Molecular dynamics simulations of the adsorption processes on ZnO nanoclusters

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Introduction and Methods

We have analyzed in detail the processes of O2 gas adsorption on ZnO nanoclusters using the molecular dynamics method. Simulation of the adsorption processes of ZnO nanoparticles, was carried out by molecular dynamics method, that is based on numerical solution of Newtonian differential equations of motion for each atom of the system with initial values of speed and coordinates. By analyzing the nature of the formation of such nanostructures and referring to sources about the interatomic potentials, we have selected Reactive Force Field (ReaxFF). This interatomic potential has been developed for a wide range of chemical compounds, including ZnO, and already has been used by us in previous work [1, 2]. To study the main parameters, the gas pressure in the system, the size of ZnO nanoparticles, and the system temperature were changed. The dependences of the total energy of the system and the radial distribution functions (RDF) were used to describe the adsorption processes, and the CSP (centro-symmetry parameter) method was used to study the surface properties. For modeling and analysis of the adsorption of zinc oxide nanoparticle, we have been used Large-scale Atomic/Molecular Massively Parallel Simulator, which was developed by a scientific group from Sandia National Laboratories (USA). Calculations were performed on a computing cluster of the Institute of Applied Problems of Mechanics and Mathematics, which is based on four Intel Xeon multi-core processors under operating system Linux ROCKS.

Results

In order to investigate the mechanism of adsorption of oxygen molecules on the ZnO surface, the adsorption of one O2 molecule on the surface at T = 300 K was simulated.

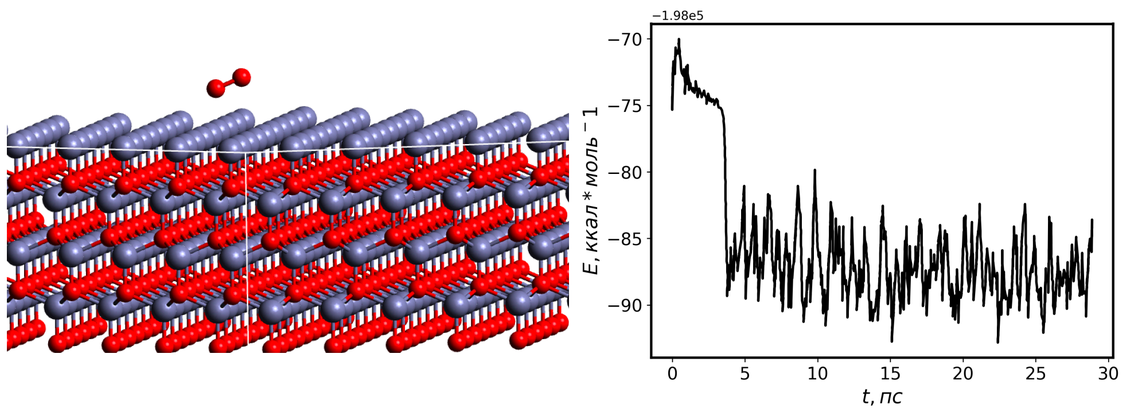

Figure 1. Snapshot of the ZnO system during the adsorption of one oxygen molecule at the initial moment of modeling (left) and change in the potential energy of the O2 molecule over time (right).

It was found that the adsorption process of one O2 molecule occurred within 4 ps from the beginning of the simulation. The adsorption process can be investigated by the change in potential energy over time. A sharp decrease of the energy of the molecule was detected near 4 ps which is responsible for the adsorption process.

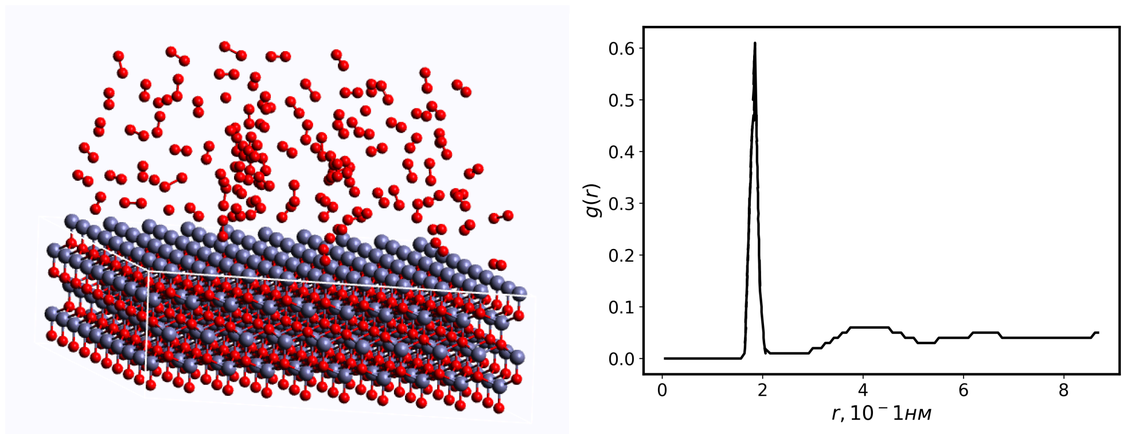

Figure 2. Snapshot of the ZnO system during the adsorption of 200 oxygen molecules at the initial moment of modeling (left) and Radial distribution function for O - Zn pairs at 300 K.

Also, we performed simulations for a higher concentration of O2 molecules in our chosen system, where the dependences of the final parameters of the system on the concentrations of O2 molecules were established. It was found that a higher concentration of O2 molecules in the system corresponds to a larger number of adsorbed particles, which subsequently diffuse into the near-surface layer, changing the crystal structure of the nanoparticle. The growth of the first peak of the radial distribution function with increasing concentration of O2 molecules in the system, which is responsible for the increase in the number of O - Zn pairs, was revealed.

Conclusion

Our research shows that the whole process of adsorption can be divided into two stages, the first stage is characterized by a rapid increase in the number of adsorbed molecules, the second - an increase in fluctuations in the change of adsorbed molecules on the surface over time. In this case, the higher the gas pressure in the system is, the greater the number of O2 molecules diffusing into the volume of the ZnO nanocluster, and the crystal structure of the surface of the ZnO nanocluster becomes amorphous with increasing concentration of gas molecules in the system.

References

[1] *S.S. Savka, D.I. Popovych, A.S. Serednytski,* Molecular Dynamics Simulations of the Formation Processes of Zinc Oxide Nanoclusters in Oxygen Environment, Nanophysics, Nanomaterials, Interface Studies, and Applications. NANO 2016. Springer Proceedings in Physics 195 (2016) 145-156.

[2] *S.S. Savka, Yu.I. Venhryn, A.S. Serednytski, D.I. Popovych,* Molecular Dynamics Simulations of the Formation Processes and Luminescence Properties of Zn-ZnO Core-Shell Nanostructures // Jouranl of Nano- and Electronic Physics 10 (2018) 03008(5).

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