

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A Molecular Dynamics Simulation Study on the Wetting Behavior of Water on Oxidized and Non-Oxidized atactic Polystyrene Surface¹

SELEMON BEKELE, MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, Ohio — All-Atomistic Molecular dynamics simulations have been carried out to study the wetting of oxidized and non-oxidized atactic polystyrene (aPS) thin films by water droplets. The dependence of the contact angle on droplet size has been studied using spherical and hemispherical water droplets of varying sizes. The effect of oxidation of the aPS surface on the contact angle has been studied as a function of oxygen concentration. Oxidation of the aPs has been achieved by randomly replacing the ortho and/or meta hydrogen on the phenyl rings within 1 nm of the aPS surface by oxygen until the desired concentration of oxygen on the surface is reached. The simulated contact angle is found to decrease monotonically with oxygen concentration consistent with recent experimental results. We will present results on the variation of water contact angle with oxygen concentration on the aPS surface. In addition, the effect of oxidization on the roughness of the polystyrene surface, the ordering of the phenyl rings and the water molecules and the number of hydrogen bonding between water molecules and the polystyrene at the interface have been investigated and will be presented.

¹This work is supported by the NSF (DMR0847580).

Selemon Bekele
Department of Polymer Science, The University of Akron, Akron, Ohio

Date submitted: 04 Dec 2012

Electronic form version 1.4