Simulations of shock waves induced by X-ray free-electron lasers and potential effects on biological samples

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X-ray free-electron lasers produce x-ray pulses with very high brilliance and short pulse duration down to a few femtoseconds. These properties allow to investigate the structure of biomolecules using nanocrystals or single particles and to observe conformational changes on the femtosecond timescale. Samples are injected into the laser beam using a liquid jet and high laser pulse repetition rates of a few Mhz are used. Due to the high brilliance of the X-ray beam atoms of the sample and the liquid jet are ionized and a hot electron gas with temperatures of about 50.000 K to 100.000 K is formed [1]. As experiments have shown, shock waves are created, which propagate through the jet and slow down to the speed of sound in water [2]. There are few investigations on effects of the shock waves on biological samples [3, 4], thus further modelling and experimental work has to be done. We use molecular dynamics simulations to model shock waves induced by heated water. The simulations are carried out with GROMACS. Thereby we will get a deeper insight in the dynamics of the experiments and we will be able to see potential effects on biological samples. In particular the effect on protein complexes, such as membrane proteins, will be studied.

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