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Research article

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MOLECULAR DYNAMICS MODELING OF THE MECHANICAL BEHAVIOR OF YSZ-CERAMICS/GRAPHENE NANOCOMPOSITE

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Abstract. Within the framework of the molecular dynamics method, the mechanical behavior of a graphene nanoinclusion in a matrix of zirconium dioxide stabilized by yttrium oxide has been simulated. The analysis of the possibility of using the existing interatomic interaction potentials developed for these crystals in model mechanical tests of the nanocomposite is carried out. It is shown that pristine graphene is an excellent reinforcing element of the composite since it is deformed without the formation of defects in the range of small and medium strain values. The artificial creation of small pores of 3 Å in diameter in the intermediate layers also makes a little effect on the destruction of the graphene nanoinclusion. The creation of pores of 5 Å in diameter and more can lead to cracking of the nanoinclusion. To improve the accuracy of the model and to observe the destruction of the sample under study, the need to develop new potential for interatomic interaction is demonstrated.
Keywords: nanocomposites, ceramics, graphene, molecular dynamics

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1. Introduction

Yttria-stabilized zirconium dioxide (or YSZ ceramics) is a promising material with a wide range of applications, for example, in catalysis [1], in refractory coatings [2,3], and in medicine [4,5]. The use of graphene as a reinforcing material in the YSZ-ceramics-graphene nanocomposite will make it possible to serve as a basis for creating an effective molecular oxygen pump with possible use in power engineering, engine building, fine chemical synthesis technologies, and in the development of new medical equipment [6-8]. There is a possibility that when the required functional properties of the material are achieved, its mechanical characteristics will deteriorate. In this regard, the aim of this work is to study the mechanical behavior of a planar graphene inclusion (a graphene interlayer) in an YSZ crystal.

2. Model of the nanocomposite "YSZ-ceramics-graphene"

The theoretical model of the composite is shown in Fig. 1a. It includes two regions of yttria-stabilized zirconium oxide (YSZ) crystal with a planar inclusion between them, consisting of

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several graphene monolayers. Mechanical tests of the composite were carried out by the molecular dynamics method implemented in the LAMMPS software package [9].

Periodic boundary conditions were applied to the modeling domain in all three spatial coordinates. Figures 1b - 1d show atomic models of the crystals under study after relaxation: with no cylindrical pore in the graphene nanoinclusion (Fig. 1b) and with a pore of 3 Å (Fig. 1c) and 5 Å (Fig. 1d) in diameter there.

