异质固液界面的预熔化相变及其更低维度的相变前驱

Heterogeneous Solid-Liquid Interfacial Premelting and Its 2d Precursor

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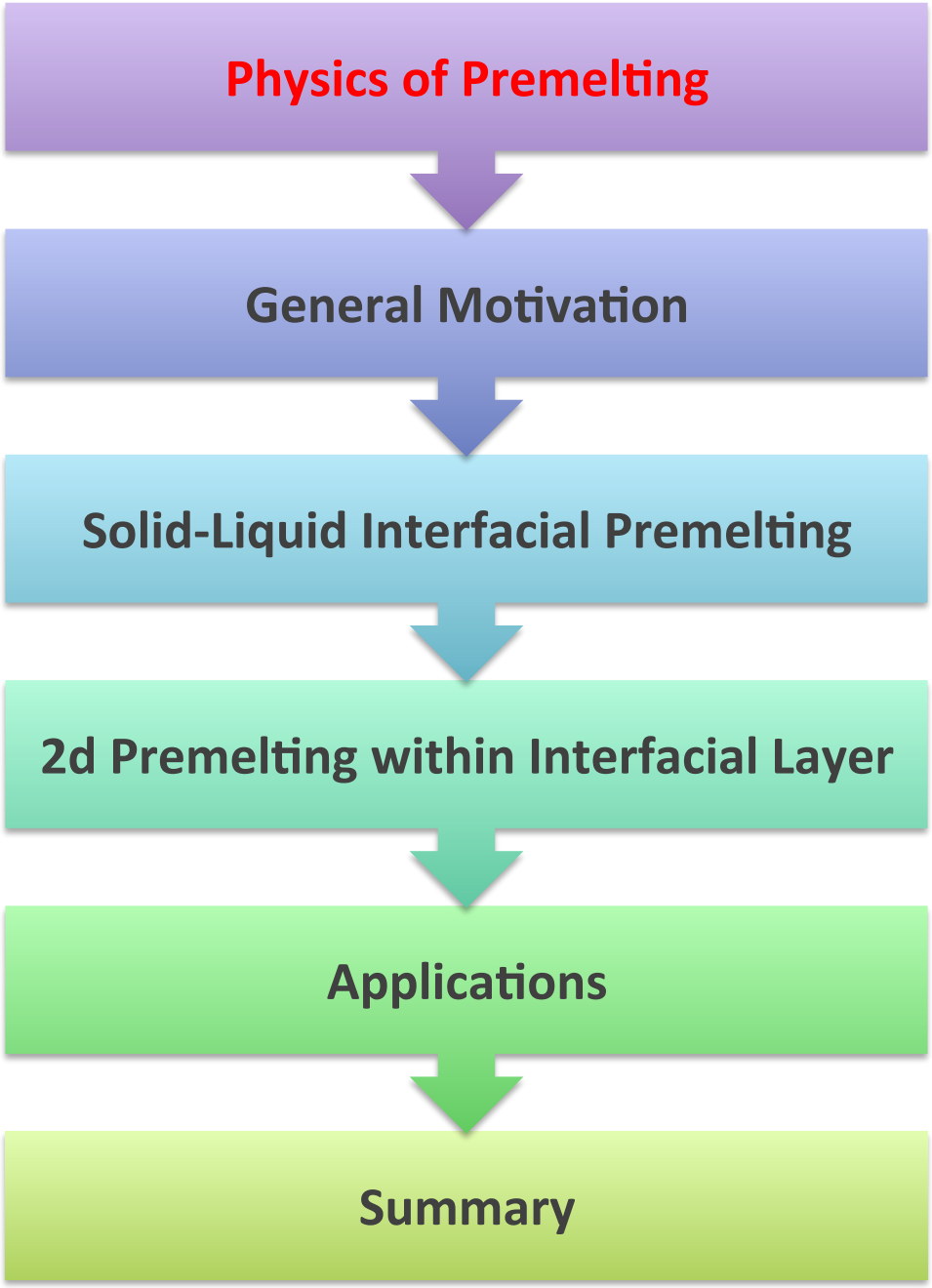
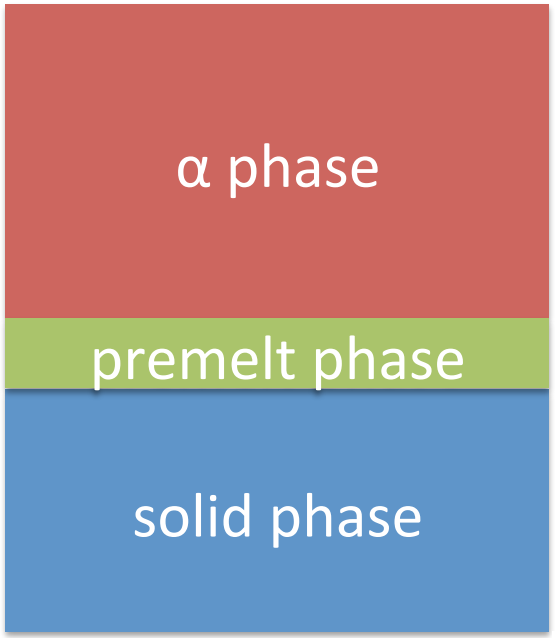

Physics of Premelting
General Motivation
Solid-Liquid Interfacial Premelting
2d Premelting within Interfacial Layer
Applications
Summary

Interfacial Premelting Transitions

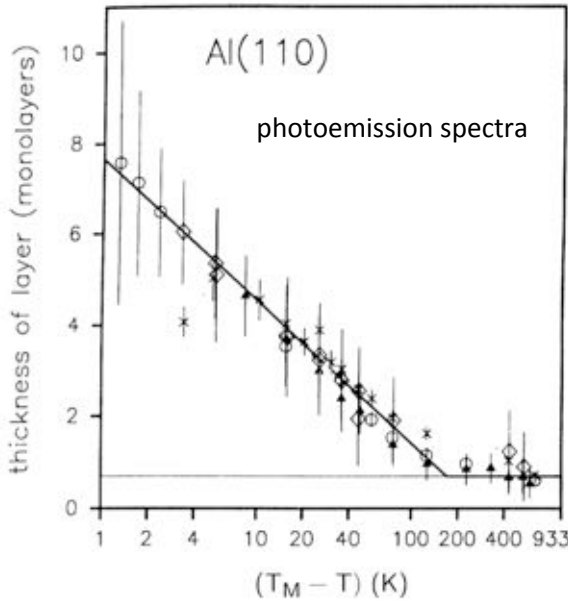


$$G(w) = w\Delta G_f + \gamma_{sl} + \gamma_{l\alpha} + \boxed{\Delta\gamma \exp(-w/\delta)}$$

