

# Maxime Dupraz

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Citations: **444**, H-index: **11**

## Education and Degrees

- 2012 – 2015 **PhD in Mechanics and Materials Science Doctor of Philosophy in Mechanics and Materials Science**, *SIMaP Laboratory, PM (Metal Physics) group, Université Grenoble Alpes*.
- PhD studies with Dr. Marc Verdier and Dr. Guillaume Beutier as my advisors.
  - Major research topics: Mechanics and Materials Science, Metal Physics, Crystallography, X-ray-Diffraction.
- 2008 – 2011 **Engineering degree with honors**, *Grenoble-INP PHELMMA (Physics, Electronic, Materials), Grenoble, France*.
- 1st year: Physics, Crystallography and Materials Science
  - 2nd and 3rd years: Materials Science and Engineering, specialization in materials for microelectronics and semiconductor physics.
- 2006 – 2008 **IUT Mesures Physics**, *Grenoble, France*.
- National diploma awarded after a two-year university course, specialization in material science, electrical engineering and physics.

## Research Activities

- Jan. 2022 – present **Beamline Scientist**, *CNRS, Institut Néel, QUEST (Quantum Electronic Surfaces and spin Tronics), CRG & grands instruments pole, BM02-D2AM beamline*.
- The French CRG D2AM beamline hosted by the ESRF is dedicated to in situ and operando material characterization. A wide panel of scattering techniques are available, taking advantage of two main endstations: a high precision kappa diffractometer and a X-ray scattering bench*
- Support for user experiments
    - Preparation and optimization of the experimental setup
    - Beamline alignment and fine tuning of the experiment
    - Development of python tools (scripts, notebooks, GUIs) to facilitate the on-line data treatment
    - Interpretation and discussion of the experimental results with the users
  - Development and implementation of coherence based techniques
    - Bragg Coherent X-ray Diffraction Imaging (nanoparticles, nanostructures)
    - X-ray Photon Correlation Spectroscopy (dynamic processes in polymers...)
    - Ptychography to characterize the beam properties
  - Technical / instrumental development
    - In charge of the development of new X-ray focalization (transfocator) in collaboration with several teams from Institut Néel
    - Involved in the development of the python based beamline control software (BLISS)
  - Collaboration with several researchers from the materials science and synchrotron community to tackle novel research topics and or implement novel experimental techniques or analysis methods on the beamline

