Velocity Dependency of Ice Melting at Polymer Interfaces: A Molecular Dynamics Investigation

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The quasi-liquid layer (premelting layer) formed on ice surfaces is a decisive factor governing interfacial properties such as friction and adhesion. However, the influence of the chemical characteristics of contacting polymer materials and dynamic sliding conditions on the molecular structure of this layer remains largely unexplored. In this study, we employed all-atom molecular dynamics simulations to analyze the melting behavior at the interface between ice (TIP4P/Ice model) and three polymers: hydrophobic polystyrene (PS) and hydrophilic polyethylene oxide (PEO) and polyvinyl alcohol (PVA). Static density distribution analysis revealed that hydrophilic polymers (PEO and PVA) significantly promote ice melting, inducing interfacial disorder characterized by the penetration of water molecules into the polymer matrix.

Furthermore, dynamic simulations conducted at shear velocities ranging from 0.04 to 0.9 m/s revealed a unique velocity dependence in frictional characteristics and interfacial heat transport. In the low-velocity regime (below 0.1 m/s), frictional heating enhanced the evolution of the premelting layer, leading to an increase in interfacial temperature. In contrast, at higher velocities, the interfacial temperature unexpectedly decreased. These findings suggest that controlling polymer hydrophilicity and sliding velocity is critical for optimizing tribological performance on ice surfaces, offering fundamental insights for the development of advanced ice-contacting materials.

Keywords:
Molecular Dynamics, Ice Friction, Interfacial Melting, Velocity Dependence, Polymer Hydrophilicity

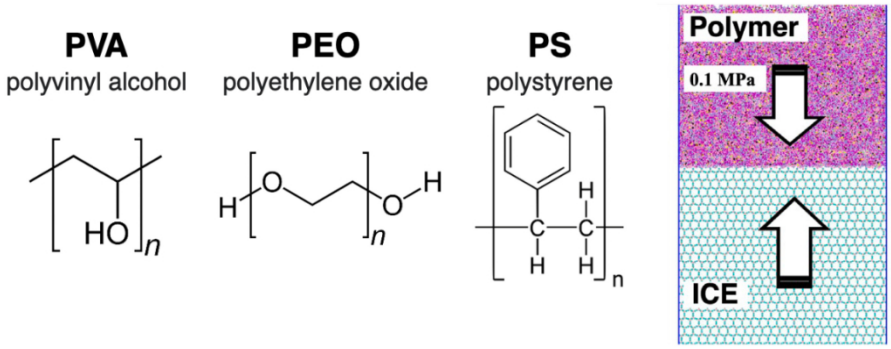

Fig. 1 Initial configuration

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