

Abstract

X-Ray free electron lasers are the next generation synchrotron radiation that uses relativistic electrons as gain medium to produce high energy, coherent (spatial and time) and pulses of extreme short duration. Interaction of an XFEL with matter is a highly non-equilibrium process. One way to visualize structural dynamics is to use monte-carlo based XMDYN and XATOM approaches. XATOM using quantum mechanics in its core deals with all the process of each individual atom present in the matter. XMDYN using classical Newton's equation of motion gives displacement of whole matter in real space. There has been proofs of 'local damage' prevalence in laser-matter interactions. The aforementioned approaches were used to determine the 'local damage' in nano-crystals of Thaumatin. The results were able to predict average charge, atomic displacements, thermalization of electronic distribution and evolution of atoms in 3-dimensions.