The main reactions initiated in polymers by irradiation are polymerizing, grafting, chain scissioning, and cross-linking. From the applications’ point of view, cross-linking is the most important of these effects. This is because it can improve the mechanical and thermal properties of the polymer, thus increasing the overall chemical, environmental, and radiation stabilities of the material.

The processing of polymeric materials by radiation has been examined and utilized by the industry since 1960s. However, some fundamental questions are still open. These questions are related to, e.g., how radicals are created near each other to induce cross-linking, and how the morphology of the material influences the cross-linking reactions.

Using molecular dynamics simulations, we have studied the irradiation effects in polyethylene and cellulose. We found that the governing reactions in both materials were chain scissioning and generation of small hydrocarbon and peroxy radicals. Recombination of chain fragments and cross-linking occurred less frequently. Crystalline cellulose was found to be more resistant to radiation damage than crystalline polyethylene.

In this work, we present our results on the statistics on radical formation, and we discuss the dynamics of the formation of radiation damage.

A cross-link between two cellulose chains, formed as a result of a 100-eV C recoil. The picture is taken from our latest publication [1].