

Standard Application for Beam Time at the ESRF

Proposal Title (175 chars maximum.)

Refinement of large-scale nanoparticle deposition for plasmonic solar cells

Keywords

#1: #2: #3: #4:

• This proposal is:

- A new proposal A proposal relating to research in collaboration with an industrial group
 A resubmission of A continuation of :

Research Area of the proposal

- CH - Chemistry MD - Medicine
 HE - Hard Condensed Matter - Electronic and Magnetic MI - Methods and Instrumentation
 HS - Crystals and Ordered Systems - Structures MX - Macromolecular Crystallography
 HD - Disordered Systems and Liquids SC - Soft Condensed Matter and Biological Materials
 MA - Applied Materials and Engineering SI - Surfaces and Interfaces
 EC - Environmental and Cultural Heritage Matters

Alternative Category:

Or specify other research areas here:

Beamline(s) requested: and
 or or

Number of shifts required (1 shift is 8 hours)
 Preferred starting time: Please select the period
 Unacceptable dates

Beam Requirements

- Multi Bunch 16 Bunch Mode 4 x 10mA Mode
 Circular polarization White beam Monochromatic beam
 Fixed energy [keV]: Tunable energy [keV] from: to:
 Beam energy resolution [meV]: Spot size on sample [μm]:
 Other:

Main Proposer (to whom correspondence will be addressed):

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Laboratory Support Facility

Chemistry Lab. Biology Lab.

Sample Environment

Items Supplied by the ESRF

- Furnace Magnet Cryostat Cryogenic gas stream Refrigerator
 Laser Class Wavelength [nm]
 High pressure Pressure range [GPa] from to

Fixed temperature Temperature range [K] from to

Detector system

Other equipment

Items Not Supplied by the ESRF

List all equipment that you will insert into the instrument

Laser Class Wavelength [nm]

Other equipment

Please indicate requirements for special equipment or facilities

Sample Description

Substance and formula

Single crystal Powder Polycrystalline Multilayer Liquid Gas

Nanoparticles Prepared at ESRF

Other

Average size [nm] Volume [mm³] Surface area [mm²]

Mass [mg] Matrix or solvent Conc. of absorb. [mmol]

Space group Cell dimensions at T= K:

a= Å b= Å c= Å alpha= ° beta= ° gamma= °

Container (capillary, flat plate, type of pressure cell, etc.)

Extra information required for Macromolecular Crystallography:

Origin and expression system

Previously observed diffraction (resolution, X-ray source, exposure/°)

Safety

Is the sample:

Radioactive? Contaminant? Corrosive? Oxidizing?
 Explosive? Biologic? None of those

Is there any danger associated with the proposed sample, with any preparation at ESRF, or with sample equipment?

Yes Uncertain No

If you have ticked Yes or Uncertain, you must give details of the associated risks in the box below:

Will you use live animals on site for your experiment (all kinds of animals are concerned)? Yes No

If yes, you will later receive a special form.

After the experiment, will the sample be: Removed by user? Stored at ESRF?

To be filled by ESRF

Sample environment code:

Comments by safety Officer:

Experience with Synchrotron Radiation

What are the technical reasons which make ESRF necessary for your experiment? Why are other synchrotron radiation sources not appropriate?

Have you used synchrotron radiation at the ESRF? No Yes

Have you used synchrotron radiation at other sources? No Yes, at:

Have you already used synchrotron radiation for this project? No Yes

Publications

Please give the references of papers published during the past 18 months as a result of experiments done at the ESRF.

Origin (1): if from data from ESRF beamlines ONLY, (2) : if from data from more than one source

Description	Origin
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Application for beam time at ESRF – Experimental Method

Refinement of large-scale nanoparticle deposition for plasmonic solar cells

Proposal Summary (should state the aims and scientific basis of the proposal) :

The prospects of plasmonics to increase the solar cell conversion efficiency are high [1]. The metallic nanoparticles having the plasmon resonance in the visible range are incorporated into various parts of solar cells. The goal of this proposal is to use the colloidal nanoparticles for plasmonic templates. The utilization of colloidal monodisperse metallic nanoparticles would significantly simplify the fabrication of suitable plasmonic templates as they are produced cost-effectively in large quantities. The main objective of the proposed project is the in-situ optimization of the nanoparticle assemblies prior to Langmuir-Blodgett/Schaefer deposition on solid surfaces. The challenge is the large-scale homogenous deposition of the nanoparticle assemblies with the different surface densities at the solar cell interfaces. We plan to influence also the size and distribution of clusters/islands composed of nanoparticles in case of sub-monolayers. We would like to perform in-situ GISAXS measurements on the Langmuir-Blodgett trough. We will investigate the nanoparticle distribution as a function of three free parameters: nanoparticle surface pressure, concentration of the free (unbound) surfactant molecules and molar fraction of acyclic alcohols in the subphase. Utilizing the in-situ GISAXS data we can find the optimum deposition conditions for nanoparticle arrays suitable for novel plasmonic solar cells.

