Modelling Diffusion in Solids

TRACK 3000- COMPUTATIONAL NATURAL SCIENCES

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ABSTRACT

Diffusion in solids is a branch of science rooted in solid state physics, thermodynamics and mechanics. The implications in applied sciences and engineering are enormous, especially in the understanding of the mechanical, thermal or electrical properties of materials. Due to the nature of crystal lattices, substitutional, interstitial and self- diffusion have been widely studied by material scientists, especially for metals and alloys.

The main purpose of this mini-symposium is to give visibility to computational advances in coupled physical problems that involve diffusion of substances through solid lattices, with a special emphasis on the coupling between mechanical deformation and transport of diffusing species through a metallic lattice. Some examples of the need of modelling mass transport through solids include diffusion of lithium ions, which needs to be understood for the prediction of degradation and performance of batteries; transport of hydrogen atoms through metals is crucial for the elucidation of the embrittlement phenomenon; and the doping process of semiconductors also requires modelling diffusion of impurities.

A multi-physics approach is usually needed and continuum modelling including electro-thermo-chemo-mechanical phenomena represents a numerical challenge due to the strong coupled character, the involved non-linearities and the instability of some solutions. Coupled processes modify ideal diffusion, including stress-driven or thermo-migration terms; thus, analytical solutions from the classical fickian approach are no longer valid, requiring advanced numerical methods. The analogy between the mass transport problem and other partial differential equations, especially the prototypical heat transfer equation, can be computationally exploited by researchers to model diffusion in solids. Similarly, the analogy of the drifting terms with advection-convection phenomena can be used to apply stabilization techniques to avoid spurious oscillations. Strategies to solve numerically the continuum Fokker-Planck equation can also be followed considering its relationship with the random walk of atoms through lattices.

Continuum micro and mesoscale approaches are covered by this mini-symposium, including finite difference and finite element frameworks. Advances on different topics, e.g. discretization, integration schemes, adaptative mesh strategies, stabilization algorithms or non-linear boundary conditions, can be considered within the field of coupled diffusion modelling. Similarly, modelling schemes from damage mechanics and peridynamics are computationally challenging when coupled with mass transport equations. Multiscale approaches with homogenization methods and continuum models informed by atomistic features are also welcome, including Molecular Dynamics or Monte Carlo simulation schemes. Due to the importance of multiscale features and the associated experimental uncertainties, machine-learning and data-driven computational methods are also powerful tools for these coupled chemo-mechanical diffusion models in solids and thus suitable for this mini-symposium. Despite the focus on metals, contributions in modelling diffusion through polymers or through soft solids, e.g. gels or tissues, are also welcome.