 ICCES, vol.18, no.4, pp.117-117

Mechanics of complex surfaces by multi-scale modeling

Yan Wang[1], Weina Li[1], Jorg Weissmoller[2, 3], Huiling Duan[1]

Summary

Surface stress plays a very important role in surface morphology evolution [1-3]. Since the bonding configurations of the atoms at surfaces become different when adsorbates are situated on the surfaces, surface stress can be altered by the presence of adsorbates. Moreover, unless experiments are carried out on high quality single crystals, the surface will typically exhibit corrugation or roughness even when it is nominally planar. We have analyzed this kind of problem and pointed out that stress can be quite significantly affected by surface roughness when the microstructure scale reaches the nanometer range [4].

Therefore, we first build a theoretical model to connect the effective surface stress and the surface morphology by using the continuum mechanics method and basic capillary equations [5]. Then, molecular statics simulation is used to estimate the line stress on a rough surface with steps [6]. Finally, we established the connections between the surface stress at the continuum level and the adsorbate interactions at the molecular level for the van der Waals interaction and the Coulomb interaction [7] while the relation between surface stress and surface topology is present.

References

1. M. Godin, P.J. Williams and V.T. Cossa (2004), Langmuir, 20, 7090.

2. R. C. Cammarata and K. Sieradzki (1989), Appl. Phys. Lett. 55, 1197.

3. C. E. Bach, M. Giesen, H. Ibach and T. L. Einstein (1997), Phys. Rev. Lett., 78, 4225.

4. J. Weissmoller and H. Duan (2008), Phy. Rev. Lett., 101, 146102.

5. Y. Wang, J. Weissmuller and H. L. Duan (2010), J. Mech. Phys. Solids 58, 1552.

6. W.N. Li, H.L. Duan, K. Albe and J. Weissmuller (2011), Sur. Sci. (Revised).

7. Yi, X. and Duan, H.L., (2009). J. Mech. Phys. Solids. 57, 1254.

[1]State Key Laboratory for Turbulence and Complex System and Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, P.R. China

[2]Institut for Nanotechnologie, Forschungszentrum Karlsruhe, Karlsruhe, Germany

[3]Technische Physik, University des Saarlandes, SaarbrCken, Germany