ECCM 2010
IV European Conference on Computational Mechanics
Palais des Congrès, Paris, France, May 16-21, 2010

Investigation of the size of plastic zones in nano indentation and nano scratching

T. Junge[1], J.-F. Molinari[1], W.A. Curtin[2] and J. Song[2]

[1] *LSMS, Ecole Polytechnique Fédérale de Lausanne, Switzerland, {till.junge/jean-francois.molinari}@epfl.ch*
[2] *Brown University, Providence RI, U.S.A, {William_Curtin/Jun_Song}@Brown.edu*

Friction and the associated wear are important but still poorly understood phenomena with strong impacts on our every day lives. Several mechanisms, such as plasticity, lattice vibration, and third-body interactions contribute to the dissipation of energy in friction phenomena. This physical complexity is further increased by the inherently multiscale nature of contact. Indeed, it is well known that roughness exists over multiple length scales, which imposes a multiscale numerical treatment.

Our objective in this study is to analyse the development of plastic events at contacting asperities in fcc metals. Dislocation nucleation can happen at the contact surface or – in special cases – as bulk nucleation [1] underneath the surface. We capture these dislocations by molecular dynamics (MD) modelling of the contact zones. As dislocation activity extends far away from the contact, it is not feasible to tackle this problem via MD alone. Therefore, to reduce computational cost, we resort to coupling MD to a discrete dislocation dynamics (DD) domain [2], into which MD dislocations may enter.

The coupling method used is the recently proposed coupled atomistics and discrete dislocations (CADD) method [3, 4, 5]. It has so far been implemented only in 2D and therefore effectively models asperities with an infinite third dimension (cylindrical asperities). In the first part of our presentation, we evaluate the systematic differences between 2D and 3D contact in pure MD calculations. We use this comparison to motivate 2D simulations. Finally, we present simulation results obtained at different scratching speeds for several normal forces and indenter sizes and shapes. We monitor the friction coefficient and scratching forces and relate them to the energy dissipated in the form of discrete plasticity events.

References

[1] L. Nicola, A.F. Bower, K.-S. Kim, A. Needleman, and E. Van der Giessen. Surface versus bulk nucleation of dislocations during contact. *Journal of the Mechanics and Physics of Solids*, 55(6):1120, 2007.

[2] E. van der Giessen and A. Needleman. Discrete Dislocation Plasticity - A Simple Planar Model. *Modelling and simulation in Materials Science and Engineering*, 3(5):689–735, SEP 1995.

[3] R.E. Miller, L.E. Shilkrot, and W.A. Curtin. A coupled atomistics and discrete dislocation plasticity simulation of nanoindentation into single crystal thin films. *Acta Materialia*, 52(2):271, 2004.

[4] L. E. Shilkrot, W. A. Curtin, and R. E. Miller. A coupled atomistic/continuum model of defects in solids. *Journal of the Mechanics and Physics of Solids*, 50(10):2085–2106, 2002.

[5] L.E. Shilkrot. Multiscale plasticity modeling: coupled atomistics and discrete dislocation mechanics. *Journal of the Mechanics and Physics of Solids*, 52(4):755, 2004.