C4-O-040502

ACCELERATED MOLECULAR SIMULATIONS OF THE LINEAR-CHAINED CARBON SYNTHESIS ON SILICON SUBSTRATE*

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Linear chain carbon (LCC) is a one-dimensional allotrope of carbon, which has a number of unique optical and electronic properties that make it a promising material for electronic applications. The LCC was first synthesized several decades ago [1] and has already found several applications due to its unique properties. However, the synthesis of linear-chain carbon is still a complex technological challenge. The cause of this problem is the extreme instability and reactivity of carbon chains.

The aim of this work is to study the synthesis of carbon chains on the surface of silicon using molecular dynamics. During the work, a simulation of the deposition of various carbon molecules and clusters (C_2, C_2H, C_2H_2, CH, C_4H_2, C_6H_2) on the silicon surface was performed (Fig. 1, left). Simulation was implemented using three methods of hybrid molecular dynamics [2]: subtractive, force-based and electrostatic. All methods show similar results when modeling a short molecule while for long molecules (C_4H_2 and C_6H_2), only advanced QM/MM methods predict mechanisms of destruction (Fig 1, right).

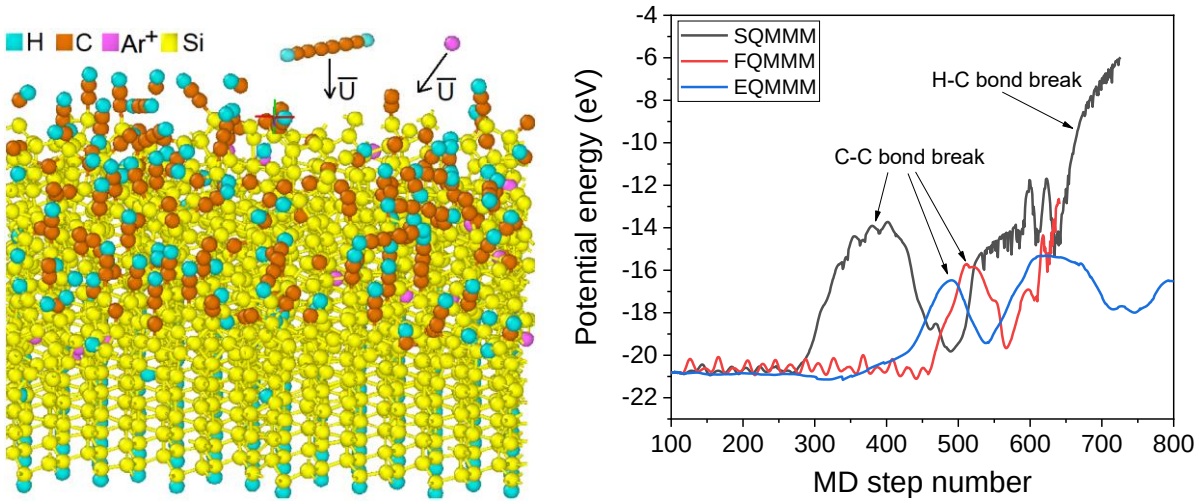

Fig.1. Structural model of the LCC plasma synthesis process (left) and energy profiles for different hybrid MD simulations (right).

The system under study has many metastable states difficult to achieve by conventional MD. In practical terms, metastability means that a system, when modeled by molecular dynamics, is likely to be in only one probability maximum for a long time. A possible way to solve this problem is to fill the free energy minima of metastable states in a controlled way, which allows the system to explore all states [3]. One of the methods for implementing this solution is metadynamics. In [4], the effect of bombardment by argon ions with different energies, bombardment angles, and flux densities on film growth was studied using the classical molecular dynamics method in the LAMMPS program to obtain linear chain carbon. However, the simulation time was not enough for significant film growth. In this work, further modeling was carried out to test the optimal conditions for the synthesis of chain structures. In order to accelerate their growth and increase the time scale of modeling, a complex of methods, including metadynamics, was used.

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* This work was supported by the Ministry of Science and Higher Education of Russian Federation (Project FEUZ-2020-0059).