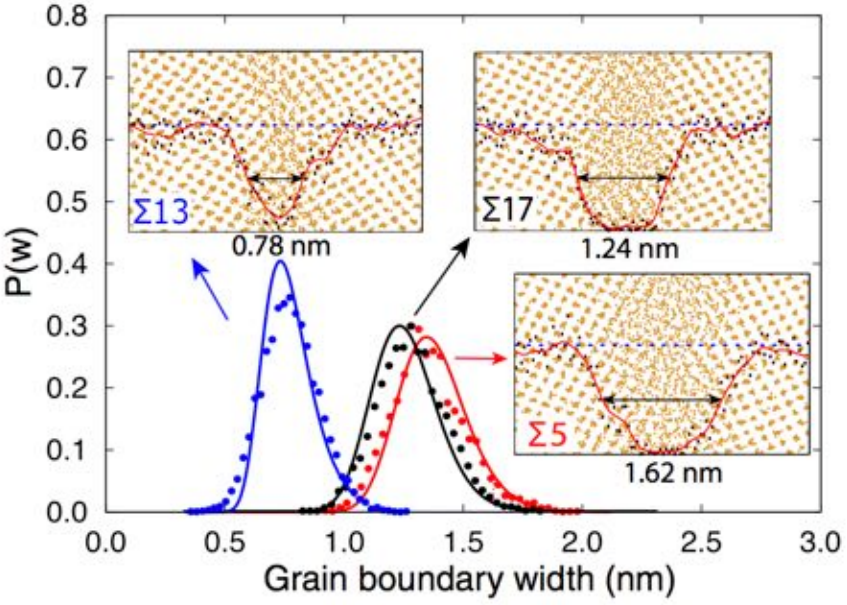
$$\Delta\gamma = \gamma_{s\alpha} - [\gamma_{sl} + \gamma_{l\alpha}]$$

$$P(w, T_i) = C_i \exp[-A_i G(w, T_i)/k_B T_i]$$

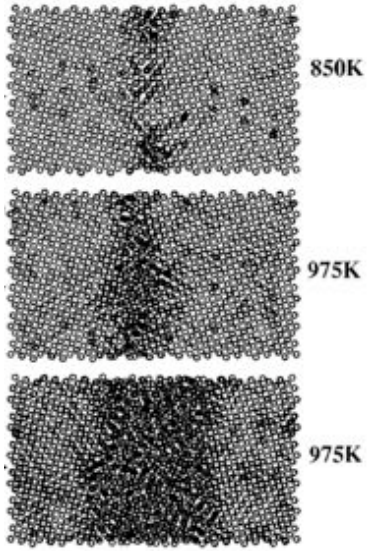
$$\frac{\partial G(w)}{\partial w} = 0 \quad w = w_0 \ln T_0 - w_0 \ln(T_m - T)$$



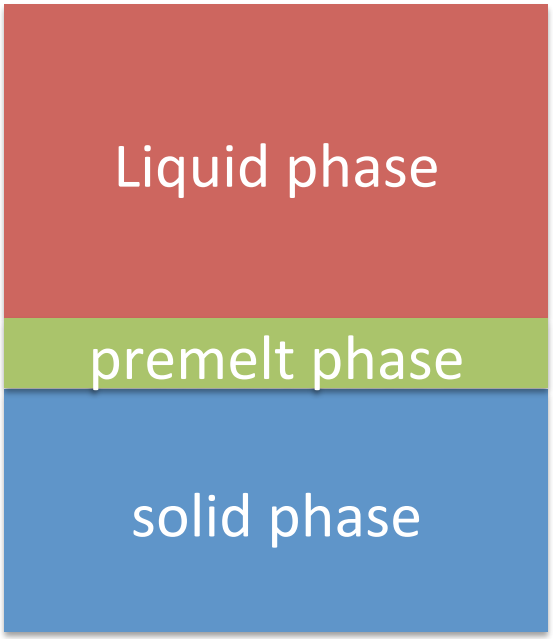
W. Theis, *PRB* (1995)

