Coherent Diffraction Imaging of Atomic Clusters in Helium Droplets

In the context of atomic resolution, coherent diffractive imaging of non-periodic samples as suggested by Neutze et al. [1] we have simulated the explosion dynamics of rare-gas clusters embedded in a Helium droplet and exposed to an intense XFEL (X-Ray Free Electron Laser) pulse as will be available from the European XFEL at DESY in Hamburg in the future. We find that the Coulomb explosion of the sample, which is the main limiting factor for this imaging technique, is significantly delayed in comparison to the case without Helium. Using quantum-mechanical transition rates for K-shell photo-ionization and Auger-decay, which are the main damage processes, combined with a molecular dynamics simulation of free electrons and ions [2] we calculate the laser induced dynamics of Ne_N clusters, with N=50-5000, and assess the decline of image quality with longer pulse lengths. We find that, embedded in a Helium droplet, the positive charge that builds up in the cluster through photo-ionization and Auger-decay is efficiently transferred to the Helium shell by ionization of the Helium atoms in the Coulomb field of the charged cluster. The Helium shell then explodes while the cluster ions are efficiently screened from each other by the quasi-free electrons originating from the Helium droplet, thus enhancing the stability of the cluster and improving the overall image quality in an imaging experiment.

[1] R. Neutze et al., Nature **406**, 752 (2000)

[2] U. Saalmann and J.-M. Rost, PRL **89**, 143401 (2002)