Supplementary Materials:

Concurrent Multiscale Simulations of Rough Lubricated Contact of Aluminum Single Crystal

Jie Zhang [1], Lihong Su [2] and Zhongnan Wang [3,*]

[1] State Key Laboratory of Tribology, Tsinghua University, Beijing 100084, China; zj517@mail.tsinghua.edu.cn
[2] School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, Wollongong, NSW 2522, Australia; lihongsu@uow.edu.au
[3] School of Mechanical, Electronic and Control Engineering, Beijing Jiaotong University, Beijing 100044, China
* Correspondence: zhn.wang@bjtu.edu.cn; Tel.: +86-010-51683746

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Validation and comparisons between MU and full MD simulations

Following the Anciaux and Molinali's work [1], we validate our multiscale (MU) model by performing a 3D Hertz contact, benchmarked with full MD simulations. Figure S1a shows the MU model for the Hertz contact, where the filled atoms and the open atoms in the substrate are free and padded, respectively. The full MD model is presented in Figure S1b, where the filled atoms and the open atoms in the substrate are free and fixed, respectively. The tip is rigid and stepped, which was obtained by cutting a face-center-cubic (FCC) crystal according to a sphere whose radius equals 50a. The size of the substrate is 90a × 90a × 110a, which corresponds to 3,564,000 atoms in MD simulation while the substrate in Figure S1a is composed of 567,000 atoms, 32,674 nodes and 178,200 elements. The top surface of the substrate was free and the bottom of the continuum region was fixed. Along both x and y directions, the periodic boundary condition was applied. The coupling strategy between the FEM and MD has been given in the main manuscript. The description of the interactions between the atoms in the MD region and the constitutive law in the FEM region are similar with the previous work [1].

The tip was initially positioned above the substrate surface with a distance of 0.5 nm. After the whole system was relaxed for the equilibrium, the tip was moved downwards in a constant speed of 10 m/s. The timestep is 2 fs. During loading, the temperature was controlled by the Langevin thermostat every 50 steps. The Langevin thermostat was used to reduce the kinetic energy of the nodes in the continuum region. During the loading, at an interval of 200 timesteps, forces, kinetic energy, stresses were recorded.

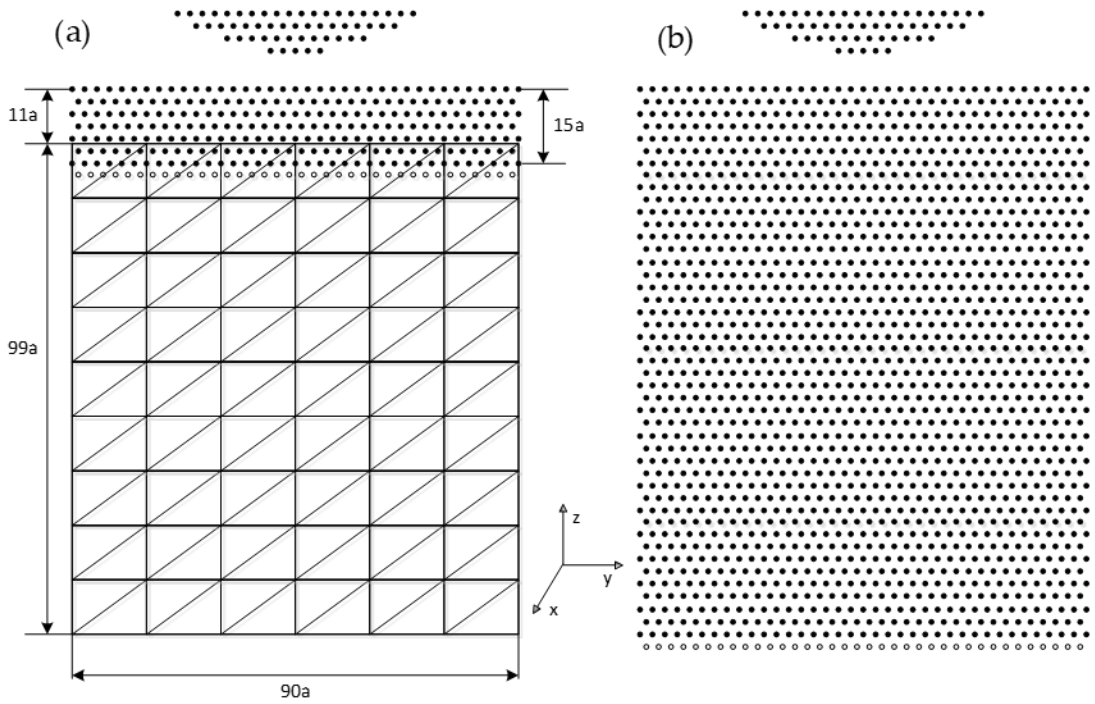

Figure 1. Geometry of the multiscale (**a**) and full MD (**b**) simulations.

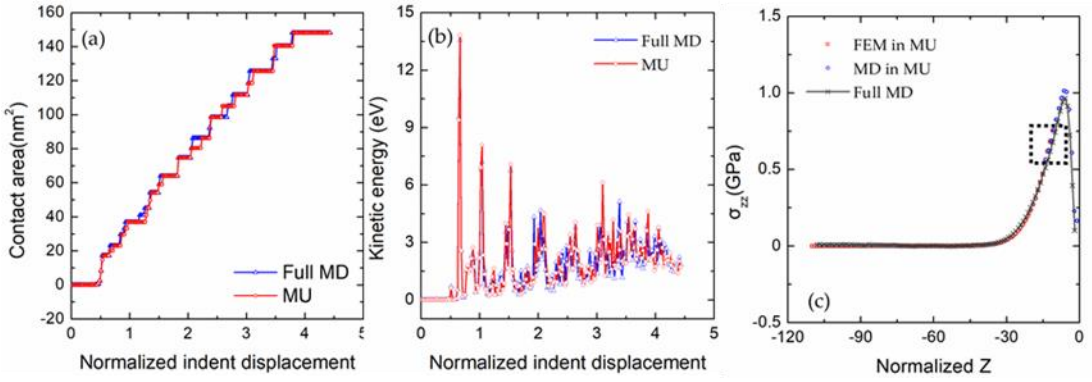

Figure S2. Comparisons between MU and full MD simulations: (**a**) Normalized contact area as a function of normalized indent displacement. (**b**) Kinetic energy near the substrate surface as a function normalized indent displacement. (**c**) Changes of stress component σ_{zz} in a line along the z direction when normalized indent displacement is 1.31a. Indent displacement and Z are normalized by lattice constant of a.

References

1. Anciaux, G.; Molinari, J.-F. Contact mechanics at the nanoscale, a 3D multiscale approach. *Int. J. Numer. Methods Engrg.* **2009,** *79*, 1041–1067.