Synthesis, structural and mechanical properties of high-entropy nanoalloys

High-entropy alloys (HEA) have evolved to one of the most popular material classes in the last decades in both fundamental and applied material science. Due to the high mixing entropy effect, these alloys, containing multiple elements (typically 4 to 6) in nearly equiatomic composition, adopt a cubic solid solution. [1] Unique mechanical, electromagnetic and electrochemical properties originate from their peculiar structural features. However, research has been focused primarily on bulk HEA, ignoring HEA nanoparticles (NPs), due to the absence of a reliable, scalable, and straightforward synthesis method for HEA NPs. The development of synthesis methods where elemental composition, particle size, and atomic structure can be precisely controlled could bring about a new repertoire of nanostructures with unprecedented functionalities, notably for mechanical applications.The Grail of any metallurgist can therefore be achieved by developing advanced materials with a substantial improvement of both strength and ductility

This PhD thesis financed by the ANR project Yosemite is a collaborative project between MPQ (at Paris-Cité University) and ICMMO (at University Paris-Saclay) that aims at:

(i) developing innovative synthesis protocols using both chemical and physical routes to gain control over the size, shape composition and structural phase of HEA NPs;

Two strategies of synthesis will be employed to ensure the fabrication of well controlled HEA NPs over a large size range (from 5 to 100 nm). On the one hand, we will use an original wet chemical synthesis method recently developed at ICMMO to synthesize small multi-metallic NPs of controlled composition. On the other hand, the MPQ laboratory has developed a pulsed laser deposition set-up to fabricate well controlled multi-metallic nanostructures in a larger size range. These two approaches have recently been used to fabricate the first HEA nanoparticles in France [2]

(ii) Exploiting *in situ* transmission electron microscopy (TEM) to rationalize the synthesis of these complex nanostructures and explore their structural properties in realistic environments.

The MeANS group uses aberration-corrected TEM to visualize with atomic resolution the behavior of nanomaterials in their formation and application media. The state of the art *in situ* TEM facilities installed at the MPQ lab will be exploited to study the nucleation and growth mechanisms of HEA NPs in liquid phase [3] and reveal their nanophase diagram in realistic application conditions. In bulk materials, the temperature–composition phase diagrams identify the stable phases at certain conditions. Once the size of materials is downscaled to nanometer dimension, significant changes in the structural properties and behavior of materials emerge because of the high surface-to-volume ratio and high surface free energy of NPs (surface segregation, coalescence, Ostwald ripening, size and shape effects…). [4, 5, 6] Understanding the thermodynamic properties of HEA NPs is an essential prerequisite to better control their size and evaluate their potential for mechanical applications, in which the nanostructures are exposed to high temperature and possibly oxidizing or reducing environments.

(iii) Preliminary mechanical testing experiments will be performed in collaboration with the CEMES (CRNS, Toulouse) to focus on the downscaling of the mechanical properties of nano HEAs.

More importantly, the interdisciplinary skills in electron microscopy and nanomaterial synthesis that will be acquired by the future PhD student will facilitate his professional insertions.

Thesis requirements and qualification

Good knowledge of materials science and/or solid-state physics (knowledge in electron optics and nanomaterial synthesis will be a major asset). Strong motivation to perform in a multidisciplinary environment at the frontier of physics and chemistry. Autonomy, ability to work in a team, synthetic/redaction ability and good knowledge of English language are requested.

Send your CV, cover and recommendation letters before September 10th to:
Damien Alloyeau (Laboratoire Matériaux et Phénomènes quantiques, CNRS – Université Paris Cité), damien.alloyeau@u-paris.fr; +33 1 57 27 69 83.

Christian Ricolleau (Laboratoire Matériaux et Phénomènes quantiques, CNRS – Université Paris Cité), Christian.ricolleau@u-paris.fr; +33 1 57 27 62 45.

Vincent Huc (Institut de Chimie Moléculaire et des Matériaux d'Orsay, CNRS – Université Paris Saclay) vincent.huc@u-psud.fr; +33 1 69 15 74 36

Website of the MeANS group at MPQ:
https://mpq.u-paris.fr/means/

Website of the inorganic chemistry group at ICMMO:
https://www.icmmo.universite-paris-saclay.fr/en/teams/lci/

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Reference

[1] Nat. Rev. Mater. 4, 515 (2019); [2] Faraday discussion. 242, 129 (2023); [3] J. Phys. Chem. Lett., 11, 2830-2837; [4] Nature Mat. 8, 940 (2009); [5] Phys. Rev. Letters 105, 255901 (2010); [6] ISBN: 978-1-4471-4013-9

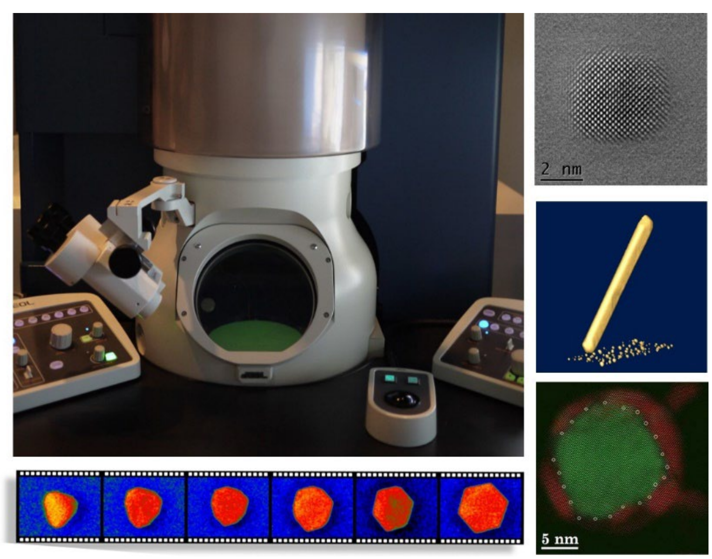

Illustration:

Possibilities of TEM to probe the atomic structure, the 3D shape, the chemistry or the growth of metal nanostructures.