CSC Joint PhD – Scientific Description
Concurrent Topology and Texture Optimisation of Anisotropic Metallic Structures Using Data-Driven Crystal Plasticity Surrogates

Thesis advisor 1	Fabrice Bernard (INSA Rennes, LGCGM EA 3913, Rennes 35700 France)
Thesis advisor 2	Balaji Raghavan (INSA Rennes, LGCGM EA 3913, Rennes 35700 France)
Thesis advisor 3	Ludovic Cauvin (UTC Compiègne, Alliance Sorbonne Universités, Compiègne 60200 France)
Collaborators (FR/EU)	Piotr Breitkopf & Salima Bouvier (UTC Compiègne, Laboratoire Roberval), Emina Hadzalic (University of Rijeka, Croatia)
Collaborators (CN)	Manyu Xiao (Northwestern Polytechnical University, Xi'an) Jianqiang Jin (Shaanxi Univ. of Technology)
Keywords	Topology optimisation · Crystal plasticity · Polycrystalline texture · Reduced-order model · Data-driven surrogate · Anisotropic metallic alloys

1. Scientific context and motivation

Structural topology optimisation (TO) determines the optimal spatial distribution of material within a design domain in order to maximise performance subject to mechanical, volumetric or manufacturing constraints. Classical TO frameworks assume an isotropic, homogeneous constitutive law — a simplification that is inadequate for the metallic alloys (aluminium, zinc, titanium, high-strength steels) used in lightweight engineering. The mechanical response of these materials is governed by crystal plasticity: the preferential activation of crystallographic slip systems depending on grain orientation and texture evolution. Neglecting this microstructural information leads to structural designs that are either unnecessarily heavy or prone to unexpected failure.

Crystal plasticity finite element modelling (CPFEM) and visco-plastic self-consistent (VPSC) homogenisation can accurately capture anisotropic plastic behaviour — including texture evolution, Bauschinger effects, and anisotropic hardening — but at a prohibitive computational cost that has, until now, prevented their direct integration within iterative optimisation loops. Bridging this gap requires two enabling technologies: (i) compact, physically admissible representations of polycrystalline texture, and (ii) fast data-driven surrogates for the crystal plasticity constitutive response.

The proposed PhD addresses precisely this challenge: to develop the first computationally tractable framework for concurrent optimisation of structural topology and local crystallographic texture in anisotropic metallic components, exploiting reduced-order modelling and manifold learning to bring the crystal plasticity fidelity inside the optimisation loop.

2. State of the art and positioning

The team's existing publications define the exact scientific boundary this PhD will cross:

- **TO with model reduction.** Xiao, Breitkopf, Raghavan et al. [1,2,3] established on-the-fly PCA-based reduced-order modelling (ROM) within large-scale TO loops, making stress-constrained 3D optimisation tractable via adaptive POD bases and primal-dual ROM strategies.
- **Crystal plasticity characterisation.** Cauvin, Raghavan, Breitkopf, Bouvier et al. [4] applied multi-scale VPSC modelling and CMA-ES inverse analysis to characterise the highly anisotropic behaviour of Zn-Cu-Ti alloys from EBSD data — directly identifying slip system parameters and predicting forming limits.
- **Data-driven texture characterisation.** Jin, Cauvin, Raghavan, Breitkopf, Xiao et al. [5] (Jin's CSC PhD thesis, UTC Compiègne) developed a data-driven paradigm for plastic anisotropy characterisation using PCA and manifold learning on orientation distribution functions (ODFs). Breitkopf, Cauvin et al. [6] further introduced Gaussian process regression with spherical-periodic kernels for ODF reconstruction.

- **Gap identified.** None of the above works integrates the data-driven texture representation into a TO design framework. The present proposal closes this gap by combining [1–3] (TO + ROM) with [4–6] (CP + texture manifold) into a single concurrent optimisation architecture.

