Energy Surface and Melting-Like Transition Modeling in Clusters

Anirudh Krishnadas

Department of Physics, York University, ON, Email: anirudhk@yorku.ca

Clusters with 100 or fewer atoms exhibit melting-like transitions that are fundamentally different from bulk melting. A better understanding of how clusters melt is important for applications of cluster materials in electronics and, especially, catalysis. We are developing a methodology for the simulation and analysis of cluster melting. We will describe it and show tests on argon clusters ranging in size from 10 to 55 atoms. We did classical Parallel Tempering Monte Carlo (PTMC) simulations with a 6-12 Lennard-Jones potential. The potential energy distribution E, heat capacity C_v, and a sample of cluster configurations {X_j} were obtained at different temperatures T. We determined the freezing temperature T_f and melting temperature $T_m > T_f$ with 3 independent criteria. The first is well-known: the maximum in the heat capacity curve C(T). The other two criteria are new. One is based on the width of the Potential Energy Distribution (PED). The third uses a machine-learned k-NN classifier which puts cluster geometries into solid-like and liquidlike categories. All three methods agree. For instance, they all show a solid-liquid coexistence region for Ar_{13} from 26K to 42K. We will discuss the computational, and conceptual, advantages of having three independent ways for estimating T_f and T_m.