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Computer simulations : from atoms to components

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In this contribution, multiscale simulations are performed in order to bridge the length scales from atoms to components: Atomistic Monte Carlo (MC) simulations are performed on the precipitation kinetics of multi-component Fe-Cu-Ni-Mn-systems. The formation of Cu-rich precipitates is analyzed and their morphology is compared with recent APFIM/TAP analyses. Annealing simulations are performed and details of the Ostwald ripening process is investigated. Coarsening rates are derived and compared with analytical data from the LSW theory. The interaction of edge dislocations with precipitates provides insight into the strengthening ability of the precipitates in the framework of Molecular Dynamics (MD) simulations. Furthermore, finite element (FE) based damage analyses are performed in order to understand the macroscopic behaviour of these materials.

Mardi 23 Octobre 2007 à 10h30

N.B : ***Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance - les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire - le Secrétariat du Service de leur entrée sur le Centre :***

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