3. Research objectives and methodology

The PhD is structured around three interlocking research axes:

Axis 1 — Compact texture representation as a design variable

Building on [5,6], the student will develop a low-dimensional parametric manifold of physically admissible polycrystalline textures. Principal component analysis on ODF snapshots — generated by VPSC simulations of target alloy deformation sequences — will yield a compact basis spanning the texture space. Gaussian process regression will enforce non-negativity and periodicity constraints inherent to ODFs. This representation transforms texture into a finite-dimensional design variable vector θ suitable for gradient-based optimisation.

Axis 2 — Data-driven crystal plasticity surrogate

A surrogate model mapping $(\rho, \theta) \rightarrow$ effective anisotropic stiffness tensor $C(\rho, \theta)$ will be trained on a database of VPSC/CPFE simulations spanning the texture manifold. Two complementary approaches will be evaluated: (i) POD-based regression, leveraging the team's established on-the-fly ROM machinery [1–3]; and (ii) physics-augmented neural network regression. The surrogate must provide not only predictions but also gradients with respect to both ρ and θ, required for adjoint sensitivity analysis in the optimisation loop.

Axis 3 — Concurrent topology and texture optimisation

The surrogate is embedded within a SIMP density-based TO framework. The optimisation problem reads: minimise compliance (or a fatigue-related objective) subject to a volume fraction constraint, over the joint design space of density field $\rho(x)$ and texture field $\theta(x)$. Adjoint equations are derived for both design variables. The method of moving asymptotes (MMA) is used as the optimiser, consistent with the team's existing TO codebase. Extensions to stress-constrained formulations and additive manufacturing texture controllability will be explored in the final year.

Target materials: Zn-Cu-Ti sheet alloy (building on [4]) as primary validation material; Ti-6Al-4V for aerospace case study.

4. Work plan

Year	Research axis	Key activities	Lead actors
Year 1	Texture representation & material database	Low-dimensional ODF parameterisation (PCA/GPR); VPSC database generation for target alloy (Zn-Cu-Ti or Ti); surrogate validation	Jin, Cauvin, Bouvier, Breitkopf
Year 2	Surrogate-in-the-loop TO	Integration of CP surrogate into SIMP/level-set loop; adjoint sensitivity derivation; 2D benchmark validation; stress-constrained extension	Raghavan, Xiao, Breitkopf
Year 3	3D concurrent geometry + texture optimisation	3D large-scale implementation with on-the-fly ROM; concurrent rho+theta design; industrial case study; dissemination	Full team (all 6 PIs)

5. Expected contributions and deliverables

- **Scientific novelty:** First TO framework coupling geometry and texture as simultaneous design variables via a data-driven CP surrogate with adjoint sensitivity.

- **Software tool:** Open-source MATLAB/Python implementation, evolution of the team's established 88/169-line TO codes.
- **Publications:** Minimum 3 journal articles (target: Structural and Multidisciplinary Optimisation; Computer Methods in Applied Mechanics and Engineering; Materials Science and Engineering A).

6. Franco-Chinese collaboration rationale

This project is a natural continuation of a productive multi-year collaboration between the French (INSA Rennes / UTC Compiègne – Roberval) and Chinese (NPU Xi'an) teams, evidenced by multiple joint publications [2,4-8].

The French side contributes crystal plasticity characterisation, manifold learning for texture, and topology optimization methodology.
Prof. Fabrice Bernard (INSA Rennes, LGCGM EA 3913), who serves as the main director of the project, brings a foundational multiscale modelling expertise that anchors the framework from the nanoscale upward. His work on atomistic simulation of crystalline phases — including characterisation of single-crystal elastic tensors and crystal morphology via molecular dynamics and density functional theory — provides a rigorous bottom-up grounding for the material parameters that feed the crystal plasticity constitutive models of Axis 2. Critically, Prof. Bernard has already demonstrated his ability to lead exactly this type of upscaling endeavour through the successful supervision of a CSC-funded PhD student (P. Wang, LGCGM, 2024), who together developed a novel molecular-dynamics-based cohesive zone model to bridge nanoscale C-S-H globule mechanics to the sub-microscale colloidal response — establishing both the methodological template and the institutional track record that the present project will build upon.

