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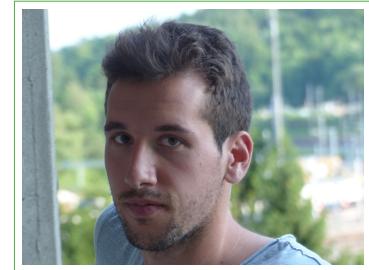
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Citations: **444**, H-index: **11**

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 PHELMA (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, taking advantage of two main endstations: a high precision kappa diffractometer and a SAXS bench. My role as a beamline scientist is to introduce new experimental techniques or analysis methods to the beamline, in addition to collaborating and providing support to researchers from the materials science and synchrotron communities to address innovative research topics.

- Support for user experiments
  - Preparation and optimization of the experimental setup
  - Beamline alignment and fine-tuning of the experiment
  - Development of python tools (scripts, python libraries, notebooks and templates, GUIs) to facilitate the online 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
- Project management, technical and instrumental development
  - In charge of the development of a new X-ray focusing device (transfocator) in partnership with several teams from Institut Néel as part of the MAGNIFIX project
  - Co-leader of the work package: "high throughput of samples & automated alignment procedures" for the CarAX@F-CRG project under the DIADEM program
  - Co-leader of the work package: "Machine learning assisted data collection and data analysis" under the NANOX-ML ANR (proposal under review)
  - Involved in the development of the python based beamline control software (BLISS)

Nov. 2019 – Dec. 2021 **Postdoctoral Researcher**, *CEA Grenoble, IRIG, MEM (Modeling and Exploration of Materials) 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 γ' 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 – Nov. 2019 **Postdoctoral Researcher**, *Aix-Marseille Université, IM2NP Laboratory, MNO (Mechanics of Nano-Objects) group.*
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 – Dec. 2021 **Visiting Postdoctoral Researcher**, *ESRF the European Synchrotron, XNP (X-ray nanoprobe), 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 – Dec. 2018 **Postdoctoral Researcher**, *Paul Scherrer Institut, PEM (Photons for Engineering and Manufacturing) group.*
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 – Nov. 2015	**PhD. Student**, *Université Grenoble Alpes, SIMaP Laboratory, Metal Physics (PM) group.* *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 – Sep. 2011	**Master thesis**, *Nanyang Technological University, Division Physics and Applied Physics.* *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. Schülli, 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. Schülli, 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. Schülli, 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. Schülli & 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. Pardoen, 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 reavealed 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. Yakhou & 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 Σ3 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. Schülli & 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 Bacherlor'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 Σ3 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 Σ5 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, Qtiplot, Spip, Gwyddion, ImageJ, Gimp, Dawn, Gnuplot, X-SOCS, PyMCA, pyFAI

Synchrotron Beamlines control softwares

Advanced	Spec, Bliss
Intermediate	GDA