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Molecular Dynamics Simulations of Melting of Nitromethane Initiated at Crystal-Rare Gas Interfaces GANESH KAMATH, University of Missouri-Columbia, ALI SIAVOSH-HAGHIGHI, University of North Texas, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia —
The melting of nitromethane initiated at the (100), (010), and (001) crystallographic faces in contact with rare gases at pressures over the interval 1 kbar to 16 kbar has been investigated using molecular dynamics simulations with an all atom force field. Simulations were performed to evaluate the melting point of nitromethane crystal in contact with He, Ar, and Kr. The calculated melting curve is in good agreement with experiment and previous simulation results. The molecular-level mechanism of melting initiated at a crystal surface in contact with rare gas was compared with that for melting at the bare crystal surface and void-nucleated melting. Orientational disordering of the molecules at the melt front precedes the onset of translational freedom of molecules both at the crystal-fluid interface and in the core of the crystal. There is an increase of the time gap between the occurence of molecular reorientation and translational mobility in the nitromethane molecules. The predicted melting points for nitromethane in contact with He, Ar, and Kr are within 20 K of each other for all state points and can be correlated to the diffusion of the rare gas atoms into the nitromethane crystal. The diffusion of rare gas atoms into the crystalline solid eliminates the dependence of melting temperature on the crystallographic orientation reported previously for melting at bare surfaces.

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