Thermodynamic calculation for surface melting of macro-crystals and melting of nano-crystal for Al, Cu and Ag

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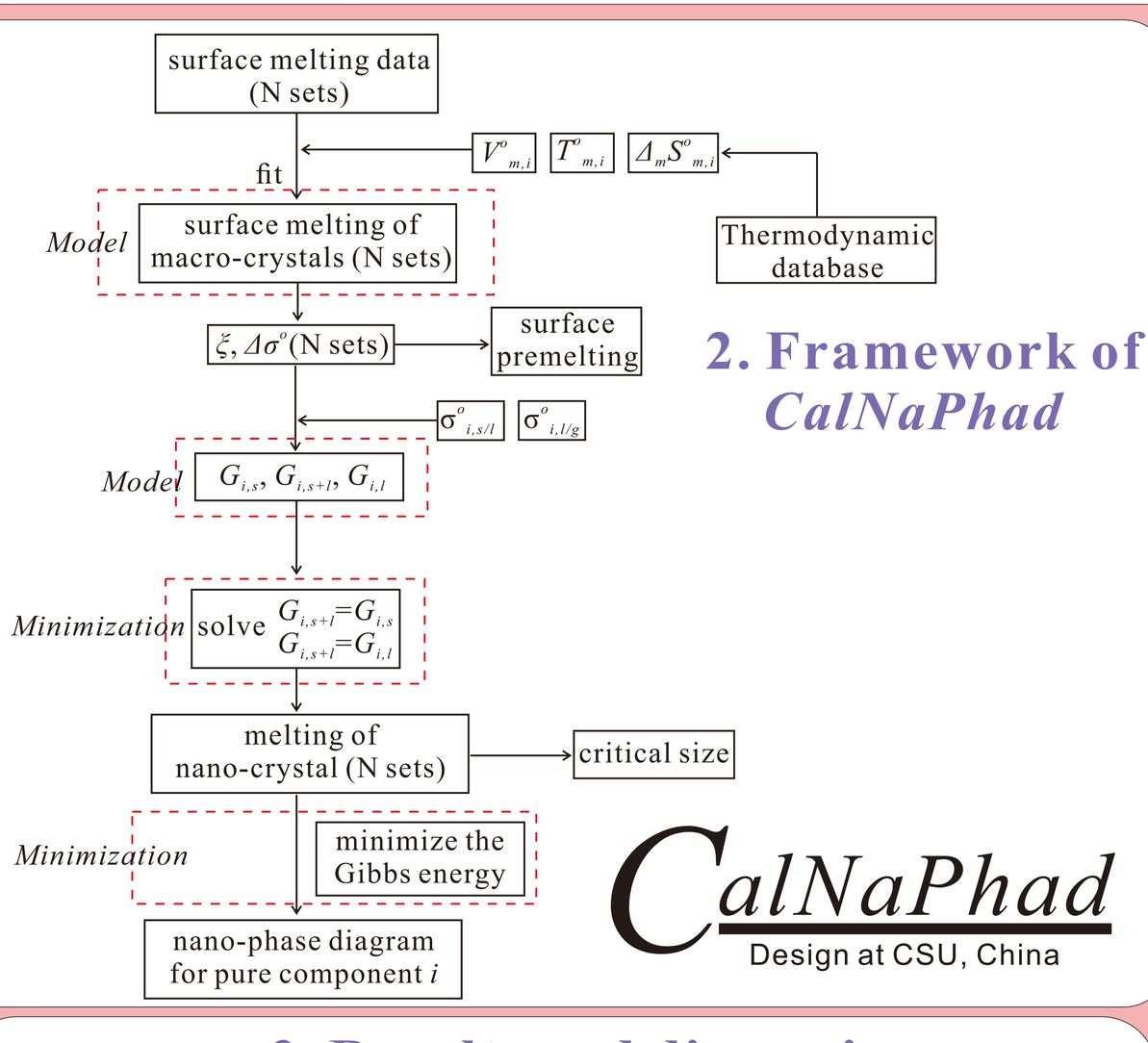
1. Background

Al-Cu-Ag ternary system is one of the most important subsystem of Al-based alloys due to the nano-structure precipitation phases. The second generation nano-Calphad model [1] considered the existence of solid/liquid interface, while the first generation model ignored the phenomenon of surface melting for macro-crystals.

