Molecular dynamics study of the effect of the substrate temperature on the self-assembly of a copper nanofilm in a gas discharge

Fairushin I I[1,2,3,@] **and Shemakhin A Yu**[1]

[1] Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan 420008, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Kazan National Research Technical University named after A N Tupolev—KAI, Karl Marx Street 10, Kazan, Tatarstan 420111, Russia

[@] fairushin_ilnaz@mail.ru

Copper-based nanostructures can serve as an alternative to noble metals for their use as catalysts in a number of chemical processes [1]. One of the methods for obtaining metal nanostructures is the impact on a massive sample of high-energy ions of a gas-discharge plasma with subsequent sputtering and deposition of individual atoms and (or) metal clusters on the substrate [2, 3]. This method can be improved with the help of computer simulation, which makes it possible to identify the optimal parameters without field experiments.

In this work, using the molecular dynamics method, we simulate the sputtering of a copper target and the subsequent formation of a copper nanofilm on a silicon substrate. The process parameters corresponded to the conditions in a low-pressure gas-discharge plasma. The obtained values of the sputtering coefficient correspond to the experimental data. The studies were carried out for various values of the substrate surface temperature.

[1] Sun Y, Yu J and Ma Q 2018 *Science Advances* **4** eaau3275
[2] Fairushin I I, Saifutdinov A I and Sofronitskiy A O 2020 *High Energy Chemistry* **54** 150–153
[3] Brault P 2018 *Frontiers in Physics* **6** 59