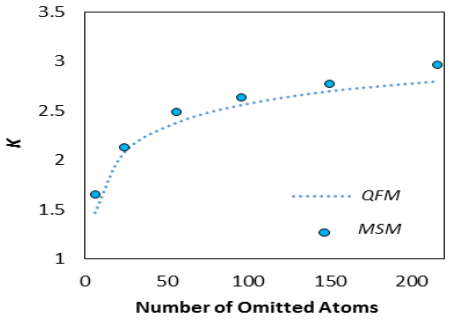

Fig.6
Comparison between stress concentration factor obtained by MSM and QFM for a circular vacancy.

Figs. 7 and 8 demonstrate the stress concentration factor for SLGSs having elliptical holes for armchair and zigzag configurations, respectively. The values of stress concentration factor are presented for various values of aspect ratio of elliptical hole, α , in logarithmic scale. One can see that for both configurations, by increasing α , the stress concentration factor increases; however, for the vacancies with $\alpha \succ 1$, the stress concentration factor rises significantly. The reason is the orientation of the crack length with respect to loading direction. When the length of crack is parallel to the loading direction ($\alpha \prec 1$), the unidirectional tension is weaker to open the crack in comparison to the case that crack length is perpendicular to the tension load ($\alpha \succ 1$). To improve the usefulness of presented results, equations for evaluating stress concentration factor for both armchair and zigzag configurations are obtained by cure fitting as follows:

$$K = 0.6 + 2\alpha\left(armchair\right) \tag{6}$$

$$K = 1 + 1.3\alpha\left(zigzag\right) \tag{7}$$

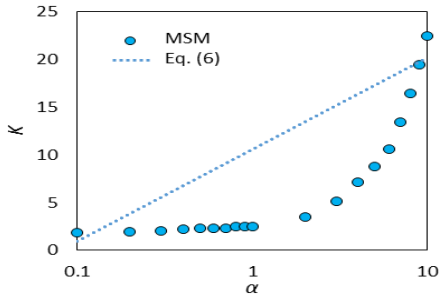

Fig.7
Stress concentration factor of SLGSs having elliptical holes for armchair configuration.

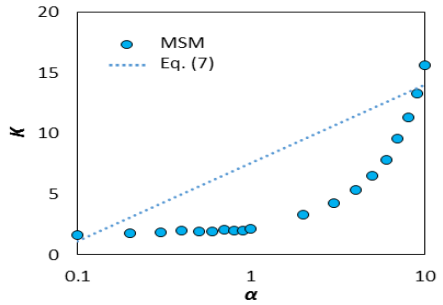

Fig.8
Stress concentration factor of SLGSs having elliptical holes for zigzag configuration.

Fig. 9 compares the values of stress concentration factor of armchair and zigzag configurations. It is seen that armchair SLGSs have larger stress concentration factor than zigzag one. Furthermore, a comparison between the results obtained by presented MSM approach and theory of elasticity for thin infinite panels having elliptical holes, i.e. Eq. (2), is presented. Results reveal that the trends of both elasticity and MSM approaches are same which

means that the proposed MSM model can successfully predict the stress concentration phenomena in nanostructures. The difference between the results is because of discrete nature of SLGSs and the assumption of infinite panel in theory of elasticity.

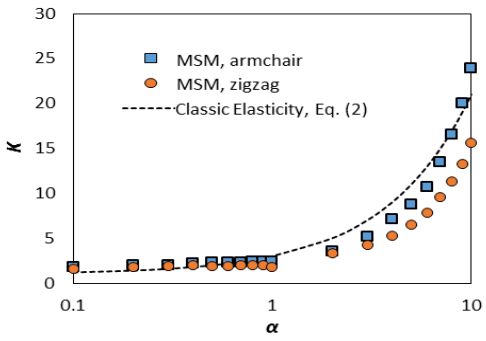

Fig.9
Comparison between stress concentration factor obtained by MSM and theory of elasticity.