Scientific background :

Three possible locations are suitable for nanoparticle inclusion in solar cells based on theoretical predictions [2-4]. The first location is the interface between the transparent conducting oxide (TCO) and the active absorption layer. Here the role of the nanoparticles is to scatter the incoming solar radiation effectively into the active absorbing layer [2]. This allows reduction of active layer thickness while keeping the optical thickness constant. The second location is the direct inclusion of nanoparticles into the active layer [3]. Here the enhanced local electromagnetic field due to the nanoparticle plasmon resonance increases absorption of the incoming radiation. The third suitable location is at the bottom metallic electrode. Here the generated surface plasmon polaritons (SPP) at the metal/semiconductor interface are increasing the absorption of the impinging solar radiation [4]. All described effects increase effectively the external quantum efficiency of solar cells. We mastered a modified Langmuir-Schaefer deposition technique capable to fabricate large-scale arrays of nanoparticles on the substrates of up to 4 inch in diameter [5]. As the nanoparticle deposition is modified by many free parameters like the surface pressure, concentration of free surfactant molecules and molar fraction of acyclic alcohols in the water phase, a systematic in-situ study is of vital importance. The GISAXS technique will provide valuable information on the nanoparticle assemblies prior to deposition on solid surfaces.

Experimental technique(s), required set-up(s), measurement strategy, sample details (quantity...etc)

For the planned experiments we would like to use the instrumentation of the ID10B beamline that can perform the grazing-incidence small-angle X-ray scattering (GISAXS) measurements on the liquid phase. We would like to use a 2D X-ray detector at the distance permitting to record the GISAXS patterns in reciprocal space up to some 5 nm^{-1} . We would prefer the beam energy in the range of 6-9 keV. The beam size available at the beamline is suitable for our application. We will record in-situ the GISAXS from the nanoparticle layer as a function of surface pressure, concentration of extra surfactant molecules and molar fraction of acyclic alcohol molecules in the subphase. If necessary we can provide our custom-made Langmuir-Blodgett trough suitable for grazing-incident measurements with an enhanced range of attainable surface pressures due to a large aspect ratio of the trough geometry. We can also provide a fast X-ray detector (Pilatus 100K) for the in-situ time-resolved measurements at the trough if there will be no

one available in detector pool at the time. The planned experiments do not involve any materials or substances that underlay special safety regulations valid for synchrotron beamlines.

Beamline(s) and beam time requested with justification :

For this proposal, we ask for a total of 12 shifts on the ID10B beamline. In the case of a reduction of this request, we are able to reduce our plans accordingly to utilize efficiently the beamtime allocated.

Results expected and their significance in the respective field of research :

The main objective of introduced proposal is to study in-situ the evolution of nanoparticle layers directly on the Langmuir-Blodgett trough. Particularly, we are interested in the dependencies of nanoparticle distributions as a function of surface pressure, concentration of free surfactant molecules and molar fraction of acyclic alcohol molecules in water subphase. The research should trigger and refine the nanoparticle large-scale deposition [5] suitable for emerging plasmonic solar cells. To support the planned activities we performed a pilot in-situ GISAXS study at a home-made laboratory system able to measure X-ray scattering from liquid surfaces.

In this study we measured GISAXS pattern of nanoparticle films at specific surface pressures. Fig. 1 shows GISAXS patterns taken at four different surface pressures. The first experiment shows that already at low surface pressure (Fig. 1a) the nanoparticles are clustered into the small islands with already well defined particle pair correlation function.

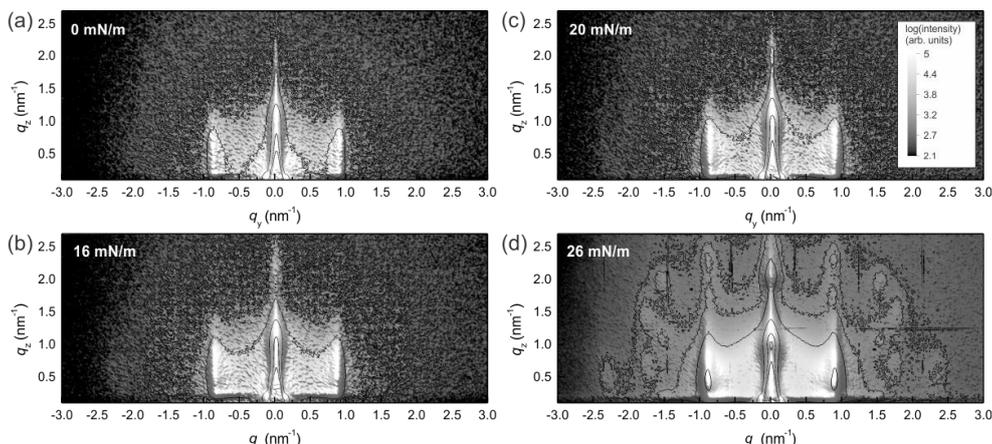


Fig. 1 The in-situ GISAXS patterns of nanoparticle films at four different surfaces pressures (a) 0 mN/m (b) 16 mN/m (c) 20 mN/m and (d) 26 mN/m.

Increasing the surface pressure (Fig. 1b, Fig. 1c) leads to the compression of the separate islands into the continuous monolayer that is indicated by an increase of intensity in the diffraction maxima located approx. at $q_y=0.8 \text{ nm}^{-1}$. Finally, at a sufficiently high surface pressure the monolayer collapses into a nanoparticle double layer. This can be clearly seen by the appearance of diffraction spots in Fig. 1d. This pilot experiment demonstrates the possibilities of the proposal to study and improve the structure of nanoparticle assemblies suitable for future plasmonic polymer solar cells.

References

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