Prof. Balaji Raghavan (INSA Rennes), Prof. Manyu Xiao (Northwestern Polytechnical University, Xi'an) and Prof. Piotr Breitkopf (Universite de Technologie de Compiègne) have worked together for close to a decade, establishing themselves as reknowned authorities in Topology Optimization and machine learning.
In addition, Prof. Raghavan, Prof. Cauvin and prof. Breitkopf have worked on crystal plasticity modeling since 2018 [1-3], including the doctoral research of Prof. Jinqiang Jin.

The Chinese side brings leading expertise in large-scale TO acceleration and aerospace additive manufacturing (NPU Xi'an's State IJR Center), together with deep knowledge of the material system from Dr Jin's prior CSC-funded PhD thesis at UTC.

Prof. Jianqiang Jin (Shaanxi University of Technology) acts as a scientific bridge, having worked on both continents under this exact combination of supervisors on data-driven crystal plasticity using machine learning [2].

Prof. Emina Hadzalic (University of Rijeka), who completed her own joint doctoral thesis at the Roberval Laboratory (UTC Compiègne) on coupled inelastic constitutive modelling and failure mechanics in poro-plastic media, contributes to the project her expertise in multiscale finite element formulations and coupled multi-physics damage models, providing the team with a complementary perspective on failure initiation and structural integrity assessment

7. Key references

[1] Cauvin L., Raghavan B., Bouvier S., Wang X., Meraghni F. (2018). Multi-scale investigation of highly anisotropic zinc alloys using crystal plasticity and inverse analysis. Materials Science and Engineering: A, 729, 106–118.

[2] Jin J., Cauvin L., Raghavan B., Breitkopf P., Dutta S., Xiao M. (2024). Towards a data-driven paradigm for characterizing plastic anisotropy using principal components analysis and manifold learning. Computational Materials Science [accepted 2024].

[3] Li B., Breitkopf P., Cauvin L. (2025). Customized Gaussian process for representing polycrystalline texture. Computer Methods in Applied Mechanics and Engineering, 440, 117934.

[4] M Xiao, J Ma, X Gao, P Breitkopf, B Raghavan, W Zhang, L Cauvin, Primal–dual on-the-fly reduced-order modeling for large-scale transient dynamic topology optimization, Computer Methods in Applied Mechanics and Engineering 428, 117099

[5] Mukherjee S., Lu D., Raghavan B., Breitkopf P., Dutta S., Xiao M., Zhang W. (2021). Accelerating large-scale topology optimization: state-of-the-art and challenges. Archives of Computational Methods in Engineering, 28, 4549–4571.

[6] Xiao M., Lu D., Breitkopf P., Raghavan B., Dutta S., Zhang W. (2020). On-the-fly model reduction for large-scale structural topology optimization using principal components analysis. Structural and Multidisciplinary Optimization, 62, 209–230.

[7] Xiao M., Lu D., Breitkopf P., Raghavan B., Zhang W., Dutta S. (2020). Multi-grid reduced-order topology optimization. Structural and Multidisciplinary Optimization, 61, 1–23.

[8] Xiao M., Ma J., Lu D., Raghavan B., Zhang W. (2022). Stress-constrained topology optimization using approximate reanalysis with on-the-fly reduced order modeling. Advanced Modeling and Simulation in Engineering Sciences, 9, 17.

[9] J Claverie, S Kamali-Bernard, JMM Cordeiro, F Bernard, Assessment of mechanical, thermal properties and crystal shapes of monoclinic tricalcium silicate from atomistic simulations, Cement and Concrete Research 140, 106269

[10] J. Fu (under F. Bernard) Multiscale modeling and mechanical properties of typical anisotropic crystals structures at nanoscale, Doctoral dissertation, 2016, INSA de Rennes, France