

ABSTRACT

X-ray free electron lasers can produce intense X-ray pulses which can initiate various photo induced process in a nanocrystals exposed to these radiation. These processes induces structural dynamics and causes damage in crystalline structure. In this thesis we discuss local damage induced in Thaumatin nanocrystal using simulation tools XMDYN and XATOM. We discuss evolution of charge and distance between two Sulphur atoms in S-S dimer and effect of environment on dynamics of Sulphur atoms. We compare our results with an experiment performed on Thaumatin nanocrystal at LCLS.