Linking Discrete Dislocations and Molecular Dynamics in 3D: a Start

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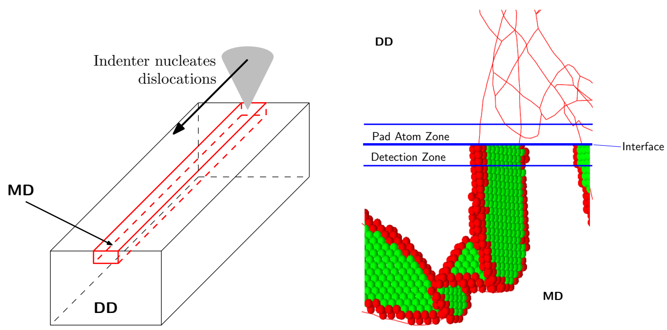
Many phenomena in crystalline metals such as friction, nano-indentation and ductile fracture are plasticity-driven and poorly understood. The physical complexity is further increased by the inherently multiscale nature of contact and fracture [1]. This study is aimed at a realistic numerical treatment of plasticity during nanoscale scratching of crystalline metal.

The principal mechanism of plasticity is dislocation nucleation and motion. Nucleation is an atomic nanoscale phenomenon and is often localised at interfaces, crack tips, etc., while dislocation motion is a microscale phenomenon occurring within grains in a polycrystalline microstructure [2]. The molecular dynamics (MD) method is able to accurately predict dislocation nucleation, however the time and length scale limitations [3] of MD do not permit for the description of the motion of entire dislocation networks. The latter are computed much more efficiently [4] with the discrete dislocation dynamics (DD) method where the details of the atomistic core are eliminated from consideration.

We present a method to extend to 3D the coupled atomistics and discrete dislocations (CADD) method [5, 6, 7]. To date, CADD has been restricted to plane strain problems with straight dislocations. In 3D CADD, the solid is split into two regions (e.g. Figure 1(a)): the MD region, where highly non-linear deformations (i.e. dislocation nucleation) and complex defect interactions are expected that require atomic resolution, and the DD region, where plastic behaviour due to dislocation motion can be computed at much lower cost. To couple these regions, the MD/DD interface (see Figure 1(b)) uses a layer in the MD region where approaching dislocations are detected and a layer in the DD region where fictitious pad atoms serve as boundary conditions for the MD region. An iterative solution permits for the tracking of dislocation lines that span the MD and DD regions, with minimal spurious forces due to the interface coupling. We apply the 3D coupling scheme to the simplest problem - motion of a straight edge dislocation under a uniform applied shear. The results will be used to show capabilities and limitations of the method, and will guide the extension to more complex problems.



(a) Separation into MD and DD

(b) Coupled representation (from [8])

Figure 1: MD-DD coupling

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