- Nov. 2019 – **Postdoctoral Researcher**, CEA Grenoble, IRIG, MEM (*Modeling and Exploration of Materials*)  
 Dec. 2021 *Laboratory*, NRS (*Nanostructure Synchrotron Radiation*) Group.  
*Catalytic properties at the nanoscale probed by Bragg Coherent Diffraction Imaging (BCDI). Project in the framework of the ERC Grant CARINE of Dr. Marie-Ingrid Richard.*
- Postdoc advisor: Dr. Marie-Ingrid Richard
  - Synchrotron experiments
    - *In situ* and operando studies of the strain evolution in catalytic metallic nanoparticles using BCDI.
    - Investigation of dislocation structures in Pt nanocrystals using BCDI.
    - Study of the strain field evolution during formation and dissolution of tertiary  $\gamma'$  precipitates in a Ni based superalloy at elevated temperatures.
  - Molecular Dynamics (MD) and diffraction simulations
    - Investigation of the surface relaxation of metallic nanoparticles by coupling BCDI and MD simulations.
    - Strain evolution in L10 AuCu precipitates during the chemical ordering of a red gold alloy.
    - Numerical study: use of superstructure reflections to study coherent and incoherent precipitates using BCDI.
  - Machine Learning and Convolutional Neural Networks
    - Defect classification in nanocrystals from the analysis of Coherent X-ray diffraction (CXD) patterns.
    - Deep generative networks for diffraction inversion.
- Jan. 2019 – **Postdoctoral Researcher**, Aix-Marseille Université, IM2NP Laboratory, MNO (*Mechanics of Nano-Objects*) group.  
 Nov. 2019 Project in the framework of the ANR T-ERC Grant CHARLINE of Dr. Marie-Ingrid Richard, also using *in situ* BCDI and atomistic simulations to understand the relationship between strain fields and crystal defects and catalytic activity in metallic nanoparticles
- Postdoc advisor: Dr. Marie-Ingrid Richard
- Jan. 2019 – **Visiting Postdoctoral Researcher**, ESRF the European Synchrotron, XNP (*X-ray nanoprobe*),  
 Dec. 2021 ID01 beamline.  
*In parallel to my position at the CEA Grenoble, I was also a visiting postdoctoral researcher at the ESRF, conducting synchrotron experiments on the microdiffraction and imaging ID01 beamline.*
- Jan. 2016 – **Postdoctoral Researcher**, Paul Scherrer Institut, PEM (*Photons for Engineering and Manufacturing*) group.  
 Dec. 2018 *Development of a compact biaxial tensile testing machine for in situ studies of changing strain paths with X-Ray diffraction techniques (at third generation synchrotron beamlines) and with Scanning Electron Microscopy (SEM). Project in the framework of the ERC Grant MULTIAX of Prof. Helena Van Swygenhoven*
- Postdoc advisor & Group leader: Prof. Helena Van Swygenhoven
  - Synchrotron experiments
    - Study of the influence of biaxial loading conditions and strain path changes on the microstructural evolution of phase transforming materials, nanocrystalline materials and bicrystals during *in situ* powder and Laue diffraction.
    - Ptychographic topography experiments to image the strain fields of metallic micropillars.
  - MD and diffraction simulations
    - Study of dislocation-dislocation and dislocation-grain boundaries mechanisms in Nanocrystalline Aluminium at reduced strain rates
    - 3D Atomic-scale simulations of the interaction of a screw dislocation with a coherent twin boundary in fcc metals
      - Parametric study to investigate the influence of the material, potential and temperature on the interaction mechanism and or transmission stress
      - Influence of the loading conditions (multiaxial loading, strain path changes,...) on the interaction mechanism and comparison with boundaries containing defects

- May. 2012 – **PhD. Student**, *Université Grenoble Alpes, SIMaP Laboratory, Metal Physics (PM) group.*
- Nov. 2015 *Coherent X-ray Diffraction applied to metal physics*
- PhD supervisors: Dr. Marc Verdier and Dr. Guillaume Beutier
  - Synchrotron experiments (20 in various facilities)
    - CXD and BCDI experiments to investigate structural properties of sub-micron metallic fcc islands and nanowires and semiconductors nanowires
    - 3D ptychographic imaging and 3D BCBI of strain and defects in in situ or ex situ nanoindented gold islands and nanowires
  - MD and diffraction simulations
    - Numerical study of the signature of crystal defects in fcc nanocrystals using CXD
    - Simulation of nanoindentation of fcc nanoparticles and thin films
    - Detailed study of a bimetallic interface (Cu-Ta) by MD simulations and Density Functional Theory (DFT) calculations
- Feb. 2011 – **Master thesis**, *Nanyang Technological University, Division Physics and Applied Physics.*
- Sep. 2011 *Optimization of the performances of a Scanning Tunneling Microscope (STM) by improving nanotips preparation process and design of a new head unit dedicated to the study of superconductors under extreme conditions (UHV, Very Low Temperature, Very High magnetic field)*
- Supervisor: Dr. Alexander Paul Petrovic
  - Design of the STM head unit
  - Calibration of the STM prototype under various experimental conditions
  - Optimization of the nanotips preparation processes

