Effect of surface roughness on cohesive bonding of polymer-solid interfaces

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 kinds 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 improves 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 step in industrial processes to prepare suited substrates for bonding with the polymeric material. Cohesive strengthening of the interface is caused by an 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 solid-polymer interface. In this work, we focus on this issue via molecular dynamics simulations of a simple and generic model system. The relative size of polymer molecules with respect to the wave length of surface undulations is varied and the mechanical response as well as the structure of the polymer is investigated under different types of loading scenarios. A comparison of results with similar systems having planar solid substrate allows quantifying the role of surface roughness on cohesive bonding.