Optimizing the geometry of aerodynamic lens injectors for single-particle coherent diffractive imaging of gold nanoparticles

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Abstract

Single-particle x-ray diffractive imaging (SPI) of small (bio-)nanoparticles (NPs) requires optimized injectors to collect sufficient diffraction patterns to reconstruct the NP structure with high resolution. Typically, aerodynamic-lens-stack injectors are used for single NP injection. However, current injectors were developed for larger NPs (>100 nm) and their ability to generate high-density NP beams suffers with decreasing NP size. Here, an aerodynamic-lens-stack injector with variable geometry and the geometry-optimization procedure are presented. The optimization for 50 nm gold NP (AuNP) injection using a numerical simulation infrastructure capable of calculating the carrier gas flow and the particle trajectories through the injector is introduced. The simulations are experimentally validated using spherical AuNPs and sucrose NPs. In addition, the optimized injector is compared to the standard-installation “Uppsala-injector” for AuNPs and results for these heavy particles show a shift in the particle-beam focus position rather than a change in beam size, which results in a lower gas background for the optimized injector. Optimized aerodynamic-lens stack injectors will allow to increase NP beam density, reduce the gas background, discover the limits of current injectors, and contribute to structure determination of small NPs using SPI.

I. INTRODUCTION

Simulations predicted the possibility of deriving high-resolution structures of biological macromolecules using x-ray free-electron lasers (XFELs) [1]. The ultra-short and extremely bright pulses of coherent x-rays provided by free-electron lasers (FELs) can outrun radiation damage processes before the particle has time to structurally respond and eventually be destroyed by the deposited energy [2]. Thus, the single-particle diffractive imaging (SPI) method at XFELs can be used to elucidate the structure of biological molecules [3,4] without the need of highly ordered crystalline sample. SPI allows to retrieve the three-dimensional (3D) structure of biomolecules by reconstruction from a large number of two dimensional diffraction patterns, assembled into a 3D diffraction volume, requiring a high probability of an x-ray pulse interacting with an injected particle [5]. High-density particle-beams with ideally one particle per pulse and focus volume are generated to use both, x-rays and sample, efficiently. However, for the atomic resolution, ~100 pm, reconstruction of a protein, 10^5 to 10^6 diffraction patterns need to be collected [6].

Delivery of high-density single-particle-beams was demonstrated using aerodynamic-lens stacks (ALS) to generate focused beams of aerosolized particles from ambient conditions into vacuum [3, 5]. An ALS contains sets of thin apertures to manipulate the particles’ lateral spatial distribution before it exits through the last aperture into vacuum. Aerodynamic lenses enable successive contractions of a flowing particle-beam and provide focusing to high particle-densities for wide range of particle sizes [7, 8]. Before adaption for SPI, they were mainly used in aerosol mass spectrometry to ensure a high transmission for a large particle size range [9]. A widely used ALS for SPI, readily available at many XFELs, is the so-called “Uppsala-injector” (TSI model AFL100), which can deliver collimated or focused beams for a range of particle sizes, e.g., 0.1–300 μm [10]. It was successfully used in various experiments at XFEL facilities [10–13]. A recent experiment we performed at EuXFEL showed the successful collection of more than 10 million diffraction patterns from single gold nanoparticles using this injector and shows the opportunities provided by careful sample preparation and injection [5]. However, currently sample injection and beam formation is the bottleneck of collecting large data sets of small bio-particle diffraction patterns and injection schemes have to be modified accordingly [14]. The geometry of the “Uppsala injector” is fixed by design and the only tunable parameter to change the particle-beam focus size and position is the inlet pressure before the ALS [15]. To circumvent the increase of inlet pressure to generate a smaller particle-beam focus and thus an increase of pressure in the experimental chamber, we designed and used a new particle injector with variable geometry, as shown in Fig. 1, i.e., the inner tube diameter and the aperture diameter can be changed [16, 17] to produce the highest particle-beam density for a given particle size. In addition, the speed of the particles is important in SPI experiments. It should be as slow as possible to allow interaction of
NPs with two x-ray pulses. For the full repetition rate of 4.5 MHz at EuXFEL [18] and an x-ray focus size of 2 μm, the particle speed has to exceed 10 m/s to enter the interaction region without interacting with the previous pulse, which can damage or scatter off the sample already. Here, we present the geometry optimization for aerosolized spherical gold nanoparticles (AuNPs) of 50 nm diameter at typical inlet conditions for SPI experiments. The size is chosen as an intermediate step from large NPs and viruses (> 100 nm) towards single proteins (< 10 nm). The numerical simulation infrastructure used is presented elsewhere [16, 19]. To validate our simulation results, we compare them with experimental data for both AuNPs and sucrose spheres. AuNPs, when synthesized and prepared well, show a narrow size distribution similar to bio-particles and are therefore good benchmark samples for sizing and focusing experiments. AuNPs have a high scattering power resulting in good detection efficiencies both in x-ray scattering and for in-laboratory detection methods [20, 21]. Furthermore, AuNPs exhibit distinct physical and chemical properties with potential applications ranging from quantum electronics to biomedicine and potential drug delivery systems [22, 23]. Sucrose particles are often used at XFEL facilities for alignment in commissioning and startup experiments [11, 12], as the number density of the generated sucrose spheres is high and the particle-beam can be observed easily while aligning the injector to the x-ray beam. Most importantly, the mass density of sucrose NPs, and thus their focusing behavior, is comparable to biological matter, rendering them a good prototypical benchmark system for bio-nanoparticles.

