

Recent Progress in Contact Mechanics Methods for Solids with Surface Roughness Using Green's Function Molecular Dynamics

I. Solovyev¹, V. Petrenko¹, Y. Murugesan², L. Dorogin¹

¹ Saint Petersburg National Research University of Information Technologies, Mechanics and Optics (ITMO University), St. Petersburg, 197101, Russia

² Department of Industrial Engineering, University of Padova, I-35131, Italy

Received: February 11, 2022

Corresponding author: I. Solovyev

Abstract. In spite of importance of tribology of solids with surface roughness, there is no synthesized theory covering adhesion yet. One of the methods to describe adhesion in tribological systems is the Green's Function Molecular Dynamics (GFMD). This work aims at reviewing the most recent GFMD techniques and applications of GFMD in contact mechanics. There are different attributes of this method that are important for its realization: model to describe surface roughness, model to describe interfacial forces, constitutive model to describe the solid deformation and algorithm to minimize surface potential energy. We organize this review using the following set of parameters: degrees of freedom of the system modelled, substrate geometry, loading control, material properties, surface topography, interfacial interaction models.

Acknowledgements. This work was supported by the Ministry of Science and Higher Education of the Russian Federation (agreement nr. 075-15-2021-1349).

Citation: Rev. Adv. Mater. Technol., 2022, vol. 4, no. 1, pp. 1–8

View online: <https://doi.org/10.17586/2687-0568-2022-4-1-1-8>

View Table of Contents: <https://reviewsamt.com/issues>

REFERENCES

- [1] B.N.J. Persson and S. Gorb, *The effect of surface roughness on the adhesion of elastic plates with application to biological systems*, The Journal of Chemical Physics, 2003, vol. 119, no. 21, pp. 11437–11444.
- [2] L. Dorogin, A. Tiwari, C. Rotella, P. Mangiagalli and B.N.J. Persson, *Role of preload in adhesion of rough surfaces*, Phys. Rev. Lett., 2017, vol. 118, no. 23, art. no. 238001.
- [3] A. Tiwari, L. Dorogin, A.I. Bennett, K.D. Schulze, W.G. Sawyer, M. Tahir, G. Heinrich and B.N.J. Persson, *The effect of surface roughness and viscoelasticity on rubber adhesion*, Soft Matter, 2017, vol. 13, no. 19, pp. 3602–3621.
- [4] H. Zahouani, R. Vargiolu and J.-L. Loubet, *Fractal models of surface topography and contact mechanics*, Mathematical and Computer Modelling, 1998, vol. 28, no. 4, pp. 517–534.
- [5] T. Gneiting and M. Schlather, *Stochastic models that separate fractal dimension and the hurst effect*, SIAM Review, 2004, vol. 46, no. 2, pp. 269–282.
- [6] M.M. Kanafi, *Surface generator: artificial randomly rough surfaces*, 2016.
- [7] B. Persson, O. Albohr, U. Tartaglino, A. Volokitin and E. Tosatti, *On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion*, J. Phys.: Condens. Matter, 2005, vol. 17, no. 1, pp. R1–R62.
- [8] A. Duparré, J. Ferre-Borrull, S. Gliech, G. Notni, J. Steinert and J.M. Bennett, *Surface characterization techniques for determining the root-mean-square roughness and power spectral densities of optical components*, Appl. Opt., 2002, vol. 41, no. 1, pp. 154–171.
- [9] T.D.B. Jacobs, T. Junge and L. Pastewka, *Quantitative characterization of surface topography using spectral analysis*, Surf. Topogr.: Metrol. Prop., vol. 5, no. 1, art. no. 013001.
- [10] D.S. Dugdale, *Yielding of steel sheets containing slits*, J. Mech. Phys. Solids, 1960, vol. 8, no. 2, pp. 100–104.
- [11] J.H. Rose, J. Ferrante and J.R. Smith, *Universal binding energy curves for metals and bimetallic interfaces*, Phys. Rev. Lett., 1981, vol. 47, no. 9, pp. 675–678.
- [12] N. Prodanov, W.B. Dapp and M.H. Müser, *On the contact area and mean gap of rough, elastic contacts: Dimensional analysis, numerical corrections, and reference data*, Tribology Letters, 2014, vol. 53, no. 2, pp. 433–448.
- [13] M. Frigo and S.G. Johnson, *The design and implementation of FFTW3*, Proc. IEEE, 2005, vol. 93, no. 2, pp. 216–231.
- [14] C. Campañá and Martin Müser, *Contact mechanics of real vs. randomly rough surfaces: A green's function molecular dynamics study*, Europhysics Letters, 2007, vol. 77, no. 3, art. no. 38005.
- [15] S.P. Venugopalan, L. Nicola and M.H. Müser, *Green's function molecular dynamics: including finite heights, shear, and body fields*, Modelling and Simulation in Materials Science and Engineering, 2017, vol. 25, no. 3, art. no. 034001.
- [16] S.P. Venugopalan, N. Irani and L. Nicola, *Plastic contact of self-affine surfaces: Persson's theory versus discrete dislocation plasticity*, J. Mech. Phys. Solids, 2019, vol. 132, art. no. 103676.
- [17] Y. Murugesan, S.P. Venugopalan and L. Nicola, *On sub-surface stress caused by contact roughness in compressible elastic solids*, Tribology International, 2021, vol. 159, art. no. 106867.
- [18] M. Khajeh Salehani, N. Irani and L. Nicola, *Modeling adhesive contacts under mixed-mode loading*, J. Mech. Phys. Solids, 2019, vol. 130, pp. 320–329.
- [19] J.S. van Dokkum, M. Khajeh Salehani, N. Irani and L. Nicola, *On the proportionality between area and load in line contacts*, Tribology Letters, 2018, vol. 66, no. 3, art. no. 115.
- [20] J.S. van Dokkum, F. Pérez-Ràfols, L. Dorogin, L. Nicola, *On the retraction of an adhesive cylindrical indenter from a viscoelastic substrate*, Tribology International, 2021, vol. 164, art. no. 107234.
- [21] S. Sukhomlinov and M. Müser, *On the viscous dissipation caused by randomly rough indenters in smooth sliding motion*, Applied Surface Science Advances, 2021, vol. 6, art. no. 100182.
- [22] J.S. van Dokkum and L. Nicola, *Green's function molecular dynamics including viscoelasticity*, Modelling and Simulation in Materials Science and Engineering, 2019, vol. 27, no. 7, art. no. 075006.