Effect of substrate topography on mechanical properties of glassy polymer coatings

Dhiraj K. Mahajan, Fathollah Varnik, Alexander Hartmaier

Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum,

Stiepeler Str. 129, 44801 Bochum, Germany

E-mail: dhiraj.mahajan@icams.rub.de

Phone: +49 234 32 29380

Abstract

Cohesively bonded polymer-solid interfaces are essentially required for all kind of applications such as metal-polymer compound systems. A feature that characterizes these interfaces is the substrate surface roughness. It is commonly believed that surface roughness improve cohesive bonding of these compound systems. Indeed, abrading of smooth surfaces using different techniques (e.g. sand blasting, wire brushing, shot peening) forms an essential industrial step to prepare solid substrates for bonding with the polymeric material. Various theories exist, describing the cohesive strengthening of the interface due to increase in the effective area of solid-polymer contact and mechanical interlocking of the polymeric material in between surface undulations. The length scale of surface undulations varies from few nanometers up to several micrometers, similar to the characteristic dimensions of the polymeric molecules (radius of gyration, chain end to end distance). It is expected that the relative length scales of surface undulations with respect to polymer characteristic dimensions should also play an important role in strengthening the soild-polymer interface. In this work, we have specifically looked at this aspect of solid-polymer bonding using molecular dynamics simulations. A solid-polymer coating system is obtained by bonding coarse-grained polymer molecules with a solid substrate, having periodic surface undulation, using simple Lennard-Jones potential. The relative size of polymer molecules with respect to the wave length of surface undulation is varied. The compound system is then subjected to different types of loading and the stress-strain behavior is monitored. A comparison of results with similar system having planar solid substrate quantifies the role of surface roughness on cohesive bonding.