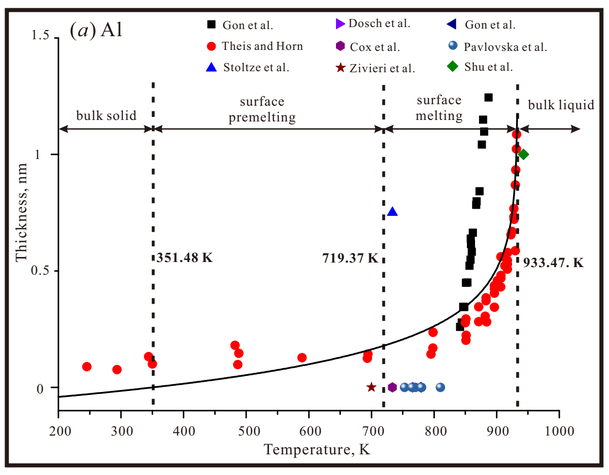
[1] A. Vegh, G. Kaptay, *Calphad*, 63 (2018) 37-50.

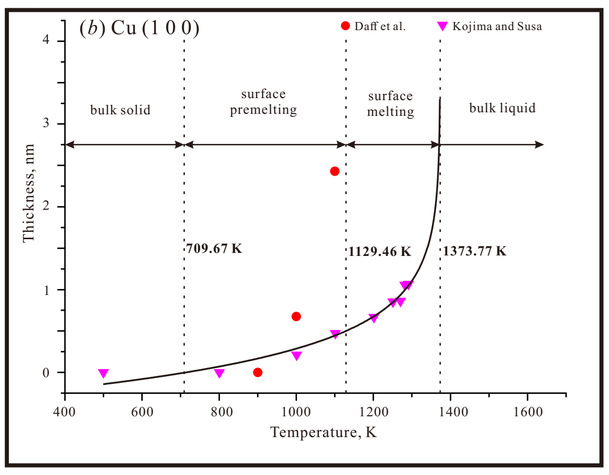
2. Framework of *CalNaPhad*

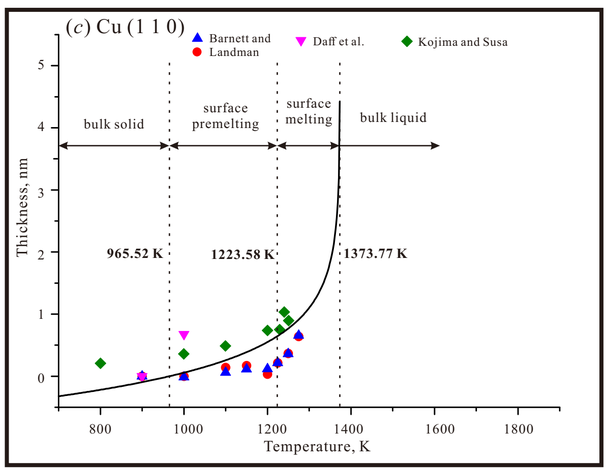


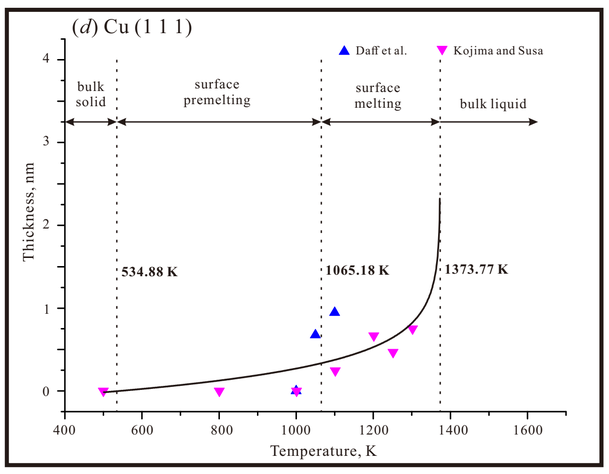
3. Results and discussion

3.1 Surface melting of macro-crystals