4 CONCLUSIONS

Atomistic evaluation of stress concentration factor for SLGSs containing elliptical vacancies are investigated. For this purpose, the carbon-carbon covalent bonds are simulated by equivalent beam elements to construct the frame-like hexagonal structure of SLGSs. In order to match the response of the equivalent finite element based beam network to the SLGS nanostructure, the strain energies of the structural beams are equaled to the potential energies of chemical bonds. As the main conclusion, results reveal that MSM approach can successfully predicts stress concentration factor phenomena in nano structures, especially SLGSs. Usability of results are improved by presenting equations for evaluating stress concentration factor of both armchair and zigzag configurations. It is seen that armchair SLGSs have larger stress concentration factor than zigzag one. Showing potential application of MSM in the case of predicting stress concentration opens an opportunity for future works in the field of investigation of fracture mechanics of nanostructures based on semi-atomistic approaches which is the main novelty of the present work. Furthermore, obtained results are applicable for designing nano devices containing SLGSs as their structural element.

REFERENCES

[1] Tourki Samaei A., Hosseini Hashemi S., 2012, Buckling analysis of graphene nanosheets based on nonlocal elasticity theory, *International Journal of Nano Dimension* **2**: 227-232.
[2] Prasanna Kumar T. J., Narendar S., Gupta B. L. V. S., Gopalakrishnan S., 2013, Thermal vibration analysis of double-layer graphene embedded in elastic medium based on nonlocal continuum mechanics, *International Journal of Nano Dimension* **4**: 29-49.
[3] Soldano C., Mahmood A., Dujardin E., 2010, Production, properties and potential of graphene, *Carbon* **48**: 2127-2150.
[4] Ansari R., Ajori S., Motevalli B., 2012, Mechanical properties of defective single-layered graphene sheets via molecular dynamics simulation, *Superlattices and Microstructures* **51**: 274-289.
[5] Mortazavi B., Ahzi S., 2013, Thermal conductivity and tensile response of defective graphene: A molecular dynamics study, *Carbon* **63**: 460–470.
[6] Adali S., 2012, Variational principles for nonlocal continuum model of orthotropic graphene sheets embedded in an elastic medium, *Acta Mathematica Scientia* **32**: 325-338.
[7] Kang J. W., Lee S., 2013, Molecular dynamics study on the bending rigidity of graphene nanoribbons, *Computational Materials Science* **74**: 107-113.
[8] Shokrieh M. M., Esmkhani M., Haghighatkhah A. R., Zhao Z. , 2014, Flexural fatigue behavior of synthesized graphene/carbon-nanofiber/epoxy hybrid nanocomposites, *Materials & Design* **62**: 401-408.
[9] Firouz-Abadi R. D., Hosseinian A. R., 2012, Free vibrations of single-walled carbon nanotubes in the vicinity of a fully constrained graphene sheet, *Computational Materials Science* **53**: 12-17.
[10] Oubal M., Picaud S., Rayez M.-T., Rayez J.-C., 2012, Structure and reactivity of carbon multivacancies in graphene, *Computational and Theoretical Chemistry* **990**: 159-166.
[11] Ozturk Z., Baykasoglu C., Kirca M., 2016, Sandwiched graphene-fullerene composite: A novel 3-D nanostructured material for hydrogen storage, *International Journal of Hydrogen Energy* **41**: 6403-6411.

