Feasibility Studies of Single Molecule Scattering Analysis with X-ray Free Electron Lasers

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The feasibility of single molecule elastic scattering analysis with the X-ray free electron laser (XFEL) sources in operation and under construction around the world was investigated for various biological and synthetic materials (pepsin, polyethylene, poly(4,4'-oxydiphenylene pyromellitimide), and ferric oxide). This study found that existing XFEL facilities provide coherent pulse X-ray beams with the required energies (8.3–12.4 keV) but their fluxes are too low for single molecule elastic scattering experiments to determine the three-dimensional structures of such molecules; for single molecule scattering, the XFEL facilities need to improve their beam flux density to 2×10^{15} to 7×10^{18} photons $\text{pulse}^{-1}\mu\text{m}^{-2}$ depending on the beam energy. However, the existing XFEL facilities' sources were found to enable the elastic scattering analysis of pepsin and the synthetic polymers in sample sizes of 1–160 μm as well as of ferric oxide in sample sizes ≥80 nm. These criteria for the sample size can be extended to other soft (biological, organic, and polymer molecules) and hard (molecules containing heavy metals) materials. In addition, the inelastic scattering, absorption, and radiation damage characteristics of the chosen materials when exposed to the XFEL sources were examined.