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Effect of tacticity on the interfacial structural properties of adsorbed polystyrene thin films YERGOU TATEK, Addis Ababa University, MESFIN TSIGE, The University of Akron — We have carried out atomistic Molecular Dynamics simulations to investigate interfacial structural properties of thin films of polystyrene (PS) adsorbed onto solid substrates. The films are made of PS stereoregular chains, that are, isotactic PS or syndiotactic PS. Three types of surfaces of different phobicity and roughness were considered in the present work: hydroxylated silica, graphite and amorphous silica. The structural properties were studied in terms of side chains, end groups and backbone concentration and orientation in the interfacial regions (substrate/film and film/vacuum). Moreover the effect of temperature was investigated by adsorbing the films at different temperatures, below and above the glass transition temperature. Our results were compared to results obtained previously by our group on the adsorption of films made of atactic polystyrene.

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