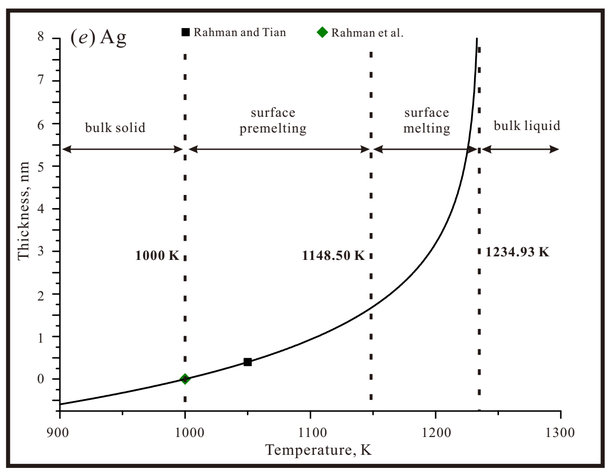
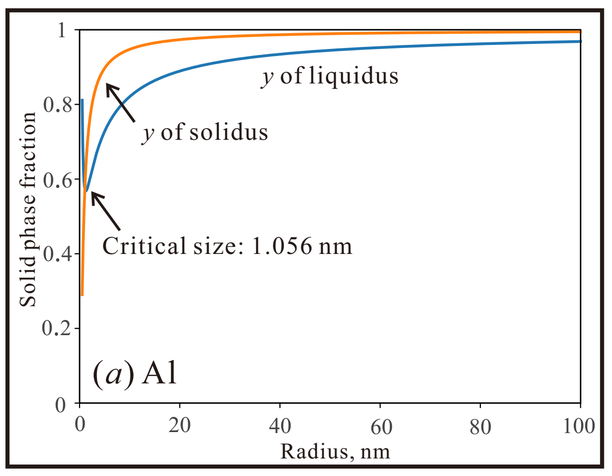
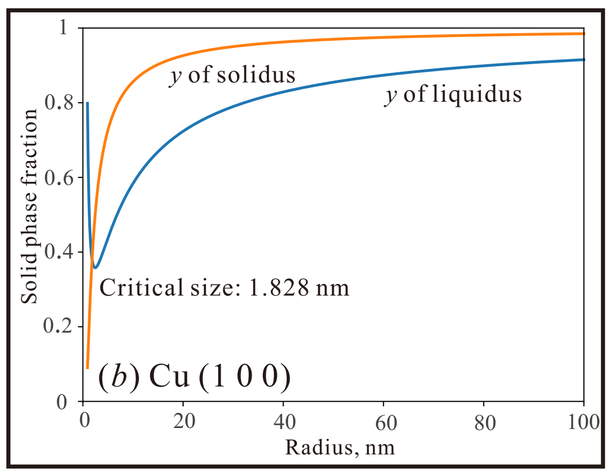
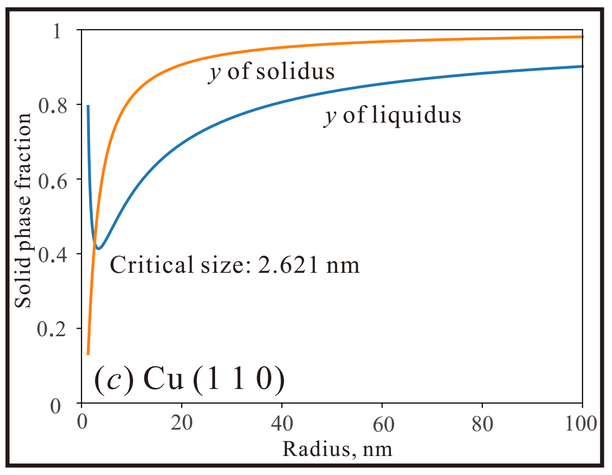


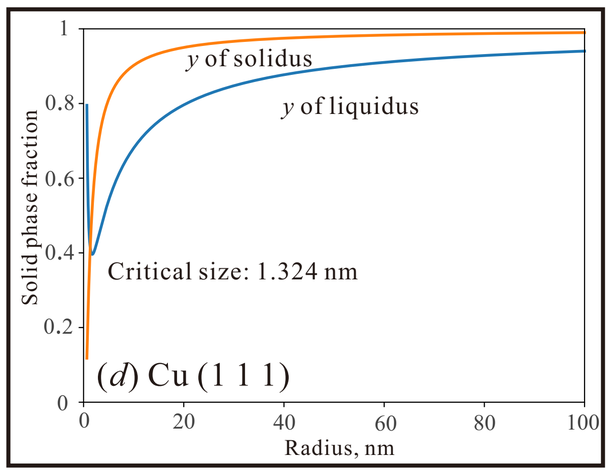
Fig.1 The temperature dependent equilibrium thickness of the liquid surface layer for: Al (*a*), Cu (*b-d*), Ag (*e*).

