PhD thesis opportunity

Data-driven Stochastic 3D Microstructure modeling for learning mechanical properties

Thesis directors

François Willot, Henry Proudhon

Doctoral school: ISMME - 621 – Systems, Engineering, Materials, Mechanics and Energy

Research labs and location

Centre for Mathematical Morphology, Mines Paris
Centre for Materials, Mines Paris

The two labs are located in Fontainebleau and Evry, in the south of Paris

Validity

October 1st, 2022

This PhD thesis is funded by a grant from French-German research agencies obtained in May 2021.

Web site

http://www.mat.mines-paristech.fr/Accueil/Propositions-de-theses/
https://www2.cmm.minesparis.psl.eu/nous-rejoindre/

Keywords

Microstructure; 4D imaging; Digital twin; Mechanics; Damage; Convolutional neural network; AI & Physics; Virtual materials testing

Summary

Damage localization, which leads to brittle or ductile failure in metal alloys, is a phenomenon induced by the local stress state within polycrystalline microstructures. The variety of observed mechanical behaviors results from the interactions between applied macroscopic stress and morphology within the microstructure. Combined with machine learning methods, phase-field and “FFT” numerical approaches allows one to explore microstructure-property relationships and identify structures of interest in terms of mechanical response. The aim of this thesis is to explore the relationships between polycrystalline texture and mechanical response using representative morphology simulations taking into account the wide range of grain shapes, granulometry or even polycrystalline texture encountered in real materials. To do this, a machine learning method using fast Fourier transform calculations will be implemented in order to determine configurations of

interest. The fracture behavior will be explored by statistical learning methods and classification methods will be implemented to explore the mechanical responses of γ-TiAl alloys.

Context

This thesis is part of the project “Smile” (Data-driven Stochastic 3D Microstructure modeling for LEarning mechanical properties) that benefits from a French-German funding provided by MESRI-BMBF.

It will be carried out in partnership with the Institute for Stochastic in Ulm University (V. Schmidt and M. Neumann). Regular visits and internships will be organized with Ulm University.

Thesis supervision

Thesis directors
François Willot – Centre de Morphologie Mathématique
Henry Proudhon – Centre des matériaux

The thesis will benefit from the expertise of Samy Blusseau, Volker Schmidt and Matthias Neumann.

Goal of the thesis

The objective of this research project is twofold. First, we want to assess and understand the influence of the polycrystalline microstructure on fracture, and on the ductile and brittle response of γ-TiAl alloys. Second, and more generally, we want to implement tools allowing rapid characterization and exploration of the mechanical behavior of polycrystalline structures.
The research program centers around three main tasks, 3D and 4D imaging, microstructure modeling, and the prediction and exploration of fracture by statistical learning. The second task, which concerns the simulation of virtual microstructures, will take place at the University of Ulm through a parallel thesis, which is part of the same research project, while the other two tasks will be the subject of the thesis at the Mines.
The first task concerns the acquisition and analysis of images of polycrystalline microstructures and local orientations in 3D of samples of γ-TiAl materials as well as in-situ microtomography at the synchrotron allowing access to the cracking facies in 3D+time. In the second task, polycrystalline microstructures will be characterized and virtually simulated using realistic random partition models, taking into account particle size distribution, grain shapes and crystallographic texture. On a smaller scale, the model will be completed by the addition of twining. The third task will concern the prediction of the failure behavior, performed using a combined phase-field/FFT method, the predictions of which will be compared with experimental data from two materials with distinct mechanical behavior.

Profile

Engineer and / or Master of Science – excellent level in science and general culture. Good level of English (B2 level) is required.

Essential qualities sought for for this international project, are: human qualities, communication, creativity, autonomy and adaptation, but also teaching skills, and a strong motivation for research.

We will particularly appreciate a good level in programming, numerical calculation methods and statistical learning, knowledge of mechanics.

Applicants could supply the following :
a detailed resume,
a covering letter explaining the applicants motivation for the position,
detailed exam results ,
the name(s) and contact details of persons whe may contact
an appreciation of the candidate,
your notes of M1, M2,
level of English equivalent TOEIC,
any other document establishing your qualities for this thesis

Please send your application to **francois.willot@mines-paristech.fr**

References

M. Neumann, O. Stenzel, F. Willot, L. Holzer, and V. Schmidt. Quantifying the influence of microstructure on effective conductivity and permeability: virtual materials testing. International Journal of Solid and Structures, 184:211–220, 2020.

H. Trumel, F. Rabette, F. Willot, R. Brenner, E. Ongari, M. Biessy, and D. Picart. Understanding the thermomechanical behavior of a TATB-based explosive via microstructure-level simulations. Part I: Microcracking and viscoelasticity. International Pyrotechnics Seminar, 2019. Online at https://hal.archives-ouvertes.fr/hal-02312483.

F. Willot. Fourier-based schemes for computing the mechanical response of composites with accurate local fields. C. Rend. M., 343(3):232–245, 2015.

M. Neumann, O. Furat, D. Hlushkou, U. Tallarek, L. Holzer, and V. Schmidt. On microstructure-property relationships derived by virtual materials testing with an emphasis on effective conductivity. In M. Baum, G. Brenner, J. Grabowski, T. Hanschke, S. Hartmann, and A. Schöbel, editors, Simulation Science: First International Workshop, SimScience 2017, Göttingen, Germany, April 27-28, 2017, Revised Selected Papers, pages 145–158. Springer, Communications in Computer and Information Science (CIS), Berlin, 2018.

H. Proudhon, M. Pelerin, A. King, and W. Ludwig. In situ 4D mechanical testing of structural materials: the data challenge. Current Opinion in Solid State and Materials Science, in press, 2020, https://doi.org/10.1016/j.cossms.2020.100834.

F. Willot, B. Abdallah, and Y.-P. Pellegrini. Fourier-based schemes with modified green operator for computing the electrical response of heterogeneous media with accurate local fields. International Journal for Numerical Methods in Engineering, 98(7):518–533, 2014.

J.-B. Gasnier, F. Willot, H. Trumel, D. Jeulin, and J. Besson. Thermoelastic properties of microcracked polycrystals. Part I: Adequacy of Fourier-based methods for cracked elastic bodies. International Journal of Solids and Structures, 155:248–256, 2018.

Funding

The PhD student will be employed by Armines.
Funding will be provided by ANR.

Salary: 2203 € (gross salary per month)

Contact

François Willot and Henry Proudhon

francois.willot@mines-paristech.fr
henry.proudhon@mines-paristech.fr