## Selected Publications

- 2023 **Imaging the Breathing of a Platinum Nanoparticle in Electrochemical Environment.**  
C. Atlan, C. Chatelier, I. Martens, **M. Dupraz**, A. Viola, N. Li, L. Gao, S. J. Leake, T. U. Schüllli, J. Eymery, F. Maillard, & M.-I. Richard, *accepted in Nature Materials*
- 2023 **Anomalous glide in fcc nanocrystals.**  
M.-I. Richard, S. Labat, **M. Dupraz**, J. Carnis, L. Gao, M. Texier, N. Li, L. Wu, J.-P. Hofmann, M. Levi, S. J. Leake, S. Lazarev, M. Sprung, E. J. M. Hensen, E. Rabkin & O. Thomas, *accepted in ACS Nano*
- 2022 **Gwaihir: Jupyter Notebook graphical user interface for Bragg coherent diffraction imaging .**  
D. Simonne, J. Carnis, C. Atlan, C. Chatelier, V. Favre-Nicolin, **M. Dupraz**, S. J. Leake, E. Zatterin, A. Resta, A. Coati & M.-I. Richard, *J. Appl. Cryst.* **55**(4), 1045-1054
- 2022 **Bragg coherent diffraction imaging of single 20 nm Pt particles at the ID01-EBS beamline of ESRF.**  
M.-I. Richard, S. Labat, **M. Dupraz**, N. Li, E. Bellec, P. Boesecke, H. Djazouli, J. Eymery, O. Thomas, T. U. Schüllli, M. K. Santala & S. J. Leake, *J. Appl. Cryst.* **55**(3), 621-625
- 2022 **Imaging the facet surface strain state of supported multi-faceted Pt nanoparticles during reaction.**  
**M. Dupraz**, N. Li, J. Carnis, L. Wu, S. Labat, C. Chatelier, R. van de Poll, J.-P. Hofmann, E. Almog, S. J. Leake, Y. Watier, S. Lazarev, F. Westermeier, M. Sprung, E. JM Hensen, O. Thomas, E. Rabkin & M.-I. Richard, *Nature Comm.* **13**, 3003  
**Nature Communications Editors' Highlight section Catalysis**
- 2021 **Twin boundary migration in an individual platinum nanocrystal during catalytic CO oxidation.**  
J. Carnis, A. R. Kshirsagar, L. Wu, **M. Dupraz**, S. Labat, M. Texier, L. Favre, L. Gao, F. E Oropeza, N. Gazit, E. Almog, A. Campos, J.-S. Micha, E. JM Hensen, S. J. Leake, T. U. Schüllli, E. Rabkin, O. Thomas, R. Poloni, J. P. Hofmann, M.-I. Richard, *Nature Comm.* **12**, 5385
- 2021 **A convolutional neural network for defect classification in Bragg Coherent X-ray Diffraction.**  
*\*indicates joint first author*  
B. Lim\*, E. Bellec\*, **M. Dupraz\***, S. J. Leake, A. Resta, A. Coati, M. Sprung, E. Almog, E. Rabkin, T. Schüllli & M.-I. Richard, *npj Comp. Mat.* **7**, 115
- 2021 **Deciphering the interactions between single arm dislocation sources and coherent twin boundary in nickel bi-crystal.**  
V. Samaee, **M. Dupraz**, T. Pardoën, H. Van Swygenhoven, D. Schryvers & H. Idrissi, *Nature Comm.* **12**, 962
- 2020 **Bragg Coherent Imaging of Nanoprecipitates: Role of Superstructure Reflections.**  
**M. Dupraz**, S. J. Leake, & M.-I. Richard, *J. Appl. Cryst.* **53**(5), 135369
- 2020 **Continuous Scanning for Bragg Coherent X-Ray Imaging.**  
L. Ni, **M. Dupraz**, L. Wu, S. J. Leake, A. Resta, J. Carnis, S. Labat, et al., *Sci. Rep.* **10**(1), 12760