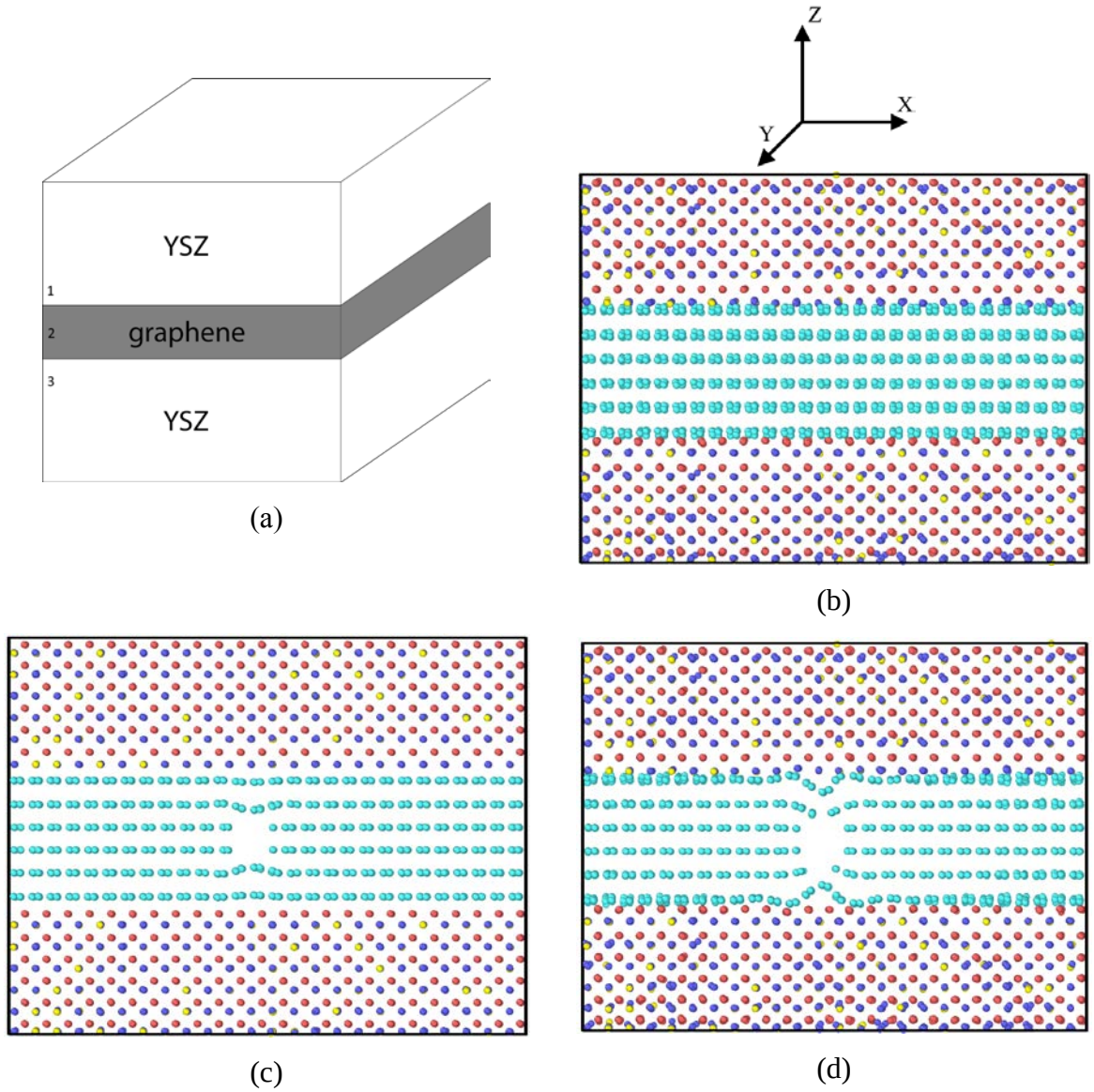

Fig. 1. Atomic models of the composite "YSZ-ceramics - graphene":
(a) Geometric model of the YSZ-ceramic – graphene nanocomposite; (b) an atomic model with a defect-free nanoinclusion consisting of several sheets of graphene, (c) with a 3 Å pore in the inclusion, (d) with a 5 Å pore in the inclusion. The red atoms are oxygen, the blue ones are zirconium, the yellow ones are yttrium, and the blue ones are carbon

3. Choice of potential

To solve the problem, it was necessary to select a potential that would adequately describe the mechanical behavior of the model under deformation. A detailed study of various interatomic potentials was carried out to refine the model and to obtain the results: (a) a combination of the Coulomb-Buckingham (CB) and Lennard-Jones (LJ) potentials, (b) the ReaxFF potential

(Reactive ForceField), (c) a combination of the Buckingham (B), ReaxFF and Lennard-Jones potentials (B-ReaxFF-LJ combination).

The first combination was considered in the model which was proposed in [10] for modeling shock loads on the YSZ / graphene composite by compressing the crystal at a high speed (300-1000 m/s). The CB potential was responsible for the interaction between oxygen atoms, as well as between oxygen atoms and zirconium and yttrium ions. The LJ potential was responsible for the interaction between carbon atoms and oxygen, yttrium and zirconium atoms. Pair interactions between yttrium and zirconium ions were described by Coulomb's law. In the present work, the simulation was carried out with parameters specified in [10]. A model composite with six graphene layers without defects at room temperature was considered. Figure 2 shows the result of modeling a composite deformed by tension along the Z-axis to the strain level of 0.1 %.