II. METHODS

A. Geometry Optimization

Simulations of the ALS were performed as follows: First, we calculated the flow field of the carrier gas inside a given 2D cylindrically symmetric geometry using a finite-element solver for the Navier-Stokes equations [24]. The flow field was calculated within the ALS geometry and extended after the exit with a quarter-circle with the radius of the last aperture serving as gas-expansion region of the vacuum chamber as shown in Fig. 1. The carrier gas was assumed to be nitrogen, as the particles were aerosolized using electrospray ionization (ESI), where the used gas mixture consists of ≈ 90 % nitrogen and ≈ 10 % CO\textsubscript{2}. As boundary conditions for the flow field we used mass-flow conservation of 13 mg/min as inlet condition and a pressure of 10\textsuperscript{-4} mbar at the end of the flow field along the semi-circle. Additional flow field calculations were performed using the inlet pressure as a boundary condition. Second, the trajectories of 100,000 particles for a given flow field were calculated with a homebuilt Python particle-tracing code [16]. Particles were introduced into the flow field with a uniform radial distribution covering the diameter of the first tube piece. We assumed the particles’ velocity to be equal to the flow field values. We simulated trajectories of 50 nm diameter spherical particles with a density of 19.32 g/cm\textsuperscript{3}, corresponding to the bulk density of gold. Transmitted particles were propagated further with their terminal speeds at the border of the flow field. Then, we determined the width of the resulting particle-beam depending on the distance from the ALS exit, i.e., the last aperture. Beam widths \(d\text{\textsubscript{70}}\) were specified as the diameter where 70 % of the particles were in; \(d\text{\textsubscript{70}}\) is a useful and robust metric as it is independent of the actual beam shape. Nevertheless, outside of the ALS all simulated particle-beams showed a peak-like radial distribution with the maximum of the particle density in the center (\(r = 0 \text{ mm}\)).

The ALS consists of \(n = 5\) aperture/tube pieces stacked onto another, see Fig. 1. The lens aperture radius \(r\text{\textsubscript{n}}\) and the inner tube radius \(R\text{\textsubscript{n}}\) can easily be adjusted. In our ALS, the aperture radius can be chosen from 0.75 mm to 5 mm in 0.25 mm steps. The lens apertures are interchangeable. The inner tube diameter could be chosen from parts with radius 2, 3, 4, 5, 6, 7, 5, 8, 10 mm, which were available in stock; in principle, any size is possible. The inner diameter of the tubes is adjusted by adding an additional tube into the standard 10 mm diameter pieces.

