Mathematical modeling of RF-plasma modification of ultra-high molecular weight polyethylene [[1]](#footnote-1)\*)

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A molecular dynamics model of UHMWPE surface modification by an Ar ion flux generated by an RF capacitive discharge in a dynamic vacuum is considered. Dynamic vacuum is understood as an average vacuum with continuous gas blowing in the pressure range p=13.3−133 Pa and gas flow rate G=0.01−0.25 g/s.

The characteristics of the RF discharge plasma in dynamic vacuum differ from the properties of the discharge without gas blowing: the degree of ionization is 10-5–10-4, the electron density ne=1015–1018 1/m3, the electron temperature Te=1–4 eV, the temperature of atoms and ions 0.03–0.06 eV. A sample placed in a plasma flow of an RF discharge in a dynamic vacuum is exposed to a flow of ions with an energy of 70–100 eV and an ion current density of 0.1–3 A/m2 [1].

The model of interaction of ions with a polymer material is described by a system of equations of classical molecular mechanics

 $\frac{dv\_{k}}{dt}=\frac{1}{m\_{k}}\sum\_{k\ne l}^{}F\_{kl}, \frac{dr\_{k}}{dt}=v\_{k}, F\_{kl}=-grad U\_{kl},$ (1)

 $v\_{k}\left(0\right)=0, r\_{k}\left(0\right)=r\_{k0}, k,l=1,…,N.$ (2)

Here $v\_{k}$ is the velocity vector of the *k*th particle, $r\_{k}$ is radius vector, $r\_{k0}$ are the coordinates of the initial position of the particles, $F\_{kl}$ is the force acting on the *k*th particle from the side of the *l*th particle, $m\_{k}$ is the mass of the *k*th particle, *t* is time, $U\_{kl}$ is the interaction potential of particles with indices *k* and *l*, *N* is the number of atoms in the model.

The model was implemented using the LAMMPS universal software package for molecular dynamics simulation. Ion bombardment of a UHMWPE crystallite 9x7.6x75 Å in size with ion energies of 10, 50, and 100 eV was simulated. The force field was modeled using the AIREBO-M potential.

As a result of modeling, it was found that at an ion energy of up to 10 eV, there are no significant changes in the structure of polyethylene. At energies of 50 eV and 100 eV, argon atoms penetrate the material to a depth of 1.8 and 2.8 nm, respectively. Along the trajectory of the atom, molecular chains break, resulting in the formation of short alkene radicals. Separate carbon and hydrogen atoms, as well as short hydrocarbon molecules, are emitted from the polyethylene surface.

The experimental results showed that active alkene radicals react with atmospheric oxygen when the treated samples are removed from the vacuum chamber after RF plasma treatment and functional carbonyl groups (–С=О) appear on the surface of UHMWPE, as a result of which the surface of UHMWPE acquires hydrophilic properties [2].

References

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2. Kudinov V. V. et al. // Inorganic Materials: Applied Research. – 2012. – Т. 3. – №. 3. – С. 257-260.
1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/L/Pt/ru/HF-Zheltukhin.docx) [↑](#footnote-ref-1)