Multiscale Simulations of Indentation: From Atomic to Continuum

In crystalline materials, indentation induced plasticity is a rather complex phenomenon that needs to be analysed at different scales in order to fully understand the underlying physics.

At the atomic level, the contact with the indenter induces dislocation nucleations that can be simulated by molecular dynamics (MD). Although the simulated volumes are very limited in sizes (typically $(20\text{nm})^3$), MD simulations give all the details of the nucleation process in term of shape and position of the indentation induced dislocations. Such geometry can then be introduced in dislocation dynamics (DD) codes that can simulate at an upper scale (typically $(2\text{m})^3$) the evolution of the dislocation microstructure during the indentation process. These simulations require coupling DD with a finite elements method (FEM) in order to enforce the boundary conditions. Although limited in term of indentation depth (typically $100\text{nm}$), DD can be used to understand the Indentation Size Effect which denotes an increase of the hardness when the indenter depth is decreased. DD simulations also give access to the surface relief, i.e. the indentation imprint left after the indenter removal. At a higher scale FEM simulations can also simulate indentation test provided physical constitutive equations are implemented. At this scale, FEM both gives access to the indentation loading curve and to the surface imprint that can be compared to experimental data. In this presentation, indentation of FCC metals like Cu or Ni is studied using these three numerical tools as shown in figure below.