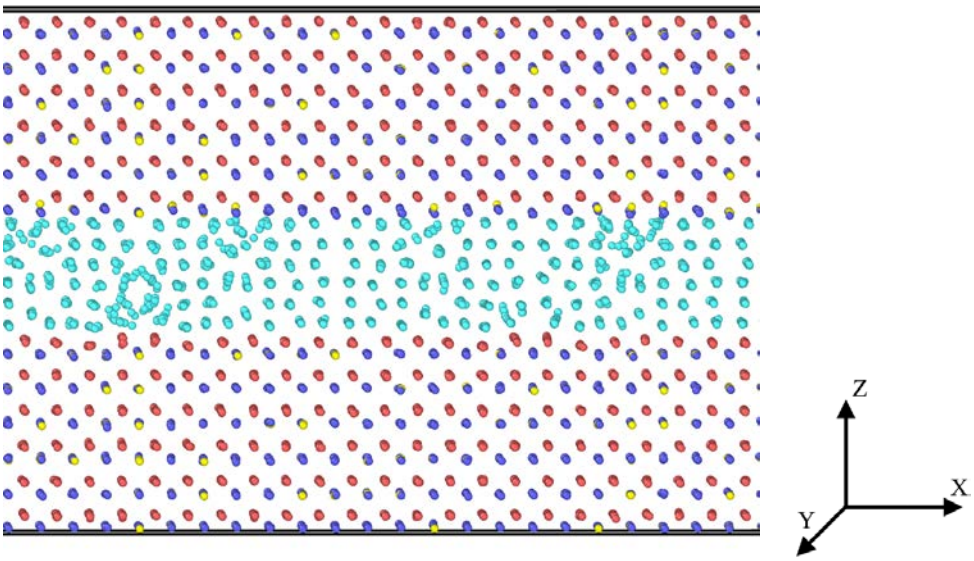

Рис. 2. The result of modeling the "YSZ-ceramics - graphene" system subjected to tension along the Z-axis, using a combination of the Coulomb-Buckingham and Lennard Jones potentials. Color designation of atoms corresponds to the description in Fig. 1

As is seen from Fig. 2, the model shows unsatisfactory results under tension due to an incorrect description of the interaction between graphene atoms under tension. The result remained unsatisfactory for stretching at all strain rates. At the same time, the use of other potentials to describe the interaction between carbon atoms, such as ReaxFF [11], AIREBO [12], or Tersoff [13], did not lead to adequate results. In the case of the Tersoff potential, atoms of YSZ ceramics began to penetrate between undeformed graphene layers, which is unlikely. In the case of the AIREBO potential, the model was unstable: graphene passed into an amorphous state. In the case of the ReaxFF potential developed for carbon materials [11], the entire composite became unstable due to poor matching of the interaction forces, as a result of which all the atoms were mixed. Therefore, this model turned out to be unsuitable for solving our task.

Then the potential of ReaxFF, proposed in [14], was considered. It was developed to simulate YSZ ceramics in fuel cells and was aimed at studying the migration of ions in the crystal lattice. This potential was applied to our model of a composite with three defect-free graphene sheets. Figure 3 shows the result of modeling a composite subjected to tension along the Z-axis to the strain level of 70 %.

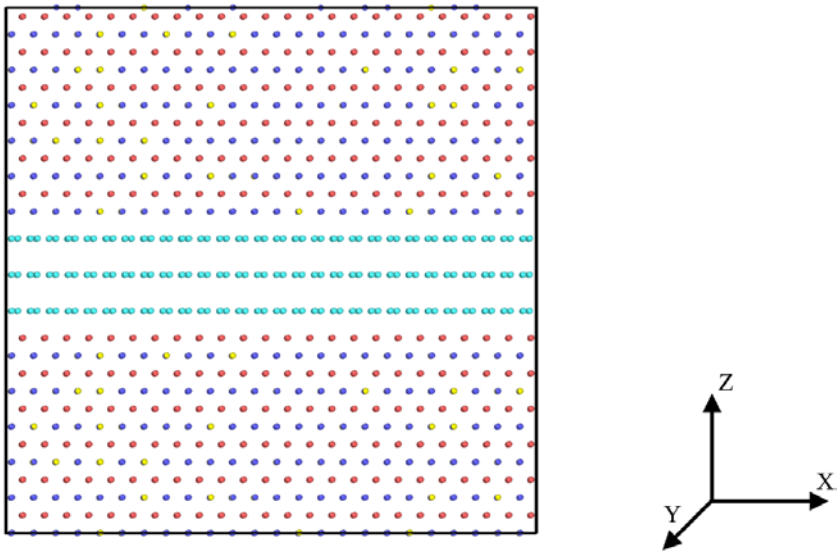

Fig. 3. The result of modeling the system "YSZ-ceramics - graphene" system subjected to tension along the Z-axis, using the ReaxFF potential. Color designation of atoms corresponds to the description in Fig. 1

According to the results obtained, the ReaxFF potential is not suitable for modeling the mechanical behavior of a composite with a graphene interlayer, since no matter how much the material is deformed, no restructuring of bonds or any destruction is observed even at a deformation of 300 %.

