

## **Abstract**

The advanced method of reconstructing the structure of Glycine in its crystalline phase is examined by X-ray diffraction. New generation X-ray sources, the X-ray free-electron lasers (XFEL), provide better opportunities for small molecular structure determination. The extreme intensity and ultrashort hard x-rays pulse duration of an XFEL pulse make it feasible to extend the diffraction technique towards nano sized crystals. . However, during a high-intensity measurement, significant atomic and electronic dynamics occur that affect the diffraction signal. Simulations of the ionization dynamics of an irradiated nanocrystal and the diffraction pattern formed are computationally examined and their pattern elucidated by spectroscopic data.