As the variety corresponds to more than \(7 \times 10\text{\textsuperscript{10}}\) combinations we approached the optimization as follows: Our optimization procedure was performed iteratively from the exit to the entrance of the ALS, as the last aperture radius \(r\text{\textsubscript{4}}\) largely determines the focus position and size of the particle beam. A larger \(r\text{\textsubscript{4}}\) aperture moves the particle-beam focus further outside or creates a collimated particle-beam and a smaller \(r\text{\textsubscript{4}}\) creates a particle-beam focus closer to the aperture or an even diverging particle-beam. We started the optimization in the last piece of the ALS, \(r\text{\textsubscript{4}}\) and \(R\text{\textsubscript{4}}\). The particles were introduced into the flow field with a uniform radial distribution covering \(r\text{\textsuperscript{\text{initial}}} = 0.02 \text{ mm}\), mimicking that the lenses before already prefocused the particle-beam. The initial particle...
velocity was set equal to the flow fields speed. The best $r_4$ and $R_4$ combination fulfills the following condition: The transmission was >90%, the focus was at $z > 4 \text{ mm}$ to suppress background scattering from the housing of the ALS, and it resulted in the smallest beam diameter. With this optimized $r_4$ and $R_4$ combination we then optimized $r_3$ and $R_3$, and this was subsequently iterated for all lenses with increasing initial radial distribution of the particles, i.e., 0.02 mm for piece 4 and 3, 0.5 mm for piece 2, 1 mm for piece 1, and the whole radius of the lens filled before the first aperture. This optimization procedure reduces the efforts to 160 combinations per lens and <1000 overall.

### B. Experimental Setup

We measured the particle-beam evolution of AuNPs from the optimized ALS geometry. The schematic of our experimental setup is shown in Fig. 2. It consists of four main parts: an aerosolization chamber, a differentially pumped transport tube, the ALS system for particle-beam formation, and the detection region for visualization of the particle-beam. To generate isolated test particles from the liquid sample, we injected spherical AuNPs with a diameter of $(27 \pm 2.25) \text{ nm}$ in 5 mM ammonium acetate (AmAc) with a concentration of $10^{11}$ particles/ml and a 2% sucrose solution in 20 mM AmAc using a commercial electrospray (TSI Advanced Electrospray 3482). The aerosolized nanoparticles passed through a differentially pumped skimmer assembly for pressure reduction. The particles were focused into the detection chamber using the ALS. The pressure above the entrance of the ALS was 1.8 mbar (Pfeiffer Vacuum CMR 361). In the main chamber, the pressure was kept at $2.5 \times 10^{-4}$ mbar. The ALS is mounted on a motorized $xyz$-manipulator to perform height scans and measure the particle-beam evolution.

Particles were detected using a side-view illumination scheme [20]. A Nd:YAG laser (Innolas SpitLight, 532 nm, pulse duration 11.5 ns, pulse energy up to 240 mJ at 532 nm, 20 Hz repetition rate) was focused into the center of the vacuum chamber intersecting the particle-beam. The light scattered off the particles was collected using a camera-based microscope system [20, 21] consisting of a long working-distance objective (Edmund Optics, 5× magnification, numerical aperture $N_a = 0.14$, working distance $d = 34 \text{ mm}$, depth of field (14 μm)) and a high-efficiency sCMOS camera (Photometrics PrimeB95, quantum efficiency 0.95 at 532 nm, 1200 × 1200 pixels). This microscope yields a nominal resolution of 0.54 pixel/μm. Images were collected with a 1 ms exposure time synchronized to the laser at 20 Hz such that every frame covered one laser pulse. For every distance of the ALS and the laser, we recorded 10000 images for the AuNP sample and 2000 images for the sucrose sample. We determined the positions of the particles by analyzing the images using a centroiding algorithm based on Hessian blob-finding [25]. The particles’ positions were converted into a 2D histogram, see Supplementary Information for details. The width of the particle beam is determined from the projection of the particle-beam onto the laser propagation axis. The beam diameter is shown as $d_{70}$.

### III. Results

#### A. Optimization and Simulation Results

The optimization process resulted in one final geometry which produced a particle beam to our specifications. The resulting optimized-lens-stack geometry is shown in Fig. 3. From entrance to exit, the lens tube radius and the aperture radius are first increasing, then decreasing. The smallest lens tube radius and aperture radius are located at the last lens piece. Values are given next to the geometry. The velocity-flow field for 13 mg/min mass flow and particle trajectories for 50 nm AuNPs at different inlet positions (black solid lines) are shown in Fig. 3, demonstrating a clear focusing effect of the ALS.

