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Supporting information for article:

The new small-angle X-ray scattering beamline for materials research at PETRA III: SAXSMAT beamline P62

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S1. Additional figures

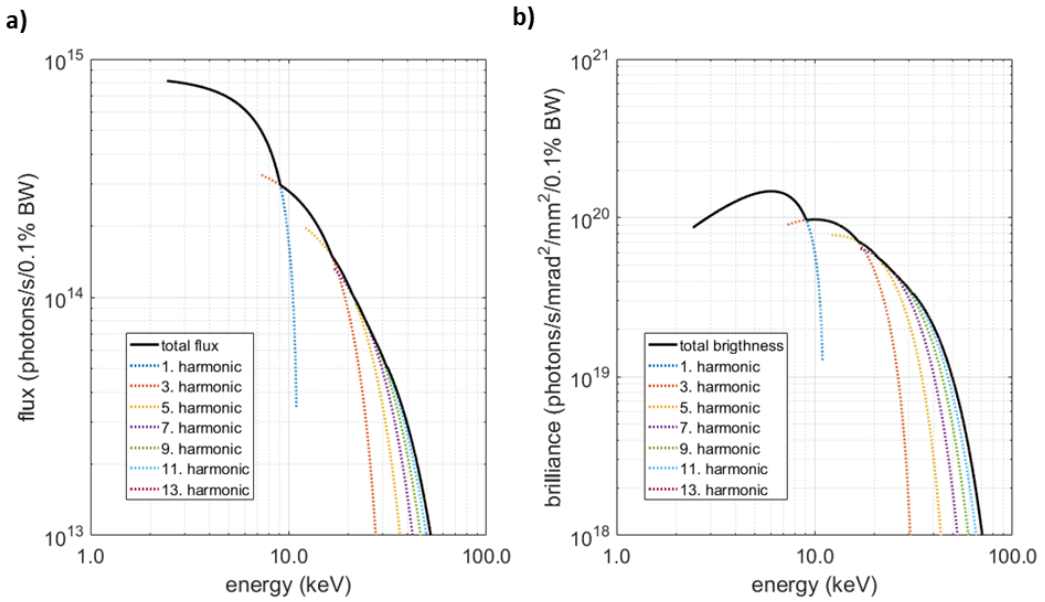

Figure S1 Flux and brilliance of the U32 undulator of the SAXSMAT P62 beamline.

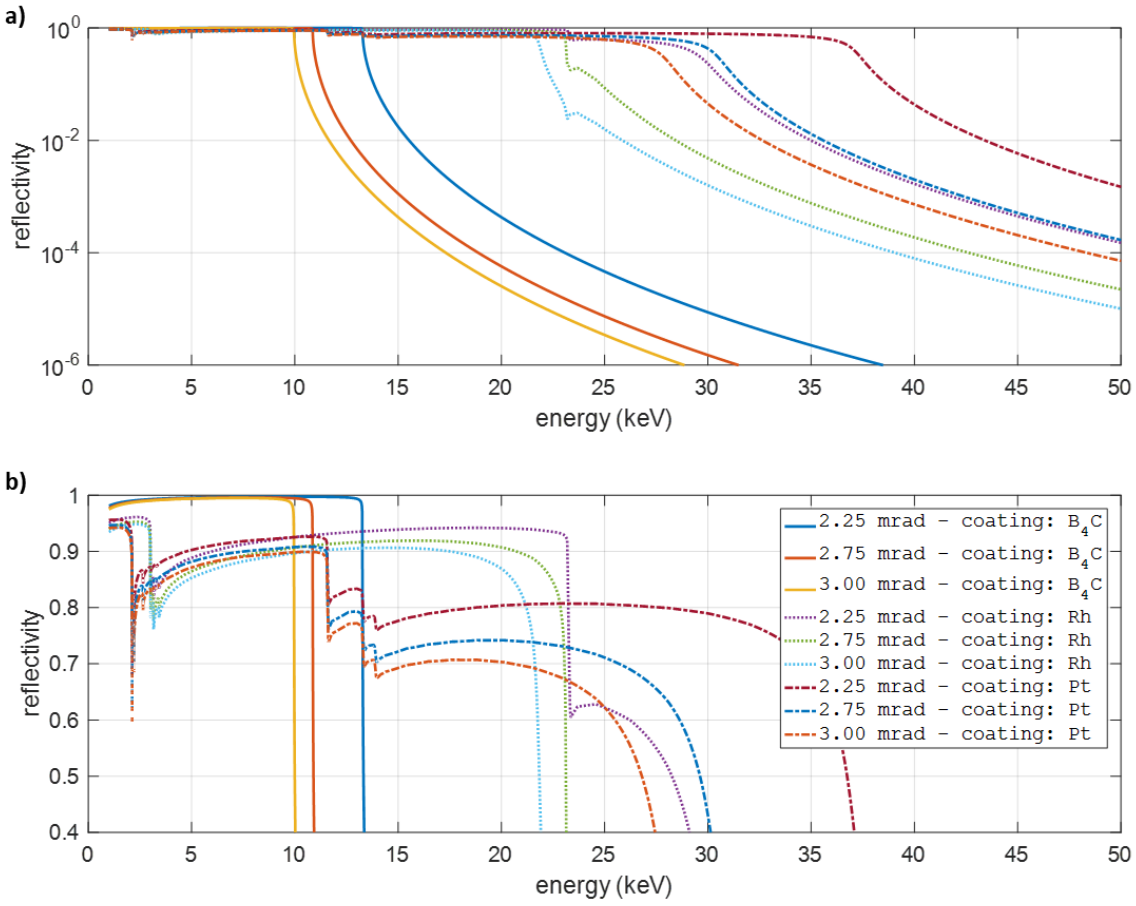

Figure S2 Calculated reflectivity curves of the double mirror system as a function of X-ray energy, pitch angle, and coating.

