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SEMIQUANTUM SIMULATION OF CELLULOSIC MATERIALS INTERACTION WITH CO_2 PLASMAS

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Abstract. The interaction of the generated ions in the gas discharge, which was modeled by using the "Particle in the cell" method see Verboncoeur et al.1993, with the surfaces of cellulose material samples (paper) exposed to CO_2 plasma treatment, i.e. the effect of fast ions near the cathode area, was quantitatively determined using a new computer code. The simulation of mentioned semiquantum plasma-ion interaction have been developed in our group and involves the breaking of interatomic chemical bonds of certain molecules, the building blocks of cellulose chains, under the influence of the electric field created by the ensemble of electrons. Since there are currently no known probabilities for the collisional interaction of an ensemble of ions and molecules of cellulose structures, the way to overcome this kind of challenge is to simulate the deformation of the electronic states of cellulose molecules by the influence of the electric field of the simulated ion created in the near-cathode CO_2 plasma region. Taking into account the ionization rate coefficients see Stankovic et al.2020, the volume of the cylinder membrane that corresponds to a certain part of the cathode potential drop, and then the concentration of electrons that occur in the modeled plasma, the number of ions that act per unit of time and per unit of the cellulose sample's surface is obtained. This data, in addition to the effective electric field strength, represents the input data of this semiquantum simulation. The obtained results show that with the increase in the intensity of the RF power supply, the percentage of breaking chemical bonds, i.e. the deformation of the molecule's electronic states of the cellulose sample's structures, also increases. Apart from the mentioned conditions, the percentage of bond breaking in polymer chains also depends on the percentage of certain molecule's presence in cellulose structures.

References

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