The Dynamics of Silica Nanoparticles Irradiated by a Femtosecond IR Laser

Dynamics of Reversible and Irreversible Nanoplasma Processes in Spherical and Fibrous Nanoparticles.

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In Short

- The description of particle edge softening, as a result of a IR-laser pulse, in framework of a suggested new theoretical model (AG Fennel, University Rostock), to be tested by the molecular dynamics procedure (MD) for the largest possible size of spherical nanoparticles with a smooth surface.
- The applicability of two alternative spatial surface plasma distribution procedures (a) generated by Mie theory for spherical particles and (b) random plasma distribution for fibrous nanoparticles as a function of IR-laser polarization should be verified.
- For spherical particles the effect of changes in the surface plasma distribution as well as of parameters describing its radial decay, given by the Fermi function, on the melting procedure will be analyzed
- In case of fibrous nanoparticles the role of fiber density, their shape, and internal structure on particle melting will be elucidated.

This project aims to model results gained from pump-probe experiments on free silica nanoparticles prepared in an aerodynamically focused beam. The pumping exciting pulsed infrared radiation at 800 nm (1 mJ/pulse, 188 kHz, 20 fs duration) is synchronized to the probing pulsed soft X-rays of 1 keV photon energy, 25 fs pulse duration, and an energy of 7 mJ per pulse, from the European XFEL Facility at the SQS instrument in the NQS chamber. The diffraction pattern of thermalized intial sphere (D=60 nm), see figure 1(a), and its real image(c), are modelled by molecular dynamics (MD) program code IMD, and compared with the experimental diffraction image of spherical nanoparticle (D=290 nm), figure 1(b). The non-uniform thin electron plasma layer, generated on the surface of particle as a result of IR laser pulse, is causing particle pole melting and elliptical deformation in the direction of laser polarization, being modelled by MD as well, figure 1(d-f). In contrast, for fibrous nanoparticles with round initial geometry given in figure 2(a-c) the final elliptical deformation occurs in the direction perpendicular to IR laser polarization, figure 2(d-f). This effect is planned to be studied as a function of S-membrane fiber density [1], the surface/volume ratio and laser power. The time dynamics of particle edge profile for polar and equatorial planes will be studied with MD as well [2]. The time recovery of the spherical particle shape after laser pulse should be analysed on the basis of fractal exponent theory [3]. Finally, the results for smooth amorphous nanospheres generated from the melt of crystalline seed will be compared with amorphous nanoparticles generated directly by using the random number generator.

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More Information

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[2] C. Peltz, C. Varin, T. Brabec, and T. Fennel, *PRL*, **113**, 133401 (2014). doi: 10.1103/PhysRevLett.113.133401

[3] C. Raschpichler, C. Goroncy, B. Langer, E. Antonsson, B. Wassermann, C. Graf, P. Klack, T. Lischke, and E. Rühl , *J. Phys. Chem. C*, **124**, 16663–16674 (2020). doi: 10.1021/acs.jpcc.0c04308

Project Partners

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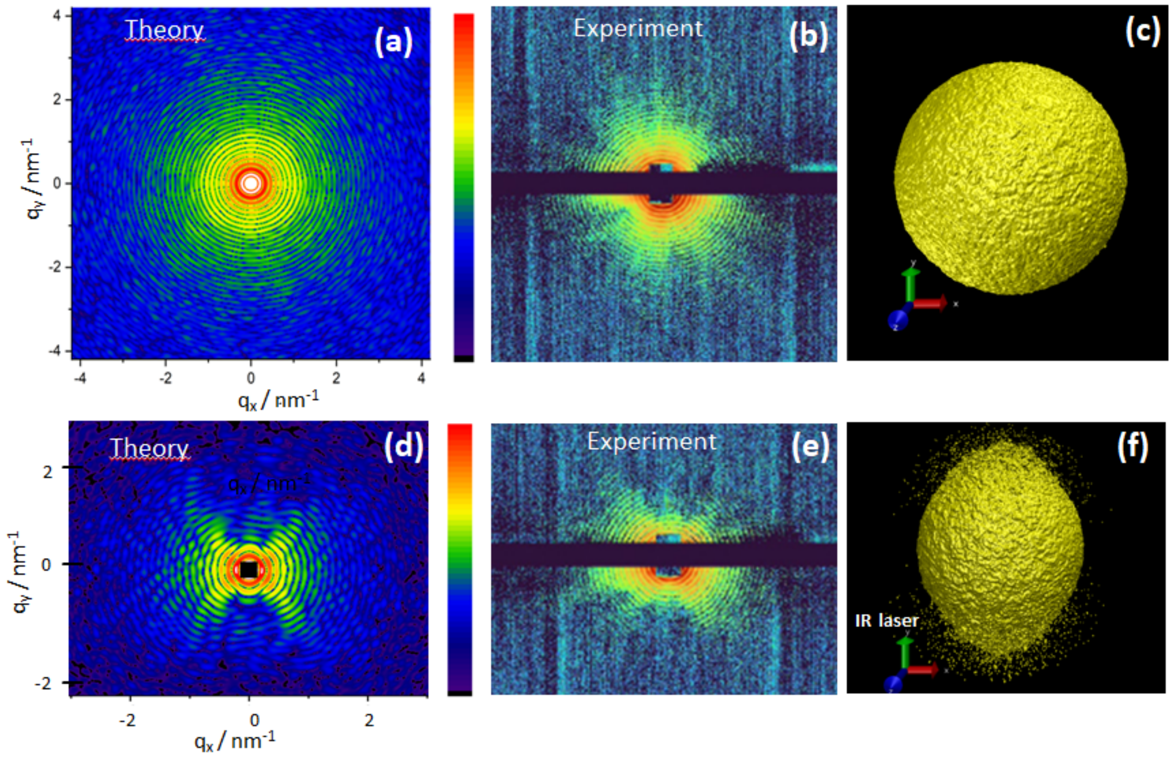

