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Effect of substrate topography on adhesion properties of polymer coatings

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Cohesively bonded polymer-solid interfaces, essentially required for all kinds of applications such as protective coatings, are characterized by substrate roughness scale of few nanometers to several micrometers. While polymer conformation is essentially independent in the case of micrometer sized roughness patterns, it may be strongly influenced in the nanometer limit, when the roughness scale becomes comparable to the characteristic dimension of polymer (determined via, e.g. radius of gyration, $\boldsymbol{R_g}$). Roughness is known to strengthen the polymer-solid bonding either by increase in the effective contact area (quantified as roughness factor: $\mathrm{RF} = \mathrm{Area}_{\mathrm{rough}}/\mathrm{Area}_{\mathrm{planar}}$) or by mechanical interlocking of polymer between surface undulations. However, little is known regarding the role of relative dimensions of polymer chains with respect to surface undulations in effecting the bonding. To this end, we have performed molecular dynamics (MD) simulations to access this information. Coating systems are obtained by bonding coarse-grained polymer molecules with planar substrate and several rough substrates with periodic surface undulation. To quantify the role of roughness, the undulation features are varied in comparison to the average $\boldsymbol{R_g}$ of the polymer. The coating systems are subjected to different loading modes while monitoring their stress-strain behavior and the work of separation. We find that polymer confinement is caused by roughness features with dimensions of the order of $\boldsymbol{R_g}$. At these dimensions, mechanical interlocking in place of increase in the effective contact area appears to play a role in improving polymer bonding. Furthermore, confinement also shows the ability to switch the mode of failure from adhesive to cohesive.