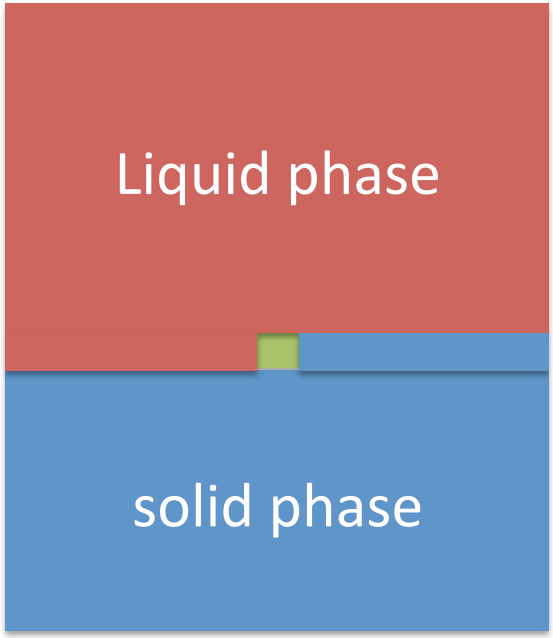


Y. Mishin, *PRB* (2016)

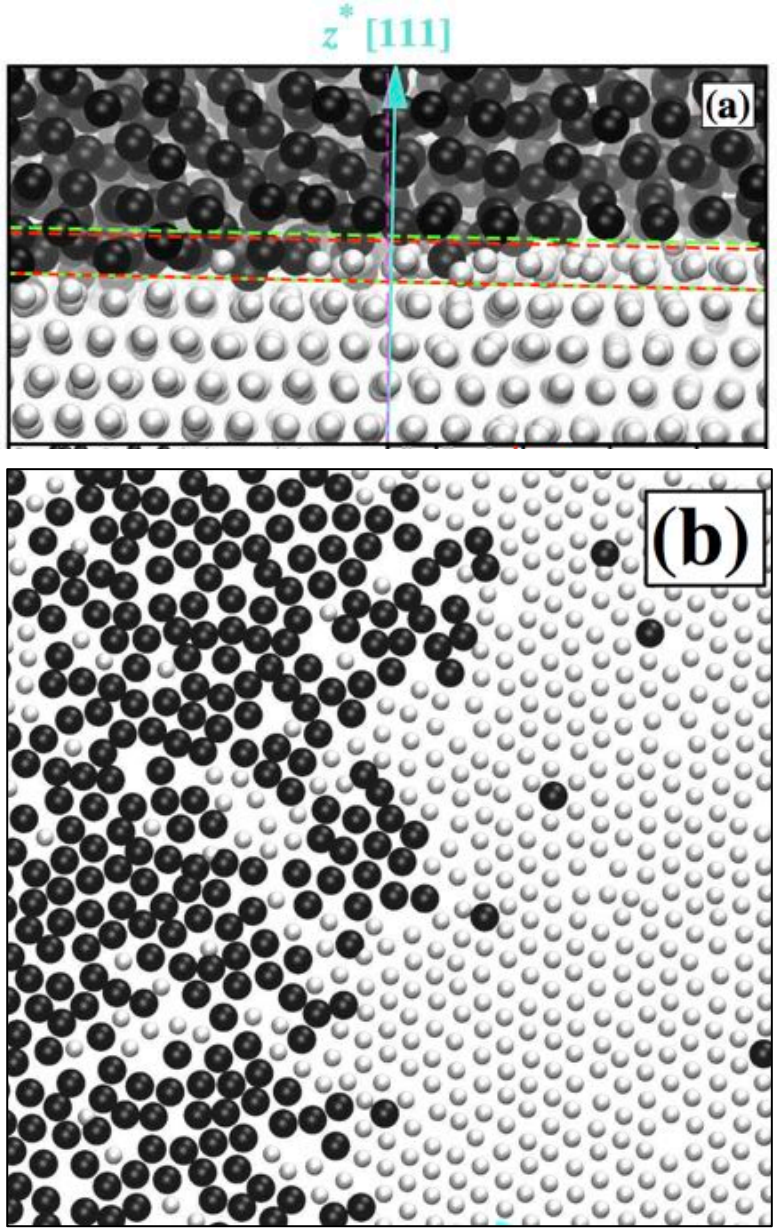


W. Fan and X. G. Gong, *PRB* (2005)

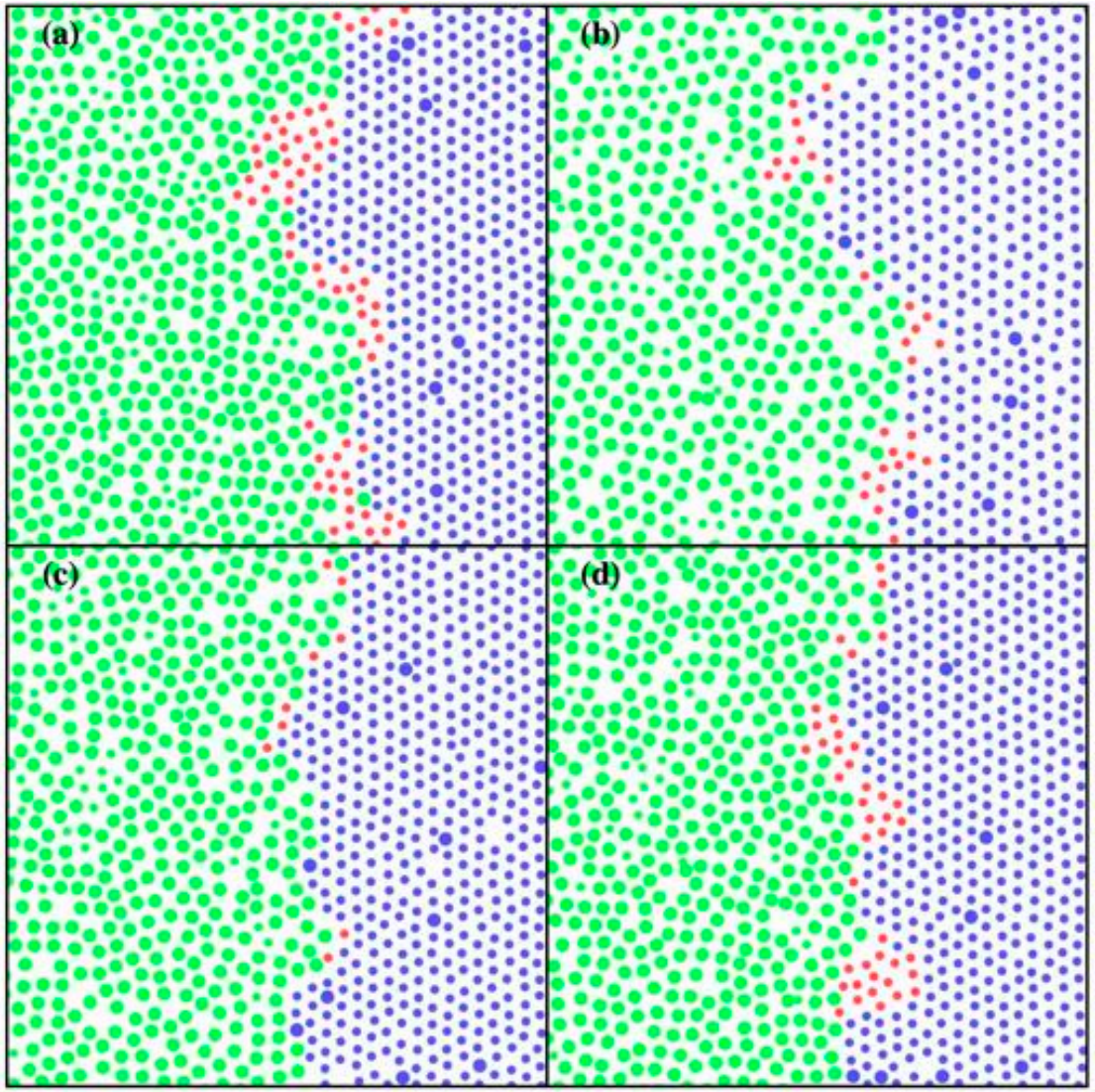

Liquid phase
premelt phase
solid phase