3.2 Melting of nano-crystal









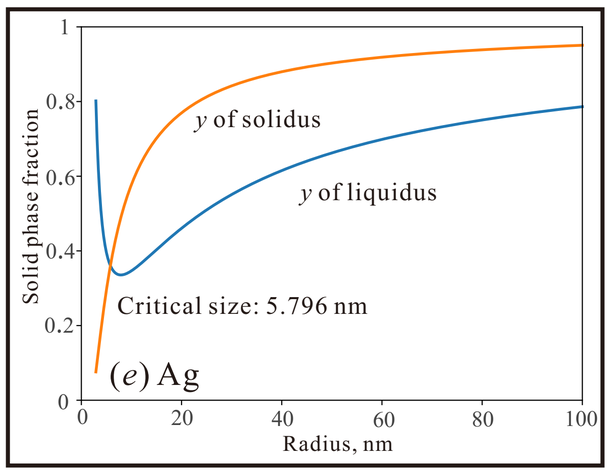
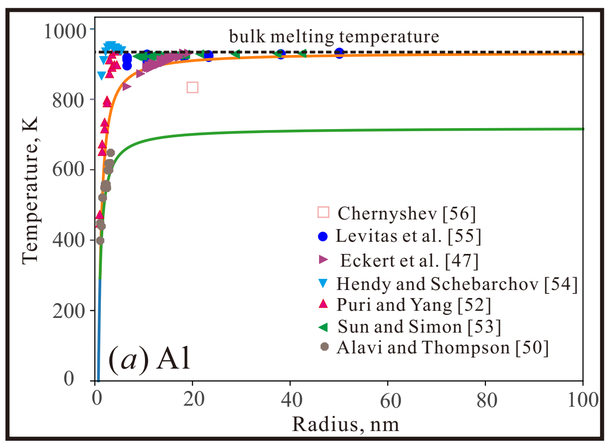
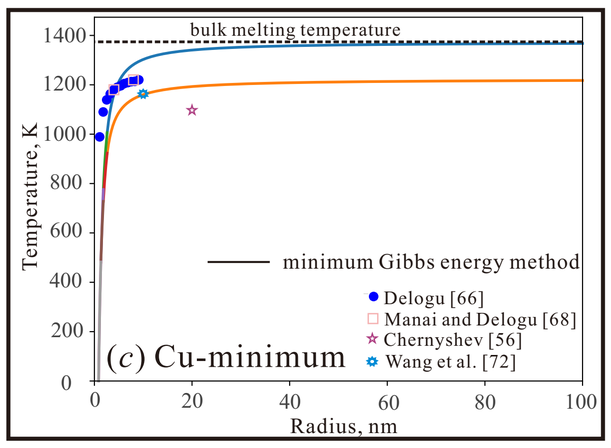
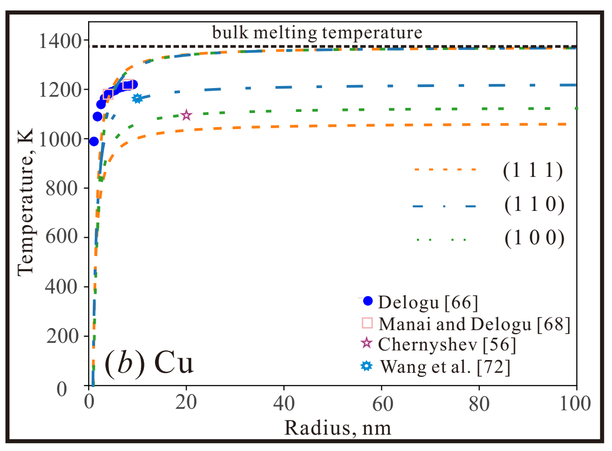


Fig.2 The solid phase fraction and critical size of solidus and liquidus for: Al (*a*), Cu (*b-d*), Ag (*e*).







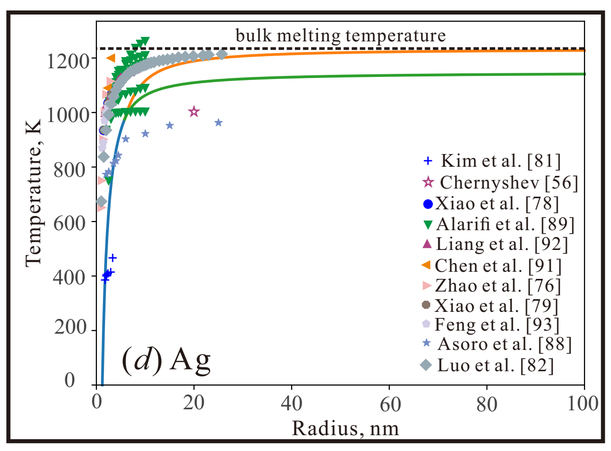


Fig.3 The nano-phase diagram for: Al (*a*), Cu (*b-d*), Ag (*e*).

4. Conclusion

- **The surface melting of macro-crystals and melting of nano-crystal for Al, Cu and Ag pure component are modeled in comparison with literature data.**
- **The relevant temperatures of surface premelting and melting, corresponding temperature dependent equilibrium thickness of liquid melted layer are obtained.**
- **The size-dependent melting behavior for Al, Cu and Ag is investigated and the critical size is determined by a home-made code, respectively.**

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