

---

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

## [PO-A2]Poster Session 2

Symposium A

2018年10月31日(水) 17:45 ~ 20:00 Poster Hall

---

### [P2-05]A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang (East China Normal University, China)

We present a substantial atomistic simulation study of the equilibrium surface tension for liquid-state binary alloy systems. Four types of spherical surface/interfaces are investigated: liquid Pb droplet embedded in bulk liquid Al, liquid Al droplet in bulk liquid Pb, a bubble in liquid state Pb-Bi eutectic (LBE) and a LBE droplet. The surface tension for these non-planar surfaces are calculated based on the calculation of the local pressure tensor in spherical coordinates. Several thermodynamics property (droplet size, temperature, capillary pressure, mutual miscibilities) dependencies of surface tension are obtained. Our results provide useful input data for the mesoscale simulations of the selective laser melting, advanced welding and bubble formation in nuclear coolants.