Liquid phase
solid phase

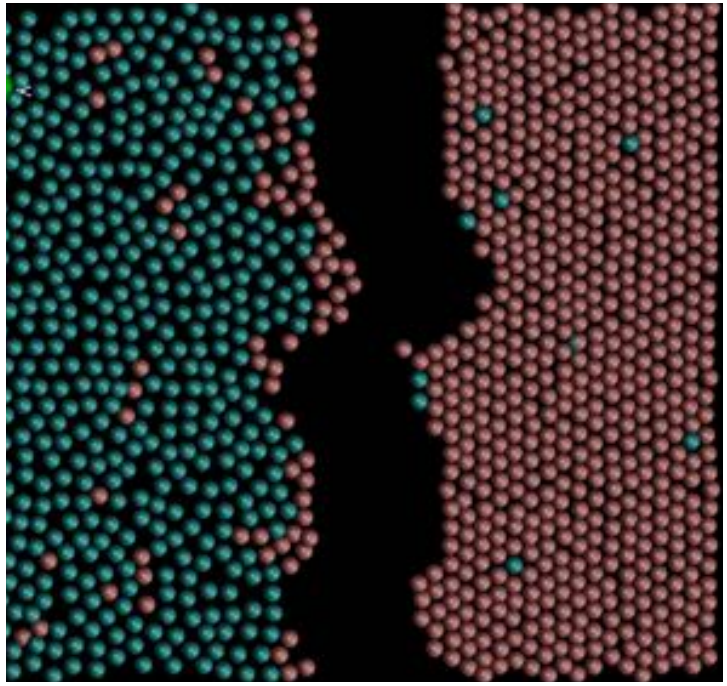
Disordering at In-plane Step-Liquid Coexistence Line

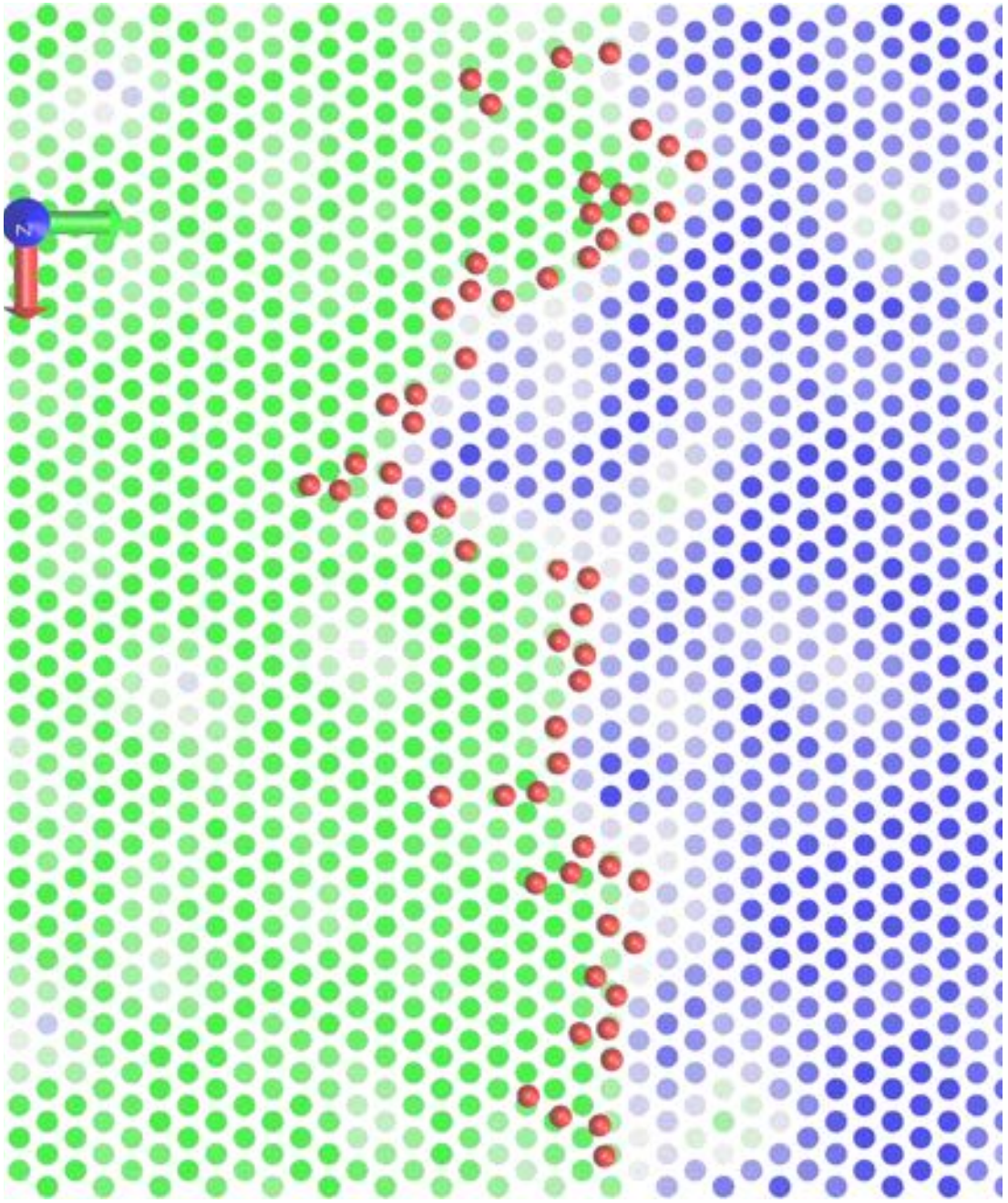


[111] interfacial step-liquid coexistence 2d plane.