[12] Gao Y., Hao P., 2009, Mechanical properties of monolayer graphene under tensile and compressive loading, *Physica E: Low-dimensional Systems and Nanostructures* **41**: 1561-1566.
[13] Li C., Chou T.-W. W., 2003, A structural mechanics approach for the analysis of carbon nanotubes, *International Journal of Solids and Structures* **40**: 2487-2499.
[14] Bocko J., Lengvarský P., 2018, Buckling analysis of graphene nanosheets by the finite element method, *MATEC Web of Conferences* **157**: 06002.
[15] Namin S. F. A., Pilafkan R., 2017, Vibration analysis of defective graphene sheets using nonlocal elasticity theory, *Physica E: Low-Dimensional Systems and Nanostructures* **93**: 257-264.
[16] Agius Anastasi A., Ritos K., Cassar G., Borg M. K., 2016, Mechanical properties of pristine and nanoporous graphene, *Molecular Simulation* **42**: 1502-1511.
[17] Sakhaee-Pour A., 2009, Elastic properties of single-layered graphene sheet, *Solid State Communications* **149**: 91-95.
[18] Scarpa F., Adhikari S., Srikantha Phani A., 2009, Effective elastic mechanical properties of single layer graphene sheets, *Nanotechnology* **20**: 065709.
[19] Lu Q., Arroyo M., Huang R., 2009, Elastic bending modulus of monolayer graphene, *Journal of Physics D: Applied Physics* **42**: 102002.
[20] Firouz-Abadi R. D., Moshrefzadeh-Sany H., Mohammadkhani H., Sarmadi M., 2016, A modified molecular structural mechanics model for the buckling analysis of single layer graphene sheet, *Solid State Communications* **225**: 12-16.
[21] Hashemnia K., Farid M., Vatankhah R., 2009, Vibrational analysis of carbon nanotubes and graphene sheets using molecular structural mechanics approach, *Computational Materials Science* **47**: 79-85.
[22] Wang C. G., Lan L., Liu Y. P., Tan H. F., He X. D., 2013, Vibration characteristics of wrinkled single-layered graphene sheets, *International Journal of Solids and Structures* **50**: 1812-1823.
[23] Yadav S., Zhu Z., Singh C. V., 2014, Defect engineering of graphene for effective hydrogen storage, *International Journal of Hydrogen Energy* **39**: 4981-4995.
[24] Wang M. C. C., Yan C., Ma L., Hu N., Chen M. W. W., 2012, Effect of defects on fracture strength of graphene sheets, *Computational Materials Science* **54**: 236-239.
[25] Liu L., Qing M., Wang Y., Chen S., 2015, Defects in graphene: generation, healing, and their effects on the properties of graphene: A review, *Journal of Materials Science & Technology* **31**: 599-606.
[26] Xiao J. R., Staniszewski J., Gillespie J. W., 2010, Tensile behaviors of graphene sheets and carbon nanotubes with multiple Stone–Wales defects, *Materials Science and Engineering: A* **527**: 715-723.
[27] Rodrigues J. N. B., 2011, Zigzag graphene nanoribbon edge reconstruction with Stone-Wales defects*, Physical Review B* **84**: 155435.
[28] Fan B. B., Yang X. B., Zhang R., 2010, Anisotropic mechanical properties and Stone–Wales defects in graphene monolayer: A theoretical study, *Physics Letters A* **374**: 2781-2784.
[29] Wang S. P., Guo J. G., Zhou L. J., 2013, Influence of Stone-Wales defects on elastic properties of graphene nanofilms, *Physica E: Low-Dimensional Systems and Nanostructures* **48**: 29-35.
[30] Surwade S. P., 2015, Water desalination using nanoporous single-layer graphene, *Nature Nanotechnology* **10**: 459-464.
[31] Cohen-Tanugi D., Grossman J. C., 2015, Nanoporous graphene as a reverse osmosis membrane: Recent insights from theory and simulation, *Desalination* **366**: 59-70.
[32] Jalali S. K., Beigrezaee M. J., Pugno N. M., 2017, Atomistic evaluation of the stress concentration factor of graphene sheets having circular holes, *Physica E: Low-dimensional Systems and Nanostructures* **93**: 318-323.
[33] Pilkey W. D., Pilkey D. F., 2007, *Peterson's Stress Concentration Factors*, John Wiley & Sons, Inc.
[34] Boresi A. P., Schmidt R. J., 2002, *Advanced Mechanics of Materials*, Wiley-VCH Verlag GmbH & Co. KGaA.
[35] Pugno N. M., Ruoff R. S., 2004, Quantized fracture mechanics, *Philosophical Magazine* **84**: 2829-2845.