For this ALS geometry, the 50 nm AuNP beam was focused at a distance of 5.8 mm from the ALS exit with a particle-beam width of 33 μm ($d_{70}$). The particle-beam evolution for 13 mg/min mass flow is shown in Fig. 4 as the cyan curve. The particle-beam evolution is shown as the beam width ($d_{70}$) depending on the distance $z$ from the ALS exit. We simulated the focusing

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FIG. 2. Schematic of the experimental setup for the characterization of nanoparticle-beams. The aerosol passed a skimmer assembly to remove most of the carrier gas and the particles were focused using an ALS and entered the main vacuum chamber, where the particle-beam was crossed by a laser beam. The light scattered off the particles was collected using a camera-based microscope system [20] [21].
FIG. 3. Optimized ALS geometry. Tube and aperture radii are specified above the device and the corresponding nitrogen-gas flow-field for the injection of 50 nm AuNPs at 13 mg/min mass flow is depicted in false color. Representative (calculated) particle trajectories are shown by black lines, with gas and particle flow direction from left to right. A clear focusing effect of the different parts of the ALS can be observed through the radial narrowing of the set of particle trajectories.

FIG. 4. (a) Particle-beam evolution curves of the optimized injector for 50 nm AuNPs at different gas-mass flows. The width of the particle-beam was determined as $d_{70}$. With increasing mass flow and thus pressure before the ALS, the particle-beam focus becomes harder, i.e., it moves closer to the ALS exit and gets smaller. At 50 mg/min mass flow, the particle-beam focus size decreased to 13 µm at a distance of 3.2 mm. Similar behavior has been shown experimentally for the “Uppsala-injector” [15]. Therefore, working at higher mass flow is desired, but it will increase the amount of gas introduced into the interaction chamber and result in a higher pressure and thus a higher gas-scattering background in diffractive imaging experiments.

At 13 mg/min mass flow the AuNPs exiting from the optimized ALS had a mean velocity of 29 m/s. Mean velocities and beam diameter values for different flow conditions are given in the Supplementary Information.

The behavior of the ALS optimized for 50 nm AuNPs was compared to smaller and larger diameters of the AuNPs as shown in Fig. 4 b. For smaller AuNPs the focus moved closer to the ALS and was larger, whereas bigger particles were focused further away and showed a smaller focus size. An interesting feature observed was the change of the convergence depending on the particle size: The smaller the particles were, the larger the convergence became. A precise positioning for small particles becomes necessary to meet the particle-beam focus. This change of the convergence is due to the larger momentum of larger particles interacting with the gas flow field.

B. Experimental Results

We measured particle-beam evolution curves of AuNPs and sucrose particles. The AuNP data with standard errors is shown in Fig. 5 a as beam diameter ($d_{70}$) de-
FIG. 5. (a) Experimental particle-beam size evolution for 
(27±2.25) nm AuNPs (black dashed line). Simulated beam 
evolution is shown for 27 nm (black solid line) with the spread 
of the beam diameter due to the size distribution of ±2.25 nm 
(grey area). (b) Experimental particle-beam size evolution 
for sucrose spheres (black). The experimental data agrees 
reasonably well with a simulated particle size of 80 nm (dark 
red).

Depending on the distance from the injector exit, along with 
simulations for the particle size of (27 ± 2.25) nm using 
the experimentally measured inlet pressure of 1.8 mbar 
above the ALS. The experimental and simulated particle-
beam diameters agree well, especially at and after the 
focus of the particle-beam. Some deviations are observed 
before the focus, where the simulation overestimates the 
beam diameter, e.g., by a factor of ~1.5 at z = 1.4 mm. 
However, the most relevant parameters for SPI experi-
ments, the focus position and focus size, are in excellent 
agreement between experiment and simulation. The same 
experiment is repeated for a 2% sucrose solution to gener-
ate spherical sucrose particles in the electrospray process 
with a broad size distribution around 80 nm, shown in the 
Supplementary Information. The sucrose-particle-beam 
evolution is shown in Fig. 5 b with standard errors (black) 
and compared to simulations for different sizes of sucrose 
spheres (ρ = 1.59 g/cm³). Overall, the experimental 
data is described well by the simulation for 80 nm su-
crose spheres. Similar to the AuNP data, the simulation 
agrees well with our data after the focus, although before 
the focus the simulation deviates by a factor of ~1.6 at 
z = 0.8 mm. This mismatch is partly due to the broad 
experimental size distribution, i.e., the experimental data 
does not correspond to a single particle-size simulation.