Disordering at In-plane Step-Liquid Coexistence Line

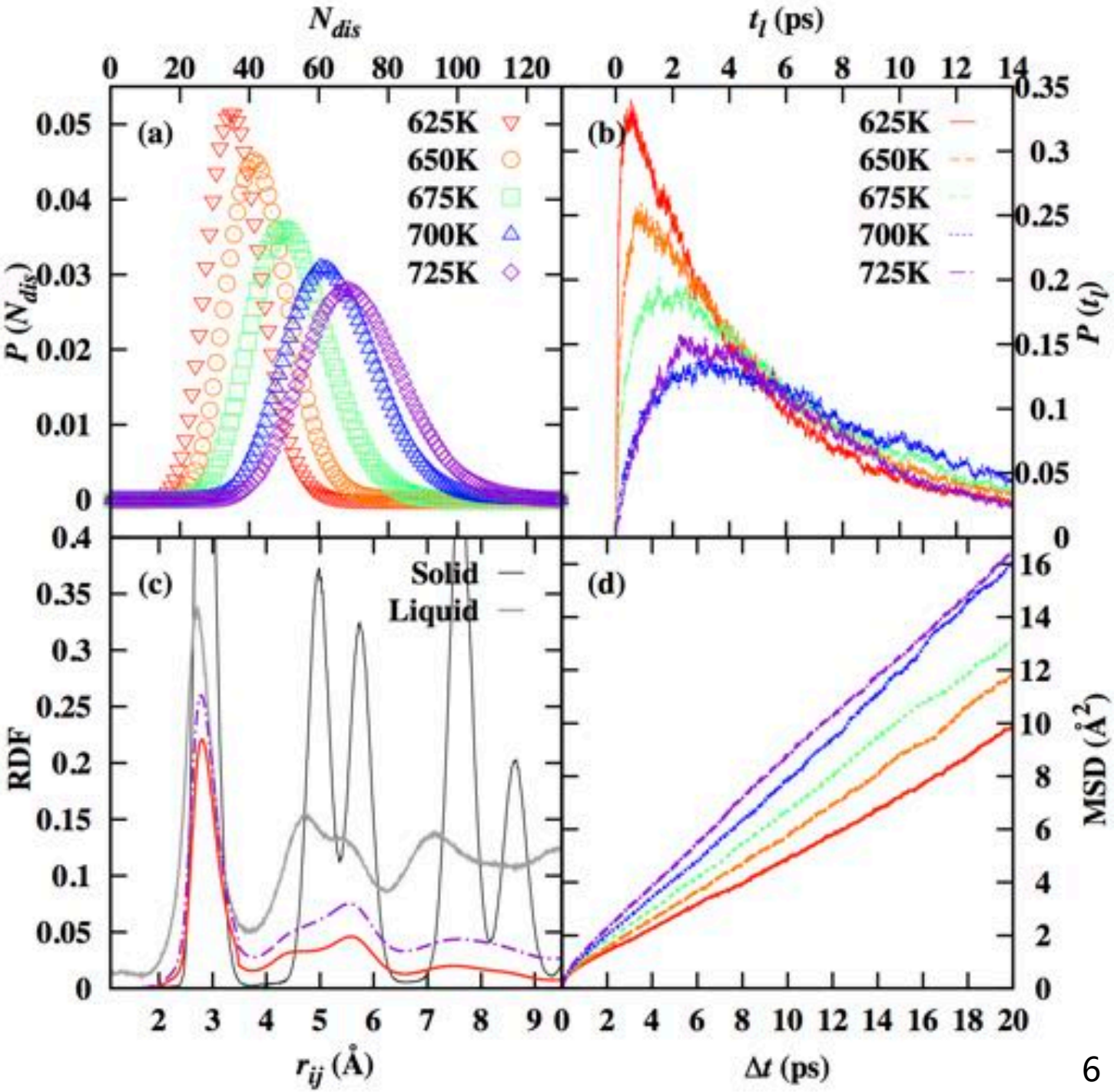




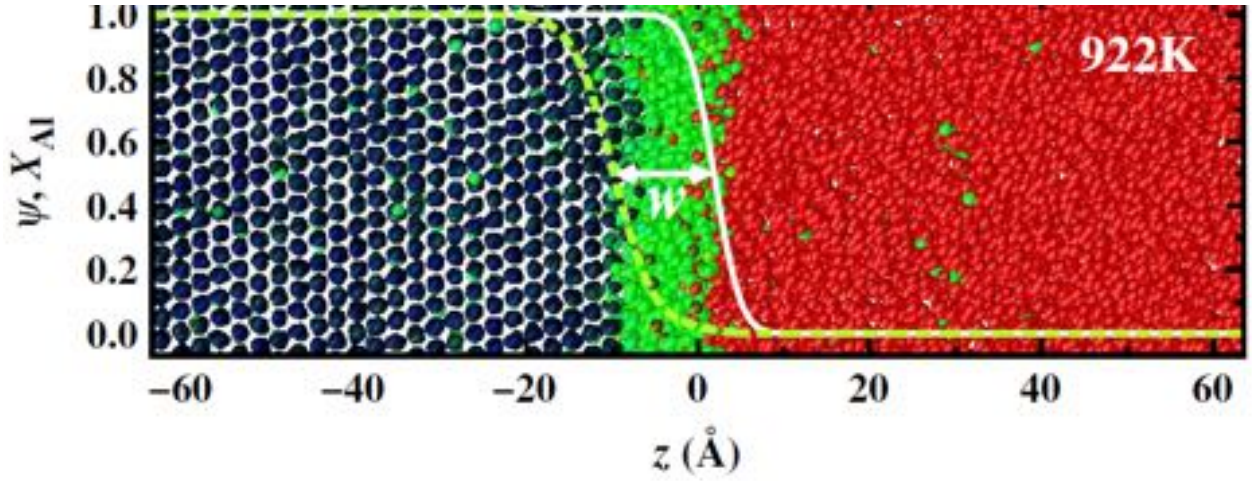
- Along with step boundary is fluctuating.
- Ultrafast (ps) disordering and recrystallization of the Al atom clusters at step boundary Al.
- Note, T is 300K below the Tm of Al.

