Monte-Carlo Simulations of Radiation Damge Produced in Protein Crystals

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The data quality and the achievable resolution in X-ray structure analysis of protein crystals is limited by radiation damage. The aim of this investigation is a better quantitative understanding of the damage produced by the absorption of photons and the subsequent processes in protein crystals by Monte-Carlo approach.

The dominating inelastic interaction for X-ray photons with an atom in a protein crystal is the photo-effect, in which high energy photo-electrons and low energy Auger-electrons are created. At higher X-ray energies Compton scattering becomes dominant. In this case most of the energy is kept by the scattered photon, which interacts for normal protein crystal sizes usually once. The produced electrons have a high inelastic cross-section, so the resulting electron cascade has a high damage-potential.

By means of the simulation the electron cascade and the spatial distribution of ions and excited atoms produced by inelastic interactions are analyzed in order to obtain more quantitative information on the damage. Also, the average time for a cascade is evaluated. One of the aims of these investigations is to find the optimum data collection energy for a given chemical composition.

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