The B-ReaxFF-LJ combination in solving the test problem made it possible to build a stable model and to obtain explainable results, in contrast to the previous two potentials. In this case, the B potential was used to describe the interaction between yttrium, zirconium, and oxygen atoms, the ReaxFF potential to describe the interaction between carbon atoms in graphene, and the LJ potential, using the Lorentz-Berthelot mixture rule, to describe the interaction between graphene and yttrium, oxygen and zirconium atoms. This combination of potentials was chosen for further modeling. When simulating the deformation of the sample, the forces were applied normally to the plane of the graphene nanoinclusion. The simulation was carried out at room temperature in the system and at a strain rate of 10^9 s^{-1}, with a time step of 0.1 fs.

4. Results of mechanical tests of the "YSZ-ceramics-graphene" nanocomposite

In Figures 4 and 5, the states of the YSZ-ceramic - graphene nanocomposite under the action of tensile or compressive forces applied perpendicular to the graphene sheets are demonstrated.

It can be seen that, in the course of tension/compression, graphene sheets experience undulating warpage, the nature of which changes depending on the method of applying forces to the sample. The crystal lattice of ceramics maintains order in the packing of atoms, breaking it only near graphene sheets: atoms in the region of ceramics adjacent to graphene penetrate into the formed bends of graphene sheets. The nucleation of a cylindrical pore of 5 Å in diameter leads to significant deformation of graphene sheets, which is not observed in the case of a similar pore of 3 Å in diameter. Further tension along the Z-axis leads to cracking of the graphene nanoinclusion (more precisely, to delamination of graphene sheets). Compressive and shear deformations in this case (at temperatures up to 1000°C) do not lead to the appearance of cracks.