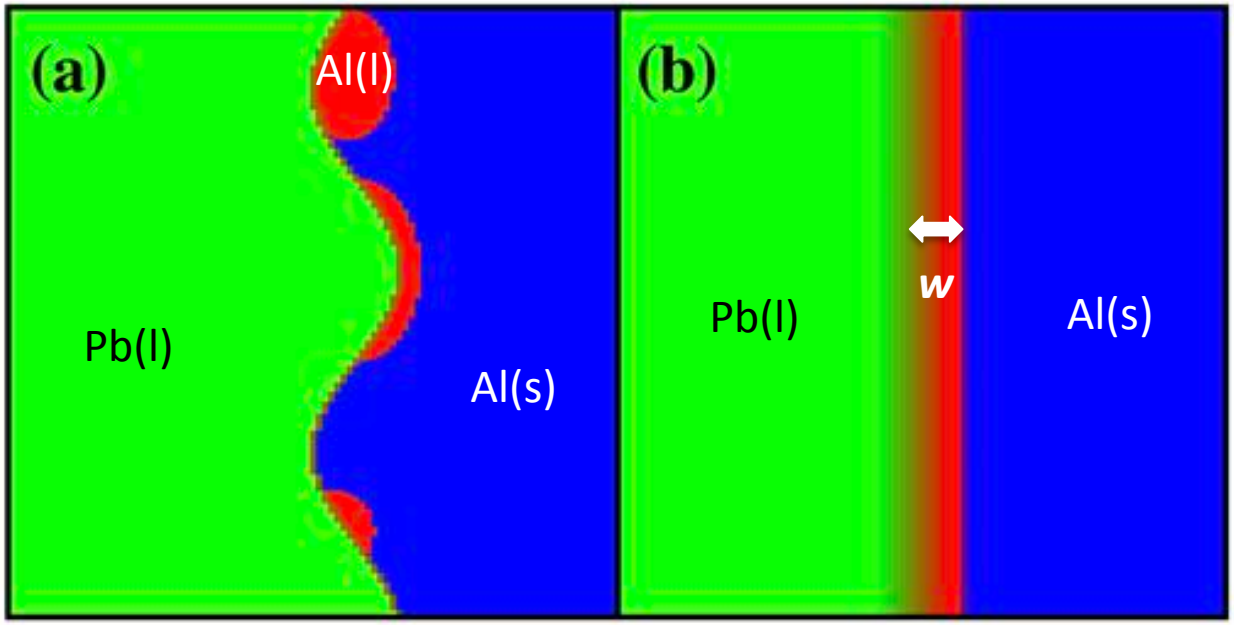
Question : Is this premelting transition? Why it happens under such low T?

- More disordering with T increases
- Life time is short, ps.
- Disordering Al atoms behaves similar to liquid.



$$G(w) = w\Delta G_f + \gamma_{sl} + \gamma_{l\alpha} + \boxed{\Delta\gamma \exp(-w/\delta)}$$





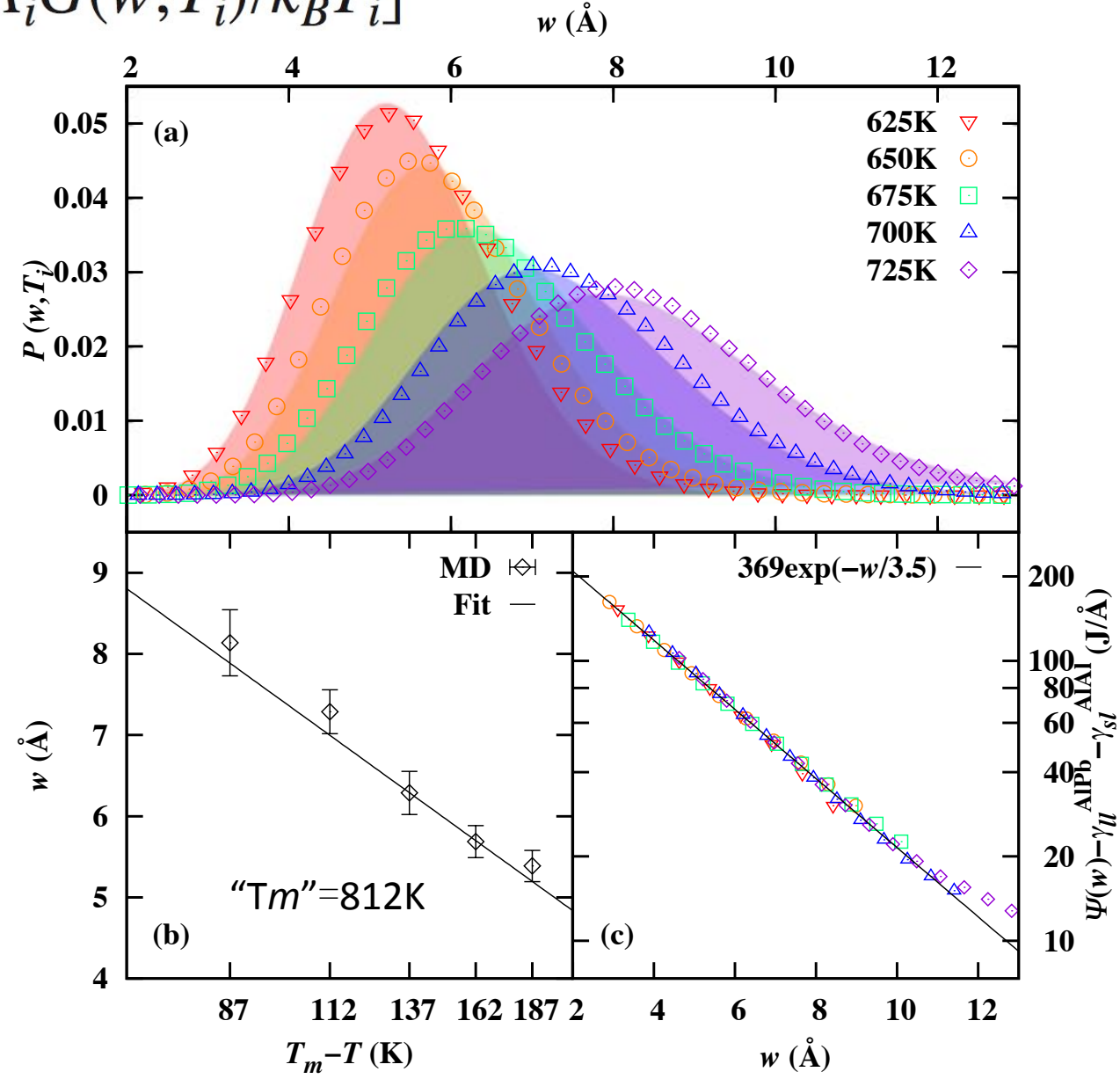
- Define the width of the premelting “film”, under an intrinsic perspective.

