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Effect of tacticity on the structure and glass transition temperature of polystyrene thin films YERGOU TATEK, SOLOMON NEGASH, Addis Ababa University, MESFIN TSIGE, The University of Akron — Detailed atomistic Molecular Dynamics simulations are performed to explore the effect of tacticity on the glass transition temperature as well as other pertinent structural properties of films of polystyrene (PS) chains adsorbed onto two distinct types of solid substrates. The investigated systems consist of thin films made of isotactic, syndiotactic and atactic PS chains adsorbed on graphite and hydroxylated silica surfaces. The structure of the films is investigated in terms of film density profiles and side chains and backbone orientations. Simulations results reveal a marked dependence of the film structure on substrate type while the absence of a strong correlation between structure and tacticity is observed. Moreover, it is found that the glass transition temperature is also substrate dependent and takes larger values for films adsorbed on graphite surface, irrespective of chain tacticity.

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