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RF PLASMA MODIFICATION OF FILLERS FOR POLYMER COMPOSITES *)

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Treatment of carbon, aramid and glass fibers, as well as fibers based on ultra-high molecular weight polyethylene (UHMWPE), used as fillers of polymer composite materials, by a flow of low-energy (up to 100 eV) ions in a low-pressure RF discharge (13.3-133 Pa) [1], significantly improves their strength and adhesion characteristics, as well as composites based on them.

The surface of the material is modified due to the effect of a flow of low-energy (30-100 eV) ions with an ion current density of 0.3-1.5 A/m^2. The results of the experiments showed that active groups on the fiber surface arise either directly in the plasma during treatment in air, or after removing the samples from the vacuum chamber – when ones are treated in an argon environment [2].

For a detailed study of the mechanism of modification of the polyethylene surface in low-pressure RF plasma, a mathematical model based on the molecular dynamic's method was created. The model of ion interaction with a polymer is described by a classical molecular mechanics equations

$$\frac{d\mathbf{v}_k}{dt} = \frac{1}{m_k}\sum_{k\neq l}\mathbf{F}_{kl}\,,\ \frac{d\mathbf{r}_k}{dt} = \mathbf{v}_k,\ \mathbf{F}_{kl} = -\mathrm{grad}\,U_{kl}, \quad (1)$$

$$\mathbf{v}_k(0) = 0,\ \mathbf{r}_k(0) = \mathbf{r}_{k0},\ k,l = 1,\dots,N. \quad (2)$$

Here $\mathbf{v}_k$ is the velocity of the *k*-th particle, $\mathbf{r}_k$ is radius vector, $\mathbf{r}_{k0}$ are the coordinates of the initial position of the particles, $\mathbf{F}_{kl}$ is the force acting on the *k*-th particle from 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 is implemented using the universal software package for molecular dynamics modeling LAMMPS. The ion bombardment of a UHMWPE crystallite measuring 9x7.6x75 Å with ion energies of 10, 50, and 100 eV was simulated. The force field was modeled using the Lennard-Jones 6-12, AIREBO-M and REAXFF potentials.

The simulation is showed that no significant changes occur in the polyethylene structure at ion energy of up to 10 eV. Argon atoms penetrate into the material to a depth of 1.8 and 2.8 nm at energies of 50 eV and 100 eV, respectively. Molecular chains are broken along the trajectory of the atom, resulting in the formation of short alkene radicals. Individual carbon and hydrogen atoms, as well as short hydrocarbon molecules, are emitted from the polyethylene surface.

References

[1]. Abdullin I.S., Zheltukhin V.S., and Kashapov N.F., Radio-frequency plasma jet treating of materials at low pressures: Theory and practice of application, 2000.
[2]. Abdullin I.S. et al. (2023) *High Energy Chemistry* **57,** Suppl 1. P. 132-136.

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