S2. ASAXS study of PVP-coated dried Au nanoparticles

S2.1. Spherical nanoparticle ASAXS model

The intensity of spherical nanoparticles with a lognormal size distribution and a structure factor in the local monodisperse approximation is given by (Glatter & Kratky, 1982; Pedersen, 1994):

$$I(q,E) = N\int_0^\infty P(r,\mu,\sigma)F_s(q,r,\rho(E))^2 S(q,r,rhs,\tau,\nu)dr + \beta_1(E)q^{-\alpha} + \beta_0(E).$$

N is the number density of particles in particles per cm³, μ and σ are the size distribution $P(r,\mu,\sigma)$ parameters (mean and polydispersity).

$F_s(q,r,\rho(E))$ is the form factor of spherical particles given by:

$$F_s\big(q,r,\rho(E)\big) = \frac{4}{3}\pi r^3\rho(E)3\frac{\sin(qr)-qr\cos(qr)}{(qr)^3}.$$

$\rho(E)$ is the energy E dependent scattering contrast of the particle phase against the solvent.

As structure factor $S(q,r,rhs,\tau,\nu)$ the sticky hard sphere model has been used (Baxter, 1970). This model includes three additional model parameters: rhs is the repulsive radius, τ the stickiness parameter characterizing the adhesive strength, and ν is the local volume fraction of particles.

The scattering background is modeled by the last two terms including two energy-dependent parameters $\beta_0(E)$ and $\beta_1(E)$ and one energy-independent parameter α that should be between 3 and 4.

S2.2. Spherical core-shell nanoparticle ASAXS model

The intensity of spherical core-shell nanoparticles with a lognormal size distribution and a structure factor in the local monodisperse approximation is given by (Glatter & Kratky, 1982; Pedersen, 1994):

$$I(q,E) = N\int_0^\infty P(r,\mu,\sigma)F_{cs}(q,r,d,\rho_{core}(E),\rho_{shell})^2 S(q,r,rhs,\tau,\nu)dr + \beta_1(E)q^{-\alpha} + \beta_0(E).$$

N is the number density of particles in particles per cm³, μ and σ are the size distribution $P(r,\mu,\sigma)$ parameters (mean and polydispersity).

$F_{cs}(q,r,d,\rho_{core}(E),\rho_{shell})$ is the form factor of spherical core-shell particles given by:

$$F_{cs}(q,r,d,\rho_{core}(E),\rho_{shell}) = F_s(q,r+d,\rho_{shell}) - F_s(q,r,\rho_{shell}-\rho_{core}(E)) .$$

$\rho_{core}(E)$ is the energy E dependent scattering contrast of the particle core phase against the solvent and ρ_{shell} is the scattering contrast of the particle shell against the solvent phase, which can be assumed to be energy independent. In the present case water. d is the shell thickness.

As structure factor $S(q,r,rhs,\tau,\nu)$ the sticky hard sphere model has been used (Baxter, 1970). This model includes three additional model parameters: rhs is the repulsive radius, τ the stickiness parameter characterizing the adhesive strength, and ν is the local volume fraction of particles.

The scattering background is modeled by the last two terms including two energy-dependent parameters $\beta_0(E)$ and $\beta_1(E)$ and one energy-independent parameter α that should be between 3 and 4.

S2.3. Summary of all fit parameters spherical model

parameter	E=11523eV	E=11823eV	E=11873eV	E=11903eV	E=11918eV	E=11922eV
α	3.52 ± 0.01					
β_0	0.0028 ± 0.0001	0.0022 ± 0.0001	0.0021 ± 0.0001	0.0021 ± 0.0001	0.0021 ± 0.0001	0.0036 ± 0.0001
β_1	0.0071 ± 0.0003	0.0064 ± 0.0002	0.0062 ± 0.0001	0.0061 ± 0.0001	0.0057 ± 0.0001	0.0058 ± 0.0001
N	5.734e-4 ± 5.97e-7					
μ	2.333 ± 0.001					
σ	0.0995 ± 0.0004					
ρ	1.163 ± 0.002	1.117 ± 0.003	1.093 ± 0.002	1.059 ± 0.001	1.024 ± 0.003	1.029 ± 0.002
rhs	3.628 ± 0.005					
τ	0.142 ± 0.002					
ν	0.069 ± 0.001					

The weighted R-value of the regression is: 0.0214425.

S2.4. Summary of all fit parameters spherical core-shell model

parameter	E=11523eV	E=11823eV	E=11873eV	E=11903eV	E=11918eV	E=11922eV
α	3.52 ± 0.01					
β_0	0.0021 ± 0.0002	0.0020 ± 0.0001	0.0020 ± 0.0001	0.0021 ± 0.0001	0.0028 ± 0.0001	0.0038 ± 0.0001
β_1	0.0070 ± 0.0002	0.0065 ± 0.0001	0.0063 ± 0.0001	0.0061 ± 0.0001	0.0058 ± 0.0001	0.0059 ± 0.0001
N	5.734e-4 ± 5.97e-7					
μ	2.323 ± 0.001					
σ	0.0998 ± 0.0004					
d	0.103 ± 0.012					
ρ_{core}	1.1864 ± 0.0002	1.1213 ± 0.0001	1.0958 ± 0.0001	1.0608 ± 0.0001	1.0049 ± 0.0001	1.0225 ± 0.0001
ρ_{shell}	0.11002 ± 0.00012					
rhs	3.626 ± 0.005					
τ	0.143 ± 0.002					
ν	0.070 ± 0.001					

The weighted R-value of the regression is: 0.0132957.