Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Free surfaces overcome superheating in simulated melting of isotactic polypropylene[1] QIN CHEN, Department of Chemical Engineering, The Pennsylvania State University, ERIC B. SIROTA, ExxonMobil Research and Engineering, MIN ZHANG, T.C. MIKE CHUNG, Department of Materials Science and Engineering, The Pennsylvania State University, SCOTT T. MILNER, Department of Chemical Engineering, The Pennsylvania State University — The equilibrium melting point (T_m) is a challenging experimental benchmark for molecular dynamics simulation of polymer melting and crystallization. T_m obtained from melting simulation of α phase isotactic polypropylene (iPP) can exhibit superheating of over 100°C. Superheating has been attributed to the use of periodic boundary conditions and ultrafast simulated heating rates, both of which inhibit melting. We have developed a simple method to overcome superheating; we replace the periodic crystal structure with a periodic array of finite thickness slabs, separated by vacuum gaps. Thermal disorder at the slab surface promotes nucleation of the melt phase. Above T_m, we observe that the melting front advances into the crystal with a velocity proportional to $T - T_m$. This correspond to a quadratic rise in the system energy versus temperature, at constant heating rate. We obtain T_m as the onset of this quadratic rise in energy, which give values consistent with experimental melting points for iPP oligomers. The same simulations allow reasonable estimates of the crystal-vacuum interfacial free energy, from the energy difference between crystalline slabs and periodic crystals.

[1]The authors acknowledge support from National Science Foundation DMR-1507980.

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Date submitted: 04 Nov 2015 Electronic form version 1.4