- 2020 **Response surface for screw dislocation - twin boundary interactions in FCC metals.**  
S. I. Rao, M. Dupraz, C. Woodward & T. A. Parthasathy, *Acta Mat.* **175**, 681-689
- 2019 **Large scale 3-dimensional atomistic simulations of screw dislocations interacting with coherent twin boundaries in Al, Cu and Ni under uniaxial and multiaxial loading conditions.**  
M. Dupraz, S. I. Rao, & H. Van Swygenhoven, *Acta Mat.* **174**, 16-28
- 2018 **Dislocation interactions at reduced strain rates in atomistic simulations of nanocrystalline Al.**  
M. Dupraz, Z. Sun, C. Brandl & H. Van Swygenhoven, *Acta Mat.* **144**, 68-79
- 2017 **3D Imaging of a dislocation loop at the onset of plasticity in an indented nanocrystal.**  
M. Dupraz, G. Beutier, T. W. Cornelius, G. Parry, R. Zhe, S. Labat, M.-I. Richard, G. A. Chahine, O. Kovalenko, M. De Boissieu, E. Rabkin, M. Verdier & O. Thomas, *Nano Lett.* **17**(11), 6696-6701  
**ESRF highlights 2017**
- 2017 **Identifying Defects with Guided Algorithms in Bragg Coherent Diffractive Imaging.**  
A. Ulvestad, Y. Nashed, G. Beutier, M. Verdier, S. O. Hruszkewycz & M. Dupraz, *Sci. Rep.* **7**(1), 9920
- 2017 **A Miniaturized Biaxial Deformation Rig for *in Situ* Mechanical Testing.**  
S. Van Petegem, A. Guitton, M. Dupraz, A. Bollhalder, K. Sofinowski, M. V. Upadhyay & H. Van Swygenhoven, *Exp. Mech.* **57**, 569-580
- 2016 **Wetting layer of copper on the tantalum (0 0 1) surface.**  
M. Dupraz, R. Poloni, K. Ratter, D. Rodney, M. De Santis, B. Gilles, G. Beutier & M. Verdier, *Phys. Rev. B* **94**, 2354277
- 2016 **Holographic imaging of magnetization in a single layer nano-contact spin transfer oscillator.**  
E. O. Burgos Parra, N. Bukin, M. Dupraz, G. Beutier, S. Sani, H. Popescu, S. Cavill, J. Akerman, N. Jaouen, P. Keatley, R. Hicken, G. van der Laan & F. Ogrin, *IEE trans. on Magn.* **52**(7), 1-4
- 2015 **Signature of dislocations and stacking faults of face-centred cubic nanocrystals in coherent X-ray diffraction patterns: a numerical study.**  
M. Dupraz, G. Beutier, D. Rodney, D. Mordehai & M. Verdier, *J. Appl. Cryst.* **48**(3), 621-644  
**Most downloaded article from Journal of Applied Crystallography of the year 2015**
- 2015 **Inversion domain boundaries in GaN revealed by Coherent Bragg imaging.**  
S. Labat, M. -I. Richard, M. Dupraz, G. Beutier, M. Verdier, F. Mastropietro, T. W. Cornelius, T. U. Schulli, J. Eymery & O. Thomas, *ACS Nano* **9**(9), 9210-9216
- 2014 **Scanning force microscope for in situ nanofocused X-ray diffraction studies.**  
R. Zhe, F. Mastropietro, A. Davydok, S. Langlais, M. I. Richard, J.-J. Furter, O. Thomas, M. Dupraz, M. Verdier, G. Beutier, P. Boesecke & T. W. Cornelius, *J. Synch. Rad.* **21**, 1128-1133
- 2013 **Holographic imaging of interlayer coupling in Co/Pt/Fe.**  
T. A. Duckworth, F. Y. Ogrin, G. Beutier, S. S. Dhesi, S. A. Cavill, S. Langridge, A. Whiteside, T. Moore, M. Dupraz, F. Yakhov & G. Van der Laan, *New J. of Physics* **15**, 023045

