Atomistic simulation of nitrogen defects in diamond with machine learning potential

Zelenina A.I.[1,2,@], **Orekhov N.D.**[1] **and Kudryashov S.I.**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereu -lok 9, Dolgoprudny, 141701, Russia

[2] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow, 119991, None

[@] zelenina.ai@phystech.edu

Defects of diamond crystal lattice have a significant impact on its physical properties. It is possible to use natural and synthetic diamonds in quantum technologies, employ defects as nanomarkers in industrial tracing and study laser generation of defects [1]. There is a lot of data on the dynamics of nitrogen atoms and the dynamics of vacancies separately, but their cooperative behavior and the transformation of one center into another has not been sufficiently figured out [2]. In this work dynamics of the "nitrogen-vacancy" point defects type was studied by the molecular dynamics method in the LAMMPS package [3] in the temperature range 3000- 3500 K. It is shown that the NV and NV_2 centers are localized, while the NV_3 center actively diffuses. A comparison of the evolution of NV_3 center and H3 center surrounded by 2 vacancies is proposed. Calculations of energy characteristics were carried out, a qualitative comparison with the available literature data and the results of first-principles approach was made. The work was carried out using a machine-learning potential of the MTP type [4].

[1] Ashfold M N, Goss J P, Green B L, May P W, Newton M E and Peaker C V 2020 *Chemical reviews* **120** 5745–5794

[2] Kudryashov S I, Danilov P A, Vins V G, Kuzmin E V, Muratov A V, Smirnov N A, Pomazkin D A, Paholchuk P P, Vasil'ev E A, Kirichenko A N *et al.* 2024 *Carbon* **217** 118606

[3] Plimpton S 1995 *Journal of computational physics* **117** 1–19

[4] Novikov I S, Gubaev K, Podryabinkin E V and Shapeev A V 2020 *Machine Learning: Science and Technology* **2** 025002