$$G(w) = w\Delta G_f + \gamma_{sl} + \gamma_{l\alpha} + \boxed{\Delta\gamma \exp(-w/\delta)}$$

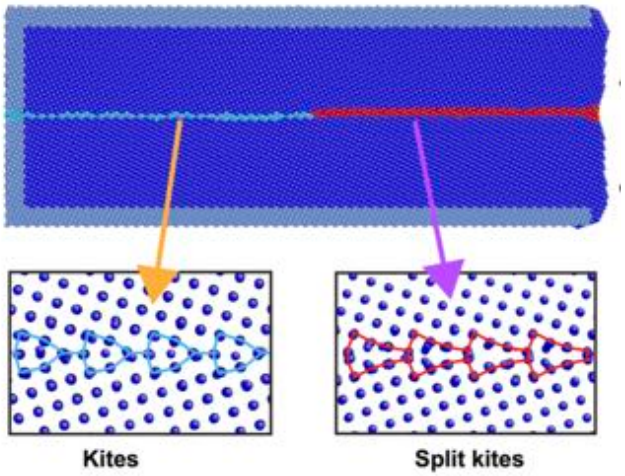
$$P(w, T_i) = C_i \exp[-A_i G(w, T_i)/k_B T_i]$$

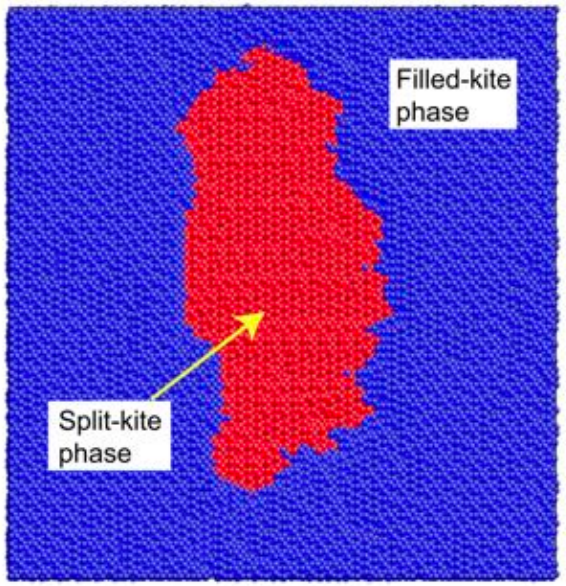
- Logarithmic dependence of *w* with respect to undercooling.
- The distribution probabilities of the premelting width at different *T*, follows the scaling relationship of the exponential decay of the disjoining potential.

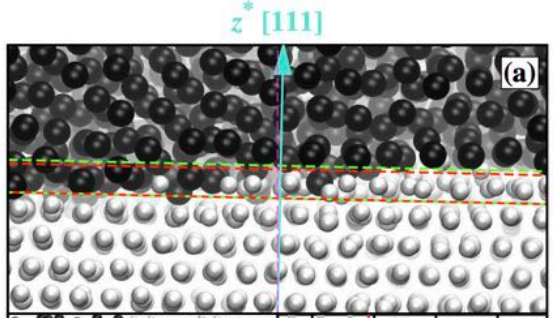
Indicating the novel disordering of the Al at step boundaries hold the nature of the premelting transition.

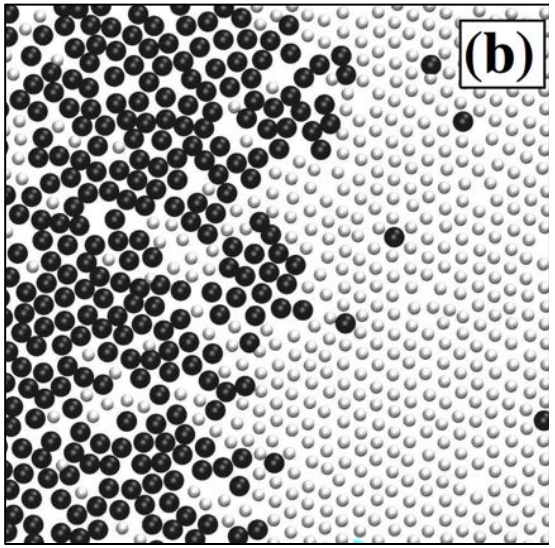


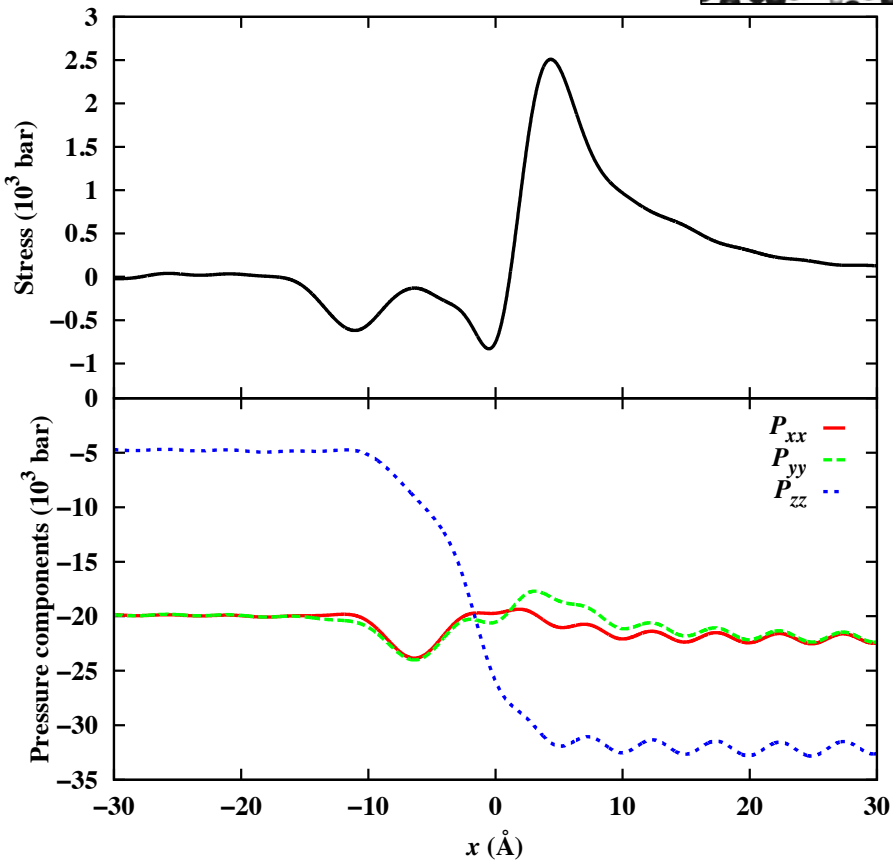
- Consistent with the concept of interfacial phase diagram.