## Dissemination of research

### Invited talks in international conferences

- 2018 **Interaction of screw dislocations with coherent twin boundaries in fcc metals: large scale 3D simulations.**  
M. Dupraz, S. I. Rao & H. Van Swygenhoven, MMM 2018, Osaka, Japan, 26/02/2018
- 2018 **Large scale 3D atomistic simulations of the interaction of screw dislocations with a  $\Sigma 3$  CTB.**  
M. Dupraz *et al.*, Schöntal Symposium, Schöntal, Germany, 26/02/2018
- 2017 **Atomistic simulations at reduced strain rates of dislocation interactions in nanocrystalline Al.**  
M. Dupraz *et al.*, TMS 2017, San Diego, USA, 27/02/2017

### Invited seminars

- 2020 ***In situ* and *operando* structural evolution of single metallic nanoparticle model catalysts.**  
M. Dupraz *et al.*, Institut NEEL, Grenoble, France, 04/12/2020

- 2019 **Coherent X-ray diffraction to investigate nanostructures.**  
M. Dupraz *et al.*, LEM, ONERA, Chatillon, France, 25/11/2019
- 2018 **Large scale 3D atomistic simulations of dislocation interactions with bicrystalline interfaces during multiaxial loading.**  
M. Dupraz *et al.*, IM2NP, Marseille, France, 16/11/2018
- 2017 **Characterization of the microstructure of small crystals using Coherent X-ray Diffraction and atomistic simulations.**  
M. Dupraz *et al.*, University of Oxford, Oxford, United-Kingdom, 16/01/2017
- Selected contributing talks in national and international conferences**
- 2021 **Imaging the facet surface strain state of supported multi-faceted Pt nanoparticles during reaction.**  
M. Dupraz, N. Li, J. Carnis, L. Wu, S. Labat, C. Chatelier, R. van de Poll, J.-P. Hofmann, E. Almog, S. J. Leake, Y. Watier, S. Lazarev, F. Westermeier, M. Sprung, E. JM Hensen, O. Thomas, E. Rabkin & M.-I. Richard, RX et Matière 2021, Aix-en-Provence, France, 25/11/2021
- 2021 **A convolutional neural network for defect classification in Bragg Coherent X-ray Diffraction.**  
M. Dupraz, B. Lim, E. Bellec, S. Leake, A. Resta, A. Coati, M. Sprung, E. Almog, E. Rabkin, T. Schüllli & M.-I. Richard, AFC 2021, Grenoble, France, 02/07/2021
- 2021 **Three-dimensional structural imaging of defects in Pt nanocrystals.**  
M. Dupraz, M.-I. Richard *et al.*, Colloque Plasticité, Lille, France, 07/04/2021
- 2020 **Evolution of the strain field in Pt nanoparticles during CO oxidation using Bragg Coherent Imaging.**  
M.-I. Richard, M. Dupraz, L. Wu, J. Carnis, S. Labat, S. J. Leake, N. Li, R. Van de Poll, J.-P. Hofmann, M. Sprung, S. Lazarev & O. Thomas, DESY Photon Science Users Meeting 2020, Hamburg, Germany, 29/01/2020
- 2019 **Large scale 3D atomistic simulations of dislocation interactions with bicrystalline interfaces during multiaxial loading.**  
M. Dupraz, S. I. Rao & H. Van Swygenhoven, Dislocations 2019, Haifa, Israel, 19/09/2019
- 2017 **3D imaging of a dislocation loop at the onset of plasticity in an indented nanocrystal.**  
M. Dupraz, G. Beutier, T. W. Cornelius, G. Parry, R. Zhe, S. Labat, M.-I. Richard, G. A. Chahine, O. Kovalenko, M. De Boissieu, E. Rabkin, M. Verdier & O. Thomas, Euromat 2017, Thessaloniki, Greece, 20/09/2017
- 2017 **In Situ X-ray Diffraction of Al-5wt% Mg Using a Miniaturized Multiaxial Deformation Machine.**  
K. Sofinowski, M. Dupraz, S. Van Petegem & H. Van Swygenhoven, TMS 2017, San Diego, USA, 26/02/2017
- 2016 **Coherent X-ray diffraction imaging of crystal defects during nanoindentation.**  
M. Dupraz, G. Beutier, T. W. Cornelius, G. Parry, R. Zhe, S. Labat, M.-I. Richard, G. A. Chahine, O. Kovalenko, M. De Boissieu, E. Rabkin, M. Verdier & O. Thomas, Coherence 2016, St-Malo, France, 08/06/2016
- 2014 **Signature of single defects in fcc nanocrystals in Coherent-X-Ray Diffraction patterns: a numerical study.**  
M. Dupraz, Guillaume Beutier, Simon Langlais, David Rodney & Marc Verdier, XTOP 2014, Villard-de-Lans, France, 19/09/2014
- 2013 **Signature of dislocations and stacking faults in fcc nanocrystals using coherent X-ray diffraction.**  
M. Dupraz, Guillaume Beutier, Simon Langlais, David Rodney, Marc Verdier, Colloque Plasticité, Paris, France, 18/04/2013

