 ICCES, vol.8, no.2, pp.81-84

Coupling Atomistic and Continuum Finite Element Models: Multi-Scale Simulations of Nanotribological Contacts of Nanometer Scale Coatings

Baolin Wang[1]

Summary

When the size of a physical system is smaller than its characteristic dimensions, the macroscopic viewpoint may not be applicable. In addition, experiments at micro/nanometer scale are difficult and the analysis of nano-experimental data is far from simple. This is mostly due to the lack of effective models that are able to study the structural characteristics and mechanics behavior of the micro/nanometer physical systems. Atomic simulation simulation has been used extensively in the investigation of nanoscale phenomena. However, the size limit of atomic simulation is far short to reach the macroscale because of the limitation in computer capacity. Therefore, the atomic simulation alone cannot predict the properties and responses of macroscopic/microscopic materials directly from their nano-structures.

On the other hand, the conventional continuum based finite element method (FEM) are not applicable to nanoscale components because they are developed for macro/microscale problems. The macro/microscale behaviors of the materials are incorporated in the conventional continuum FEM via the constitutive models of solids, which are usually determined from macroscopic experiments. These constitutive models represent the collective behavior of many atoms, and cannot accurately predict the response of discrete atoms.

Since the atomistic and continuum simulations have difficulties to investigate the material behavior at micro- and nano- scales, respectively, recently developed multiscale simulation approaches have emerged as a viable means to study materials and systems across different length scales [1-7]. Such multiscale approaches utilize the atomic simulation and the finite element method for the atomistic and continuum descriptions, respectively. The basic idea is to combine the atomistic simulation methods which capture the nanoscale physics laws with the continuum FEM which represents the collective behavior of atoms but significantly reduces the degrees of freedom [8-12].

Tribology is the science and technology of interacting surfaces in relative motion. It is of immense economic importance [13-15]. Tribology has found wide acceptance in both science and engineering. The study of rolling element bearings, seals, gears, cams, viscous dampers, human joints, and magnetic storage devices, are some of the applications in which tribology is currently used. Tribology is also

[1]Centre for Advanced Materials Technology (CAMT), School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, Sydney, NSW 2006, Australia

critical for the design of MEMS/NEMS and BioMEMS/BioNEMS [16, 17]. For example, adhesion between biological molecular layers and the substrate, and friction and wear of biological layers are important for BioMEMS/BioNEMS applications. In nanotriboligical contact of nanocoating/substrate systems, the coating and its tribological contact are at atomic scale while the much thicker substrate can be at micrometer scale. To fully understand the mechanics behavior and the role of coating/substrate interface, the atomic structure of the coating/substrate interface has to be determined by an atomistic description [18-24]. The fundamental structure of such coating/substrate system should be reflected in theoretical model. This is a multiscale problem: the nanocoatings and the heterostructure interface should be described by an atomistic model, while the much thicker substrate should be modeled by the traditional finite element method. The typical description of this multiscale approach for the nanotribological contact of a nanocoating/substrate system is shown in Fig. 1.

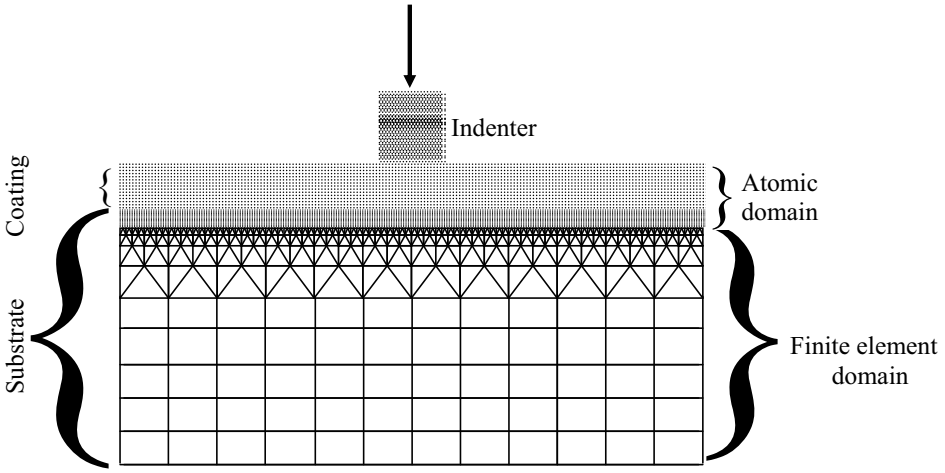

Figure 1: Atomic configuration/finite element multiscale computation of a nontribological contact (through an indenter) of a nanometer coating on a much thicker substrate (a 2-D example).

