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Optimizing aerodynamic lenses for single-particle imaging

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Abstract

A numerical simulation infrastructure capable of calculating the flow of gas and the trajectories of particles through an aerodynamic lens injector is presented. The simulations increase the fundamental understanding and predict optimized injection geometries and parameters. Our simulation results were compared to previous reports and also validated against experimental data for 500 nm polystyrene spheres from an aerosol-beam-characterization setup. The simulations yielded a detailed understanding of the radial phase-space distribution and highlighted weaknesses of current aerosol injectors for single-particle diffractive imaging. With the aid of these simulations we developed new experimental implementations to overcome current limitations.

Keywords: aerodynamic lens, aerosol, coherent diffractive imaging, simulation, single-particle imaging

1. Introduction

Single-particle diffractive imaging (SPI) is one of the key applications enabled by the advent of x-ray free-electron lasers (XFELs) [1, 2]. Short-duration XFEL pulses were predicted to allow the collection of diffraction patterns from radiation-sensitive samples without resolution limitations due to radiation damage [3, 4], although some open questions remain [4–6]. A series of two-dimensional diffraction patterns of randomly oriented isolated particles can be used to reconstruct the full three-dimensional structure, without the need for large highly ordered crystalline samples [2, 7, 8].

As every intercepted particle is destroyed by the intense x-ray pulse [9], a new and preferably identical sample particle has to be delivered into every pulse. This can be achieved with aerosolized particle beams, which, furthermore, offer significantly reduced background levels compared to liquid jet based delivery methods [10, 11]. The most widespread aerosol injectors for SPI experiments are aerodynamic lens stacks (ALS) [1, 12]. However, other aerosol injectors, e. g., convergent nozzles, have also been demonstrated [11,

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