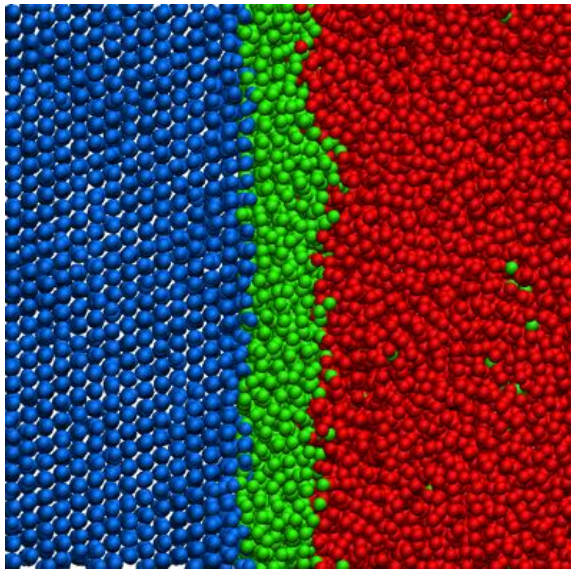


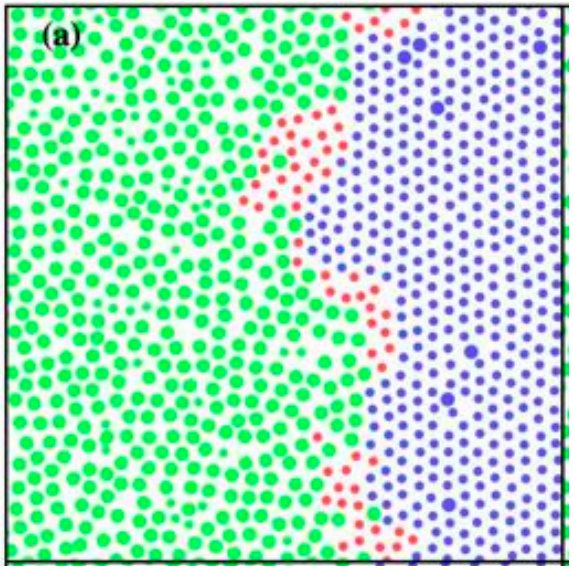


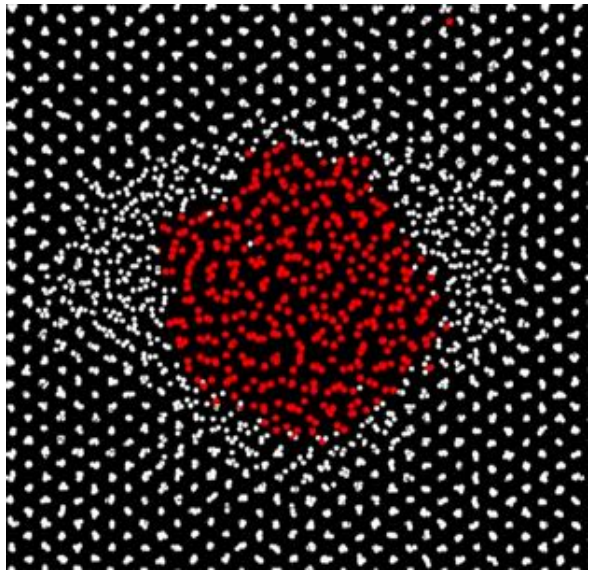


Interfacial layer pressure components are different from which hold in bulk liquid and solid "T*m*"=812K

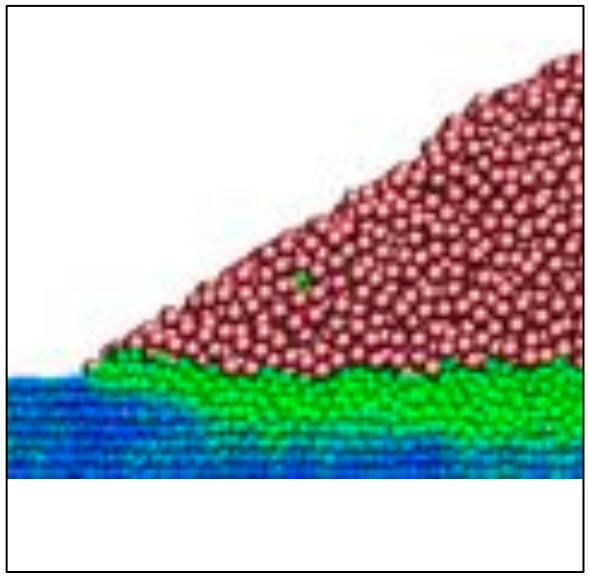
Summary







1. MD simulation predicted premelting transition in heterogeneous solid-liquid Al-Pb interface.
2. Found in-plane rapid disordering of the Al boundary, hold the premelting nature.
3. MD study of Pb liquid inclusion in Al matrix and spreading/wetting behavior with premelting transition.



Thank You for Your Time and Attention !

Have a Wonderful Day !