C. “Uppsala-injector” simulation

The “Uppsala-injector” (AFL100) was introduced before 
and used in various experiments at XFELs [10–13]. We 
simulated its focusing of 50 nm AuNPs and compared it 
to our optimized ALS.

The beam evolution curves for 50 nm AuNPs at dif-
ferent mass flow conditions for this injector are shown in 
Fig. 6 (dashed lines), along with the focusing curves for 
our optimized injector (solid lines). The simulated trans-
mission of 50 nm AuNPs through both injectors was above 
90%, i.e., at 13 mg/min mass flow the transmission was 
91.9% for the AFL100 and 93.4% for our optimized injec-
tor. At the same mass flow the AFL100 showed slightly 
smaller mean velocities of the exiting particles than our 
optimized injector. As an example, at 13 mg/min mass 
flow, 50 nm AuNPs exiting the “Uppsala-injector” showed 
a mean velocity of 27 m/s. In comparison, particles in 
our injector reached a velocity of 29 m/s. A detailed 
list of velocities depending on mass flow is shown in the 
Supplementary Information.

IV. DISCUSSION

Our simulations show that the focus size is compara-
ble for both injectors, but the difference is in the focus
position and the convergence. Our injector focuses the particles further downstream and the focusing is not as hard as for the AFL100. Generating a focused particle-beam further away from the injector exit has the advantage of a lower background from the nitrogen and CO₂ gas. Light gas diverges fast from the exit of the ALS into the vacuum chamber.

The focus position of the AFL100 is closer to the injector exit and can cause problems when using smaller particles and particles with lower sample density, such as bio-particles: The smaller and lighter the particles are the closer the focus position. As an example, we performed simulations for 10 nm AuNPs at 13 mg/min nitrogen mass flow for the AFL100 showing the focus position moves very close to the ALS exit, below \( z = 1.5 \text{ mm} \); the transmission is reduced to 59%. Our 50 nm-optimized injector still shows a transmission of 79% for those particles and a focus position above \( z = 2 \text{ mm} \); see Supplementary Information for details. The same behavior holds for the particle density: The lower the particle density (biomolecules), the closer the particle-beam focus becomes. For isolated proteins, it is almost impossible to focus the particle-beam with these injectors. In this case, an appropriate geometry optimization could result in a particle-beam focus further away from the injector exit.

V. CONCLUSION

We presented an optimization procedure of an ALS for 50 nm AuNPs using our previously developed computer-simulation framework for ALS injectors [16, 19] including the results of this optimization. We experimentally benchmarked the optimized geometry for beams of spherical gold and sucrose nanoparticles. Both particle-beam-evolution curves are in good agreement with the simulations. This validates our simulation framework, which can be used to get further insight into the fluid-dynamics focusing process and to develop optimized particle injectors for different sizes and materials, as well as for different experimental conditions, such as inlet pressure and gas type.

We compared our optimized injector to the widely used AFL100 “Uppsala-injector” for 50 nm AuNPs. Both injectors create a focused particle-beam for different inlet mass flow conditions, and the main difference is observed in the particle-beam focus position, which for our optimized injector is further downstream, which reduces the carrier gas background at the focus and will be greatly beneficial for x-ray diffractive imaging, especially of small bio-particles that exhibit only small scattering signals.

Our variable injector geometry allows us to vary the particle-beam focus independent from the inlet pressure by varying the geometry and thus keeping the pressure after the injector, i.e., in the x-ray interaction region, constant. Generating high-quality particle-beams of nanoparticles does not only allow for structure determination by an increased number of collected diffraction patterns, but in addition it opens the field of time-resolved imaging of nanoparticle dynamics in future pump-probe-type experiments at XFELs.

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