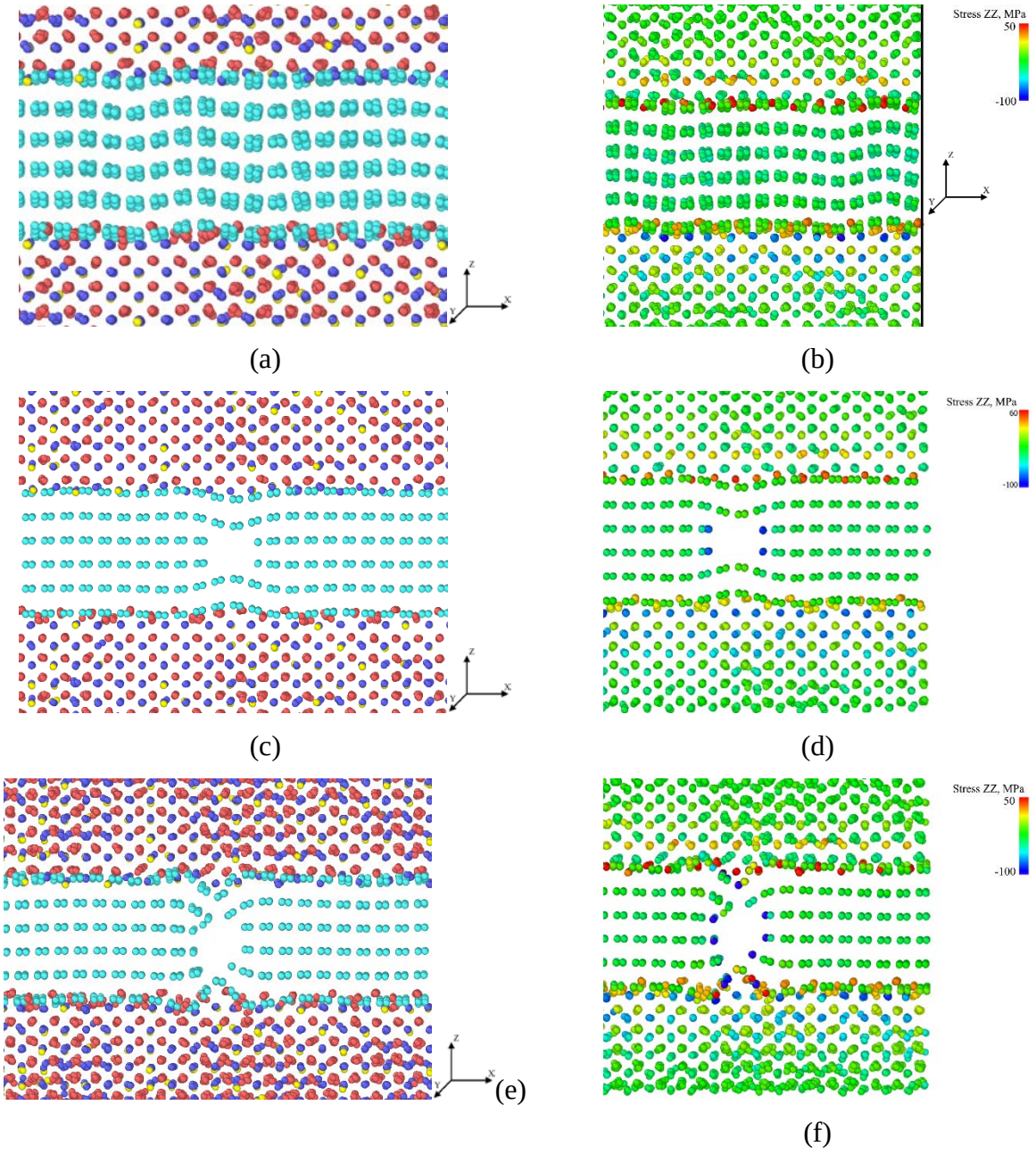

Fig. 4. Nanocomposite "YSZ-ceramics - graphene" deformed by 15% compression along the Z-axis. Atomic model and stress map of the composite (a) - (b) with a defect-free planar nanoinclusion, (c) - (d) with a pore of 3 Å in diameter in the inclusion, (e) - (f) with a pore of 5 Å in diameter in the inclusion. The modeling used the B-ReaxFF-LJ combination of potentials. Color designation of atoms corresponds to the description in Fig. 1

