Université de Paris

2021-2022

Master thesis proposal

MPQ
10 rue Alice domon et Leonie Duquet
75013 Paris
Director: Cristiano Ciuti

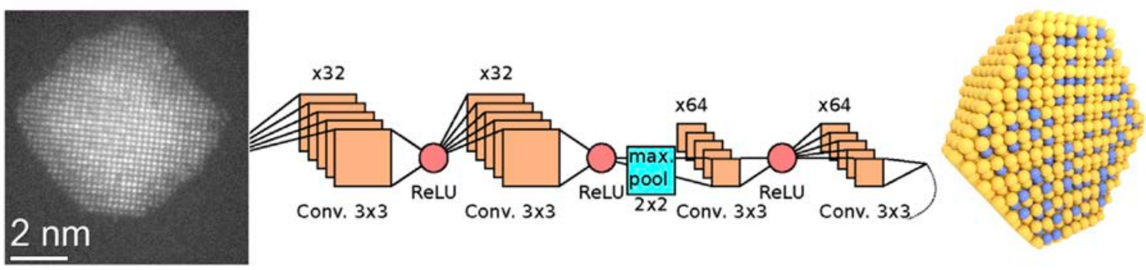
Title:

Quantitative 3D atomic reconstruction of bimetallic nanoparticles using machine learning

Keywords:
TEM, Machine learning, atomic structure, nanoalloys

Scientific description:

Bimetallic nanoparticles (BiM NPs) are emerging as a class of critical materials for applications in electronics, optics and medicine, among others, thanks to their unique physical and chemical properties. In recent years, the structural properties of this family of materials has received increasing interest as it has been shown that their properties can be tailored through particle size, morphology, composition and the arrangement of the constituent atoms [1]. Thus, determining structure–property–functionality relationships in these materials requires a thorough knowledge of their exact 3D atomic structure which can deviate from the periodic atomic arrangement of their bulk counterparts due to quantum size and/or surface effects. While various microscopy and spectroscopy techniques, including transmission electron microscopy (TEM), have been deployed for elucidating the structure and chemistry of BiM NPs, none is capable yet of retrieving their 3D atomic structure. In this internship, we aim to develop a deep-learning approach to determine the 3D atom arrangement in BiM NPs with single atom sensitivity by counting atoms in atomic-resolved 2D-projected chemically-sensitive high angle annular dark field (HAADF) images acquired in scanning TEM (STEM) mode.
In an HAADF-STEM image, the pixel intensity around each atomic column scales with its composition and arrangement of its constituent atoms. In homogeneous nanomaterials where the atomic composition varies linearly with the HAADF scattering cross-section, this relationship has recently paved to the automatic retrieval of the 3D atomic structure of single element nanomaterials by atom-counting methods using a model-based statistical approach [2]. In BiM NPs, atom-counting from HAADF-STEM images by statistical approach remains a challenging task as there is no unique relationship between image intensity in projection and atomic colum composition [3]. In this internship, we aim to overcome this limitation in bimetallic NPs by exploring the possibility of using Convolutional Neural Networks (CNNs, cf. Figure) for disentangling and quantifying the complex relationships between image intensity and atomic column composition and organisation. As test experiment, we will study the 3D atomic structure of gold-copper nanoalloys grown by pulsed laser deposition. Such BIM NPs, whose MPQ has a great expertise, are particularly studied for its remarkable catalytic properties [4].



This internship, at the frontier of Material Science, electron microscopy and computational science, will take place at MPQ laboratory in the Advanced electron mircroscopy and nanostruture (Me-ANS) group. The candidate will (i) set-up the production and advanced STEM study of the structural properties of the Au-Cu BiM NPs by atomic-resolved HAADF-STEM imaging on a state-of-the-art aberration-corrected TEM and (ii) participate in the training and optimisation of the CNNs for atom counting using synthetic HAADF-STEM images of bimetallic NPs generated by atomistic computer simulation [5] and the testing of the networks on experimental images.

References:
[1] Nanoalloys : Synthesis, Structure & Properties, Ed. D. Alloyeau, C. Mottet, C. Ricolleau, Springer Eds (2012)
[2] A. De Backer et al., Ultramicroscopy 134, 23 (2013).
[3] N. Baladés et al., Journal of microscopy 273, 81 (2019).
[4] A. Chmielewski et al., Phys. Rev. Lett. 120, 025901 (2018).
[5] G. D. Förster, A. Castan, A. Loiseau, J. Nelayah, D. Alloyeau, F. Fossard, C. Bichara, H. Amara, Carbon 169, 465 (2020).

Techniques/methods in use: Pulsed laser deposition, electron microscopy, Convolutional Neural Networks

Applicant skills: Physicist with a good knowledge of materials science, nanoscience and programming (python, fortran and knowledge of artificial intelligence will be a major asset). Strong motivation to perform in a multidisciplinary scientific environment at the frontier of physics, data modelling and computing. Autonomy, ability to work in a team, synthetic/redaction ability and good knowledge of English language are a necessity. Several collaborations (ONERA, IFPEN, IPCMS/Univ. Strasbourg) are expected, and therefore scientific exchanges will be encouraged.

Applications in English or in French should include:
- A short cover letter.
- Names and contact information of at least one reference.
- Up-to-date CV with education history and any research experience.
- Copy of university marks at the bachelor and Master levels.

Industrial partnership: N

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Website: https://mpq.u-paris.fr/?-microscopie-electronique-avancee-&lang=en

Internship location: Laboratoire MPQ, Université de Paris, Paris 13e

Possibility for a Doctoral thesis: YES. Thesis grants funded within ANR project ARTEMIA on IA-assisted analysis of in situ TEM images (2022-2026, Principal Investigator: J. Nelayah). Application to these grants will be opened in Spring 2022.)