# Study of the sorption capacity of a flake of crumpled graphene with different lengths and diameters

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Today, many works are devoted to the hydrogenation of crumpled graphene (CG), which has many unique properties [1]. An essential advantage of carbon structures for transporting various gases is a large specific surface and a high gas adsorption rate, which makes it possible to predict their use in hydrogen energy as a container for storing and transporting hydrogen [2]. In this regard, the purpose of this work is to study by molecular dynamics simulation the effect of the length and CG flake diameter on the sorption capacity at different temperatures (77 and 300 K) and external pressures (1 and 140 atm).

The computational simulation cell consists of one crumpled graphene flake placed in a hydrogen atmosphere. The flake diameter is $D_1$ = 9.5 nm and $D_2$ = 20 nm with length $l_1$ = 2.5 nm, $l_2$ = 5.0 nm and $l_3$ = 10 nm for each diameter. Molecular dynamics simulation is carried out using the publicly available and extensively software package LAMMPS. The interatomic interaction is described by the Airebo potential [3].

It is found that the gravimetric density of a crumpled graphene flake depends on its structural parameters, such as the diameter and flake length. The most optimal value of the sorption capacity is observed for a structure with a smaller diameter $D_1$ and length $l_1$ at a combination of a temperature of 77 K and a pressure of 140 atm.

REFERENCES

1. N.G. Apkadirova, K.K. Krylova, R.R. Mulyukov. Materials Physics and Mechanics. 47 (6), 817 (2021)
2. Krylova, K.; Baimova, J.; Mulyukov, R. Letters on Materials 85 (5), 1 (2019)
3. S. Stuart, A. Tutein, J. Harrison. Journal of Chemical Physics. 6472, 14 (2000).