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Structural Properties of Polystyrene Adsorbed onto a Solid Surface YERGOU TATEK, Addis Ababa University, MESFIN TSIGE, Southern Illinois University — The understanding of the structural properties of polymer layers adsorbed onto a solid surface is of paramount importance in a wide variety of technical applications. For instance, an area where surface coating is important is the solar cell technology. It has been shown that the performance of solar cells can be greatly enhanced by polymer coating. In the present work we are studying the local conformation of chains in a thin film of polystyrene (PS) adsorbed on a solid substrate by using atomistically detailed simulations. The simulations are carried out by using the readily available and massively parallel molecular dynamics code known as LAMMPS. In particular, a special emphasis is given to the density and orientation of side chains (which consist of phenyl and methylene groups) at solid/polymer and air/polymer interfaces. Three types of substrate were used in our study: α -quartz, graphite and amorphous silica. Moreover, we investigated the adsorption of PS chains of different tacticity. Our preliminary results show the presence of a peak of concentration of phenyl rings near the substrate/PS interface. This is tantamount to the existence of a local ordering in that region. Rings at both interfaces tend to point outward the film whereas rings away from the interfaces have no preferred orientation. Our results are in a large part in good agreement with previous experimental and simulation results.

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