STUDY OF THE INTERACTION BETWEEN A LOW-ENERGY FLOW OF IONS AND ultrahigh molecular weight polyethylene [[1]](#footnote-1)\*)

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Ultra-high molecular weight polyethylene (UHMWPE) is widely used as a filler for high-strength composite materials. Low pressure (13.3-133 Pa) capacitive coupled radio-frequency plasma is used for modifying UHMWPE for increasing the adhesion between the filler and the matrix [1-2]. The main factor of plasma action is the low-energy (50-100 eV) ion bombardment by an ion current of 0.5-1.0 A/m2 [3]. A molecular dynamic model of interaction between a low-intensity stream of low-energy ions and the of polymer surface is developed for a more detailed study of the process.

A unit cell of 9×11×17.6 nm3 is considered in view of the pronounced anisotropy of the UHMWPE crystallite. Full atom model is used. The interaction of ions with polyethylene in this model is described by a system of equations of classical mechanical motion of particles.

The Lennard-Jones pair potential as well as the many-body potentials both ReaxxFF and AIREBO-M is used as the force field for polyethylene atoms. The Coulomb interaction of an incident particle with PE atoms was not considered because the ions are recombined before impact. The Verlet algorithm is used for solving the system of motion equations. Calculations were performed with a time step δt = 0.1 fs by the LAMMPS package. Visualization of the results was carried out in the VMD package.

The most realistic results were obtained by the AIREBO-M potential. The depth of penetration of the fast Ar atom into the PE crystallite is 0.85 nm at an ion energy W= 10 eV, it is 1.81 nm at W=50 eV, and it is 2.81 nm at W = 100 eV. No significant structural changes occur at the energy of the bombarding atom W = 10 eV., a rarefaction is formed in the center of the target at W = 50 as well as at 100 eV, polyethylene molecules is broke in the vicinity of the track, and short alkene radicals is formed. The temperature of atoms in this region rises significantly, which qualitatively coincides with the thermo-elastic peak theory.

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References

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1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLVII/Cm/ru/KG-Zheltukhin.docx) [↑](#footnote-ref-1)