

Hydrodynamic Model of X-Ray Irradiated Biological Molecules

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X-ray free electron laser (XFEL) synchrotron radiation sources can produce extremely short and intense X-ray pulses that potentially allow the three-dimensional structure determination through single-molecule diffraction imaging. One of the critical issues is the deterioration of a molecule induced by X-ray irradiation.

Recently, molecular-dynamics calculations of the damage dynamics of biological molecules have been presented by Neutze et al. (*Nature* **406**, 752 (2000)). In contrast, we have developed a simpler hydrodynamic model, but added several physical effects that strongly affect the dynamics. Most important is the effect of trapped electrons that have been stripped from the atoms but that are trapped by the electrostatic field of the molecule.

In this paper, we will present a simple dynamics model that includes an approximate description of the dominant physical effects. We used this model to survey a wide range of parameters to obtain the image resolution as a function of molecule size, particle composition, and beam parameters. Classification of individual diffraction images according to the molecule orientation constrains the beam parameters further (G. Huld et al., to be submitted). We determined the optimum resolution as a function of beam and molecule parameters considering both radiation damage and image classification.

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