Phase-field methods and their applications to study dislocation behavior in Ni-base superalloys

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Phase-field methods are numerical methods that allow us to describe physical, chemical and mechanical properties in a heterogeneous material seen as a continuum medium. The popularity of these methods is due to their ability to describe complex non-equilibrium processes using only a few concepts that originate from the variational formalism of the classical field theory. Models where relevant properties of a material stand on field variables that can vary in space and time punctuate history of science: van der Waals (1893), Bloch (1932), Frenkel and Kontorova (1938), Ginzburg and Landau (1950), Cahn and Hilliard (1958), etc. However, only since the 90s and the increase of computational resources have such approaches spread in the material science community as a ubiquitous tool to describe microstructural evolution.

In this presentation, I will present the main features of phase-field methods that allow for the reproduction of dislocation dynamics. As an example, I will expose some recent results on the interaction between gliding dislocations and a microscale cavity that have allowed us to characterize some fundamental mechanisms that occur during the annihilation of pores in CMSX-4 superalloys when they are treated with Hot Isostatic Pressing.

In the second part of the presentation, I will show how phase-field methods can also be used to simulate dislocation climb in interaction with a cavity. I will take this opportunity to provide details on the numerical aspects of the phase-field approaches (finite difference scheme, spectral solver…).

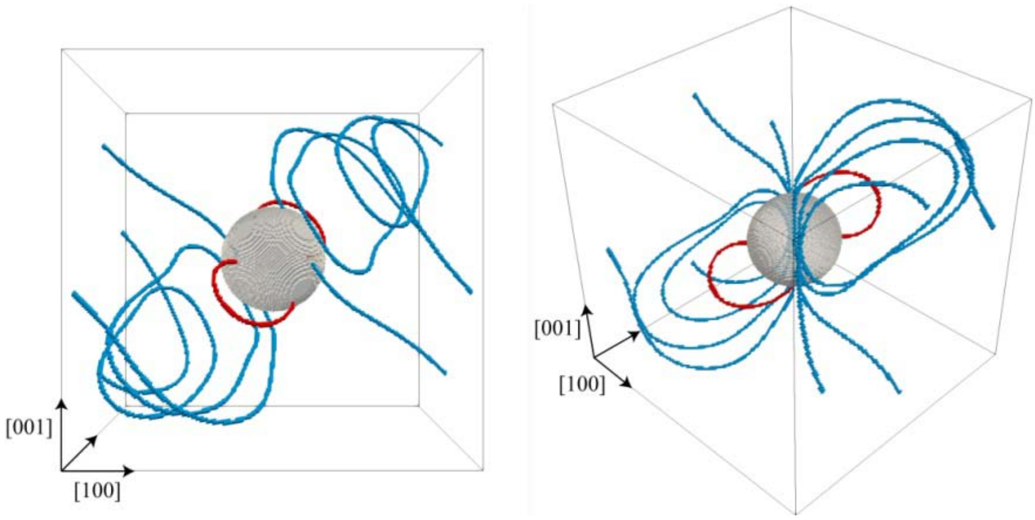

Figure 1: Phase-field simulations of gliding dislocations interacting with a pore of 3.71 micrometers radius in an elastically anisotropic FCC single crystal (CMSX-4 superalloys) under a pressure of 103 MPa.