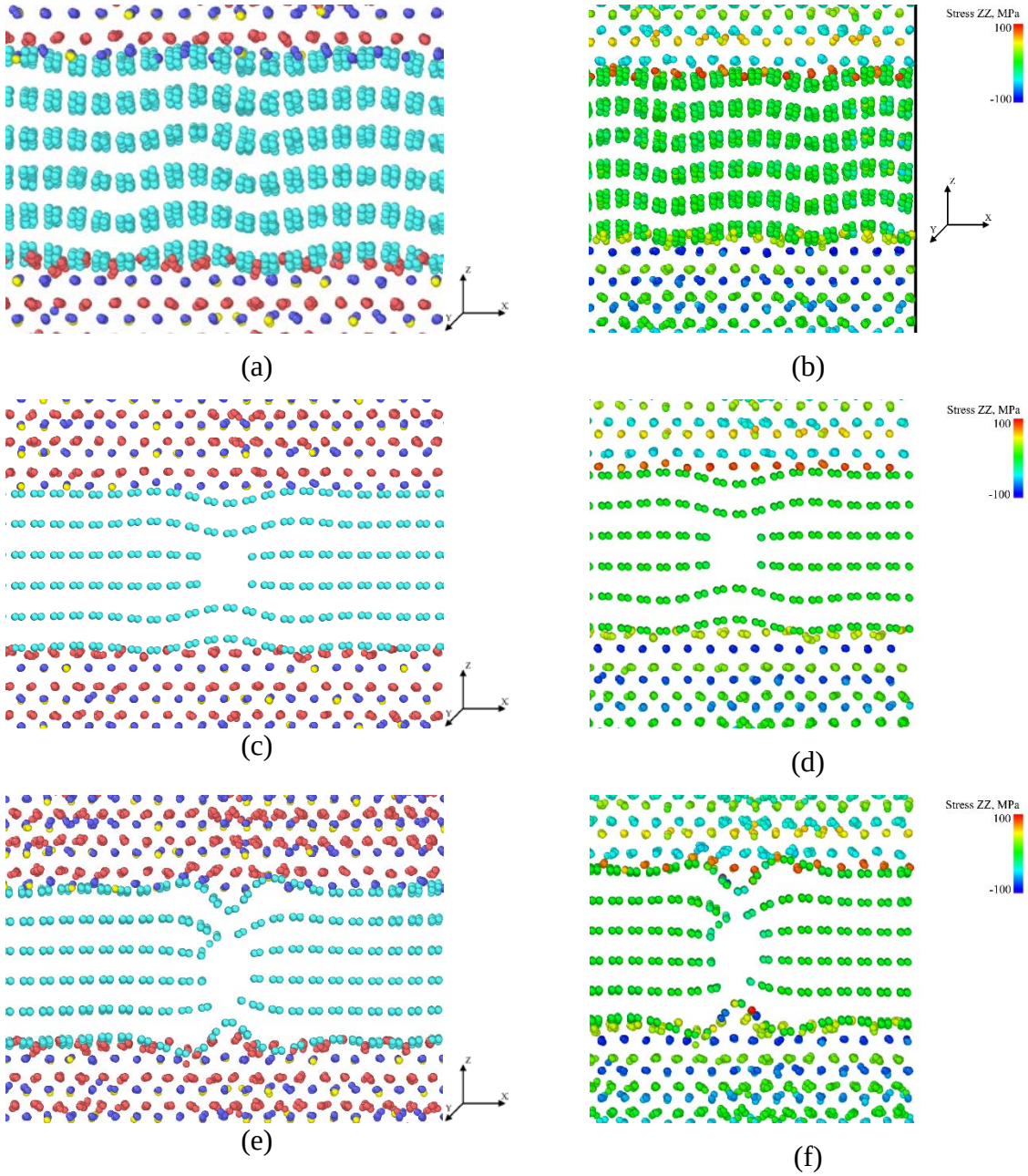

Fig. 5. Nanocomposite "YSZ-ceramics - graphene" deformed by 15% tension along the Z-axis. Atomic model and stress map of the composite (a) - (b) with a defect-free planar nanoinclusion, (c) - (d) with a pore of 3 Å in diameter in the inclusion, (e) - (f) with a pore of 5 Å in diameter the inclusion. The modeling used the B-ReaxFF-LJ combination of potentials. Color designation of atoms corresponds to the description in Fig. 1

5. Discussion

Model mechanical tests of the YSZ ceramics - graphene nanocomposite showed that the presence of a 5 Å pore in a 6-sheet graphene inclusion leads to significant deformations of this nanoinclusion as a whole. With further deformation by tension, the graphene starts cracking and delaminating from the ceramics. Unfortunately, the potentials for YSZ ceramics and their interaction with graphene are not sufficiently stable at high degrees of deformation (see Fig. 6). This indicates that, in order to analyze the destruction of this model sample, it is necessary to clarify the interatomic interaction potential. At the moment, there is not a single potential that could give adequate results for the interaction between YSZ ceramics and

graphene in the region of high deformations. At the same time, the potentials for these materials were tested separately and gave good results [15,16]. Simplifying the model and searching for similar potentials is not possible, therefore, a possible way to cope with this situation is to carry out calculations by the density functional method and to select parameters for a new potential of interatomic interaction. The PotFit [17] program, which is distributed free of charge, has similar functionality. However, calculating large systems using the density functional method takes a large amount of computer time, which should be taken into account in the possible development of new potential.

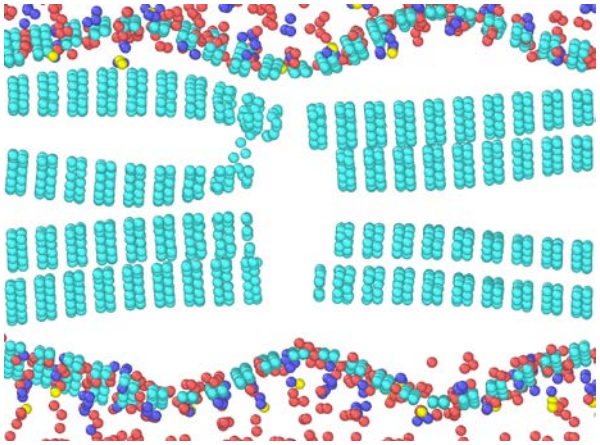

Fig. 6. Nanocomposite "YSZ ceramics - graphene" deformed by 25% tension along the Z-axis. The graphene interlayer has initially contained a pore of 5 Å in diameter. The modeling used the B-ReaxFF-LJ combination of potentials. Color designation of atoms corresponds to the description in Fig. 1

6. Conclusions

According to the constructed model and the chosen potentials of interatomic interaction, defect-free graphene manifests itself as an excellent reinforcing element of the composite. It deforms without the formation of defects at small and medium strain values. The artificial creation of small pores with a diameter of 3 Å in the intermediate layers also has little effect on the destruction of the graphene nanoinclusion. The creation of pores with a diameter of 5 Å and more can lead to cracking of the nanoinclusion and its delamination from the ceramics. To improve the accuracy of the model and to observe the destruction of the model sample under study, it is necessary to develop a refined interatomic interaction potential.

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