

Imaging of Atom Clusters by hard X-ray free Electron Laser Pulses

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We study the possibility of imaging a small cluster of atoms by short x-ray free electron laser pulses. A special molecular dynamics model has been developed to describe the Coulomb explosion of the clusters [1]. We use numerical modeling based on the non-relativistic classical equation of motion. Quantum processes are taken into account by the respective cross sections. The explosion dynamics is examined for various conditions: pulse length, constituent atomic number, number of photons in a pulse. We use our model to get an estimate of the time available for imaging before the cluster deteriorates significantly. Based on these results we calculate the continuous elastic scattering pattern of the sample and try to reconstruct the original atomic order from this pattern. We use a density modification type algorithm analogous to the Fienup hybrid input output reconstruction method [2,3]. Since this method needs a 3D dataset in the reciprocal space, scattering patterns have to be taken at various sample orientations. That requirement leads to a multi shot experiment. Therefore the full dataset have to be built from scattering patterns of several independent exploding clusters. We included this complication in the calculations. We found that the shorter the pulse the higher the ratio of the photons useable for imaging. The conclusion of the calculations is that the pulse length of the presently planned x-ray free electron lasers is too long.

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