Figure 1: *Solid nanosphere (a) initial diffraction image, theory (D=60nm) (b) experimental diffraction pattern (D=290nm) (c) real image from MD calculation (d) diffraction image at t=12 ps, theory (e) corresponding diffraction pattern, experiment (f) final real image from MD*

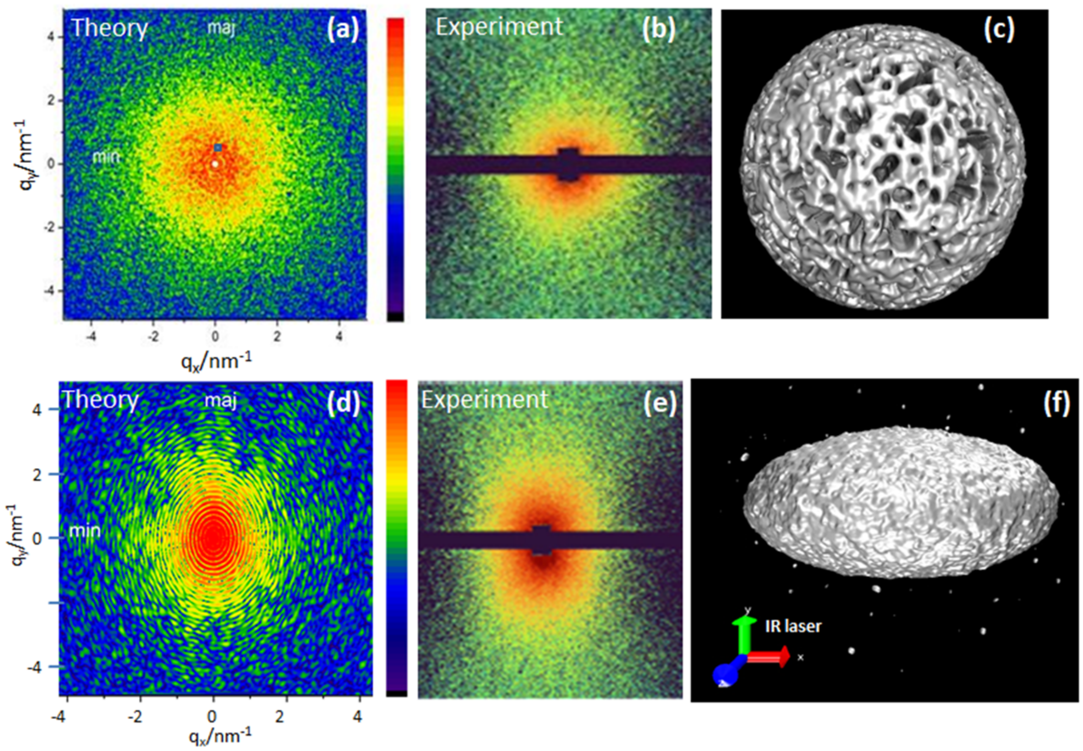

Figure 2: *Fibrous nanoparticle (a) initial diffraction image, theory (D=60nm) (b) experimantal diffraction pattern (D=650nm) (c) real image from MD calculation (d) diffraction image at t=12 ps, theory (e) corresponding diffraction pattern, experiment (f) final real image from MD*