## Awards

- 2016 "PhD prize from the Association Française de Crystallographie (AFC), Physics", for my PhD work on Coherent X-ray Diffraction applied to metal Physics

## Supervision

### Master's and Bachelor's Thesis students

- Jun. 2021 – **Licheng Xie**, *Grenoble INP, PHELMA*.  
Sep. 2021 Classification of complex defect structures in nanocrystals from the analysis of Coherent X-ray diffraction patterns using convolutional neural networks.
- Jun. 2020 – **Bruce Lim**, *Grenoble INP, PHELMA*.  
Oct. 2020 Defect classification in nanocrystals from the analysis of Coherent X-ray diffraction patterns using convolutional neural networks.  
This work was published in npj Computational Materials in 2021.
- Jun. 2020 – **Jacopo Iollo**, *Grenoble INP, ENSIMAG*.  
Sep. 2020 Deep generative networks for diffraction inversion.
- Jun. 2018 – **Todd Freeman**, *Oxford University*.  
Aug. 2018 Transmission behavior of screw dislocations with incoherent twin boundaries in FCC metals.
- Jun. 2017 – **Prune Truong**, *ETH Zürich*.  
Aug. 2017 Parametric study of the interaction between screw dislocations and a coherent  $\Sigma 3$  boundary.  
Parts of this work were published in Acta Materialia in 2019.
- Jun. 2017 – **Andrew Boardman**, *Oxford University*.  
Aug. 2017 Investigation of the interaction of dislocations with a  $\Sigma 5$  boundary using atomistic simulations.

## Teaching

- 2015 **Supervisor of 1 engineering project (10h)**, *Grenoble INP, PHELMA*.  
Failure analysis of a golf club
- 2014 **Practicals with master students (16h)**, *Grenoble INP, PHELMA*.  
Introduction to Atomic Force Microscopy (AFM)
- 2014 **Supervision of 1 research and 2 engineering project involving a small group of masters student (30h)**, *Grenoble INP, PHELMA*.
- 2013 **Practicals with master students (32h)**, *Grenoble INP, PHELMA*.  
Electromigration and electrical characterization

## Languages

French (native), English (fluent), Spanish (fair working knowledge), German (basic knowledge)

## Programming and computer skills

### Operating systems

- Advanced Linux/Unix  
Intermediate Windows

### Programming

- Advanced Python  
Intermediate Matlab  
Basic Fortran, Labview, C

### Machine learning, Convolutional Neural Networks

- Intermediate Tensorflow, Keras

### Computer Aided Design (CAD)

- Intermediate Solidworks  
Basic Catia

### Numerical Simulation (Finite Elements Modeling and Molecular Dynamics)

- Advanced LAMMPS, Ovito

Intermediate Abaqus

Basic Comsol, Ansys

High performance computing clusters / Job schedulers

Advanced SLURM

Intermediate OAR

Data analysis

Paraview, Ana, Ave, Rod, Lauetools, Qtiplo, Spip, Gwyddion, ImageJ, Gimp, Dawn, Gnuplot, X-SOCS, PyMCA, pyFAI

Synchrotron Beamlines control softwares

Advanced Spec, Bliss

Intermediate GDA