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"Plunger" Method for Simulating Polymer Crystal-Melt Interfacial Tensions QIN CHEN, The Pennsylvania State University, DANIEL KOZUCH, Princeton University, SCOTT MILNER, The Pennsylvania State University — Crystal-melt interfacial free energies are important ingredients in predicting the nucleation barrier for polymers to crystallize. Experimental measurement of polymer crystal-melt interfacial tensions is extremely challenging. We propose a simple way to obtain the interfacial free energy for any polymer crystal surface and melt using molecular dynamics simulation. We measure the force on a simulated nanoscale "plunger", that restrains a melt from flowing into the gap between two crystals. This gives the difference between the crystal-vacuum and crystal-melt interfacial free energies. Separately, the crystal-vacuum interfacial free energy is obtained by measuring the force required to hold two crystals apart and integrating the force with respect to distance. We obtain the crystal-melt interfacial free energy by subtracting the above values. Results from this method applied to n-alkanes can be compared to measurements of the homogeneous nucleation barrier.

Qin Chen
The Pennsylvania State University

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