This paper contains two parts. The first part is the development of a coupling atomistic and finite element model to simulate the systems with micrometer and nanometer length scales. The second part is the application of this multi-scale coupling model to the analysis of the tribological contact analysis of a nanocoating/substrate system. In the simulation, it is important to understand that the characteristic length scales of the atomistic and continuum systems are inherently different. The atomistic system's length scale is invariably set by the bond lengths and is the same throughout the system. The continuum system's length scale, on the other hand, is set by the size of the finite elements used, and it can vary within

the system. These two systems must be properly coupled together so that their characteristic length scales will match. For this, fine meshing in the substrate towards the coating direction is made until atomistic dimensions are reached. Therefore, the finite element grid and the atomistic lattice coincide each other at the connection face between the atomic domain and the finite element domain.

In principle, both nanocoating and the much thicker substrate can be modelled by atomic model. But this is apparently not practically since the time taken for the calculation of a huge number of atoms is not affordable. The proposed atomic model, coupled with finite element method, is especially efficient for the multi-scale simulation of nanocoating/substrate systems. The approach uses the atomistic simulation methods for domains in which the discrete motion of atoms is important and must be accounted for, and use the continuum FEM for the rest part of the structure where the response of materials and systems can be represented by the continuum models. The method is introduced for reducing the degrees of freedom in simulations of mechanical behavior of materials without sacrificing important physics. By simulating nanoscale contact region, the nanocoating, and the coating/substrate interface via atomic model, more physical phenomena can be revealed than by using continuum model alone. Numerical results in this paper include the local stresses and deformations underneath the indenter and at the coating/substrate interface. Cracking mechanisms of coating and delamination of the coating/substrate interface are explored. In addition, the effects of residual stresses, coating/substrate interface adhesion strength, coating thickness, and the indentation load are also investigated.

Acknowledgement

This research is supported by Australia Research Council (#DP0346037 and #DP0665856).

References

1. S. Kohlhoff, P. Gumbsch, and H. F. Fischmeister, Philos. Mag. A 64, 851(1991).
2. E. B. Tadmor, M. Ortiz, and R. Phillips, Philos. Mag. A 73, 1529(1996).
3. J. Knap and M. Ortiz, J. Mech. Phys. Solids 49, 1899(2001).
4. O. A. Shenderova, D. W. Brenner, A. A. Nazarov, A. E. Romanov, and L. H. Yang, Phys. Rev. B 57, R3181(1998).
5. F. F. Abraham, J. Q. Broughton, N. Bernstein, and E. Kaxiras, Comput. Phys. 12, 538(1998).
6. R. E. Rudd and J. Q. Broughton, Phys. Status Solidi B 217, 251(2000).

7. E. Lidorikis, M. E. Bachlechner, R. K. Kalia, A. Nakano, P. Vashishta, and G. Z. Voyiadjis, Phys. Rev. Lett. 87, 086104(2001).
8. S. Curtarolo, G. Ceder, Dynamics of an inhomogeneously coarse grained multiscale system, Phys. Rev. Lett. 88, 255504(2002).
9. W. E, Z. Huang, Matching conditions in atomistic-continuum modeling of materials, Phys. Rev. Lett. 87, 135501(2001).
10. S. Kohlho, P. Gumbsch, H.F. Fischmeister, Crack-propagation in bcc crystals studied with a combined finite-element and atomistic model, Philos. Mag. A 64, 851-878(1991).
11. H. Rafii-Tabar, L. Hua, M. Cross, A multi-scale atomistic/continuum modelling of crack propagation in a two-dimensional macroscopic plate, J. Phys.: Condens. Matter 10, 2375-2387(1998).
12. X.T. Li and E. Weinan. Multiscale modeling of the dynamics of solids at finite temperature. Journal of the Mechanics and Physics of Solids, 53, 1650-1685(2005).
13. B. Bhushan, Handbook of Micro/Nanotribology, Second ed., CRC, Boca Raton, Florida, 1999.
14. B. Bhushan, Nanotribology and Nanomechanics-An Introduction, Springer-Verlag, Heidelberg, Germany, 2005.
15. B. Bhushan, Springe Handbook of Nanotechnology, Second ed., Springer-Verlag, Heidelberg, Germany, 2006.
16. X.D. Li, B. Bhushan, K. Takashim, C. Baekc, Y. Kim. Ultramicroscopy 97, 481-494(2003).
17. B. Bhushan. Microelectronic Engineering 84, 387-412(2007).
18. W. Yu and A. Madhukar, Phys. Rev. Lett. 79, 905(1997).
19. M. A. Cusack, P. R. Briddon, and M. Jaros, Phys. Rev. B 54, R2300(1996).
20. M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. 3 Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, Appl. Phys. Lett. 72, 1969(1998).
21. A. Omeltchenko, M. E. Bachlechner, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, Phys. Rev. Lett. 84, 318(2000).
22. C. Pryor, J. Kim, L. W. Wang, A. J. Williamson, and A. Zunger, J. Appl. Phys. 83, 2548(1998).
23. M. A. Makeev and A. Madhukar, Phys. Rev. Lett. 86, 5542(2001).
24. Y. Kikuchi, H. Sugii, and K. Shintani, J. Appl. Phys. 89, 1191(2001).