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MODELING THE SURFACE INTERACTION OF CELLULOSIC MATERIALS WITH CO_2 PLASMAS

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Abstract. Within this research, the modeling of the interaction of plasma ions with the surfaces of cellulose samples, i.e. with the molecules of repeating cellulose structures, is presented. Low pressure RF plasma in a working CO_2 gas atmosphere was modeled using the "Particle in cell" method. The mentioned method represents a modified computer code of the group from Berkeley, University of California see Verboncoeur et al.1993 in terms of the database of CO_2 effective cross sections which is presented in detail in the earlier work of our group see Stankovic et al.2020. The calculations were performed within the cylindrical spatial geometry of the CCP reactor (plasma sheath), which is characterized by a significant drop in the cathode potential that favors the acceleration of plasma ions towards the electrode. The main data obtained by the simulation were the volume of the cylindrical area (cathode potential gradient of the plasma sheath) as well as the concentration of electrons in a unit volume of the plasma sheath. In the next stage the total and partial ionization rate coefficients were obtained by the Monte Carlo method and averaged over the half-period of the reduced RF electric field oscillation see Stankovic et al.2020. This enabled us to calculate the number of ions that act on the cellulose sample surface per unit of time by using the probability for the ionization collision process. In final stage the physical breaking of certain chemical bonds in repeating cellulosic structures of the sample (paper) is modeled by semiquantum simulation of the interaction where the major role has impact electric field influence of the accelerated ions ensemble on cellulose chains. The breaking of chemical bonds is modeled as a consequence of extreme deformation of their electron clouds induced by interaction with fast accelerated ions. In order to verify the modeling of the plasma-sample interaction, paper samples were also experimentally treated in a RF CCP reactor in the power range from 20 to 100 W and then subject the treated surfaces to the FTIR test method. Comparative analysis showed good agreement between experimental and simulation data of modeled plasma-surface interaction.

References

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