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Structure of thin polystyrene films of varying tacticity adsorbed on solid substrates YERGOU TATEK, Addis Ababa University, MESFIN TSIGE, College of Polymer Science, The University of Akron — Atomistically detailed molecular dynamics simulations are used to investigate conformational properties of thin films of polystyrene (PS) adsorbed on two types of solid substrates. The substrates considered are graphite and hydroxylated silica which are known to be of different phobicity. The conformation of the PS chains was studied in terms of side chains, backbone and end group concentration and orientation. As expected, the films structure is different in all the three regions which are the two interfaces and the bulk of the film. Moreover, the film structural properties are also dependent on the nature of the substrate. We have also investigated the effect of chain tacticity on the films conformational properties. Preliminary results show the absence of a strong correlation between tacticity and structure.

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