



DEPARTEMENT PMDM : PROCESSES METALLURGIE DURABILITE MATERIAUX

MASTER INTERNSHIP M2 PPN (5 months)

2023-2024

Title of the project: Microstructure at the interfaces in diffusion bonding: microscopic study of the grain growth, grain boundary mobility and Zener pinning.

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Laboratory / Department / Team : ICB/PMDDM/MaNaPI & M4OxE

Collaborations: This research will be developed in the context of the Equipex+ CALHIPSO: Collaborations with the Ecole des Mines (Sophia-Antipolis) and CEA (Grenoble).

Summary:

Diffusion bonding is a deformation-free solid phase joining process that can be implemented by uniaxial pressing or hot isostatic pressing (HIP). The HIP technique allows the assembly of large components with complex geometries. The components can be of different composition (heterogeneous assembly). Bonding is of better quality by HIP due to isostatic stress. One of the objectives of the Equipex+ CALHIPSO project is to understand and model the evolution of the microstructure of materials and interfaces during and after the assembly of components by HIP for industrial needs.

In the HIP process, it is important to control the microstructure in order to obtain an isotropic continuous medium with appropriate mechanical properties (fatigue and creep). A recurrent issue is the behavior of grain boundaries at interfaces. Grain boundary crossing can be inhibited by obstacles (pores, oxides and carbides). The goal is to detect the influence of the rise in temperature and the pressure on the behavior of a polycrystalline material at interfaces.

As part of this internship, we propose to adopt an atomic scale description and develop molecular dynamics (MD) simulations. This modelling allows *in-situ* investigations of metallic systems, in temperature and under pressure.

First, we will study the mobility of grain boundaries as a function of temperature and grain boundary energy. The aim is to assess the validity of empirical laws such as the Burke-Turnbull law that relates the grain size to grain boundary mobility. In a second part, we will consider defects such as pores or inclusions (carbides or oxides). This will allow us to appreciate the behavior of the grain boundaries when they encounter these defects and to detect the fine microstructure depending, for example, on the location of the defects. We will also look at Zener pinning.

Type of project (theory / experiment): theory and modelling, molecular dynamics

Required skills: A basic knowledge in materials science and statistical physics is required. A skill in numerical methods and computational languages is expected. The candidate will learn the necessary tools to develop molecular simulations with open-source software (LAMMPS). The scientific curiosity of the candidate will be appreciated.