Modeling of Radiation-induced Excitation and Damage of Macromolecules and Clusters

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Abstract: When molecules are irradiated with energetic particles, a complex sequence of reactions takes place. Excitation and decay of molecules are consequences of them. All these reactions are connected. Foremost irradiation produces excitation of molecular at the shortest time and length scales, which evolve over longer scales to produce changes in microstructure and properties through hierarchical and inherently multiscale processes. All of them can be divided into three groups of radiation-induced processes with substantially different characteristic periods. Therefore we can consider they are relatively independent. In the first place there are the processes of excitation of the molecule and especially its electron subsystem. The process of creating the excitation is stochastic. Place of generation and value of excitation are random. Secondly it is processes of excitation evolution, development and migration. As a rule, the radiation-induced excitations and their kinetics are nonlinear as result of localization of excitation and high concentration of energy. A computer modeling allows studying the long-living local states. Interest presents the collective and synergetic behavior of clusters of molecules and types of states like breathers. At last there is the decay of the molecules. It depends on magnitude of excitation, patterns of its migration and the spatial structure of the molecule because the decay of the molecule is determined mainly by its "weak points". Due to the migration of excitation decay of macromolecule can take place far away from place of excitation generation. When macromolecule has complex structure, it has a large number of possible ways of migration. Excitations can be joined and divided. In this case computer simulation is necessary because to obtain analytical expressions is not possible. Thus, to determine the probability of macromolecule collapse is necessary to consider its structure, "weak points", redistribution and extinction of excitation.

A model of the evolution and migration of radiation-induced excitation is built. Algorithm for calculating the probability of macromolecule damage is obtained. Damage of macromolecules such as fullerene is investigated by means of computer simulation. It is shown that if the structure of the macromolecule becomes more complex, the lifetime of the excited molecule and dispersion increase. It is analyzed the influence of local collective excitations.

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