Atomic scale simulations with Lammps in material science: from polymers to metallurgy

Michel Perez (INSA Lyon)

LAMMPS has been widely used at MATEIS group on all classes of materials for more than 15 years. This presentation focuses on three examples in three classes of materials: the simulation of buckling in nano-layered polymers, the formation of Cottrell atmosphere in steels and the mechanical properties of silica aerogel. Each example focuses on a particular use of lammps: *e.g.* as a library, within a new “fix” or interatomic potentials development/validation.