材料计算模拟及其与实验研究结合

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Outline

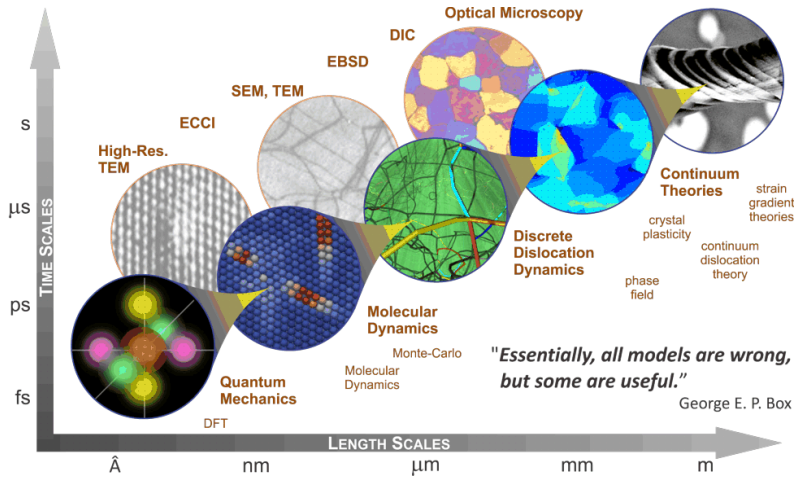
1 为什么需要计算模拟

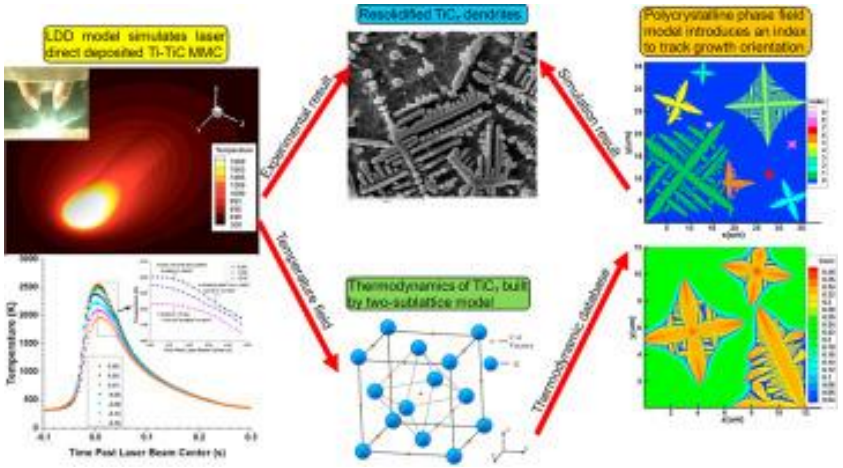
2 计算模拟可以做什么

3 如何与实验研究相结合

为什么需要计算模拟

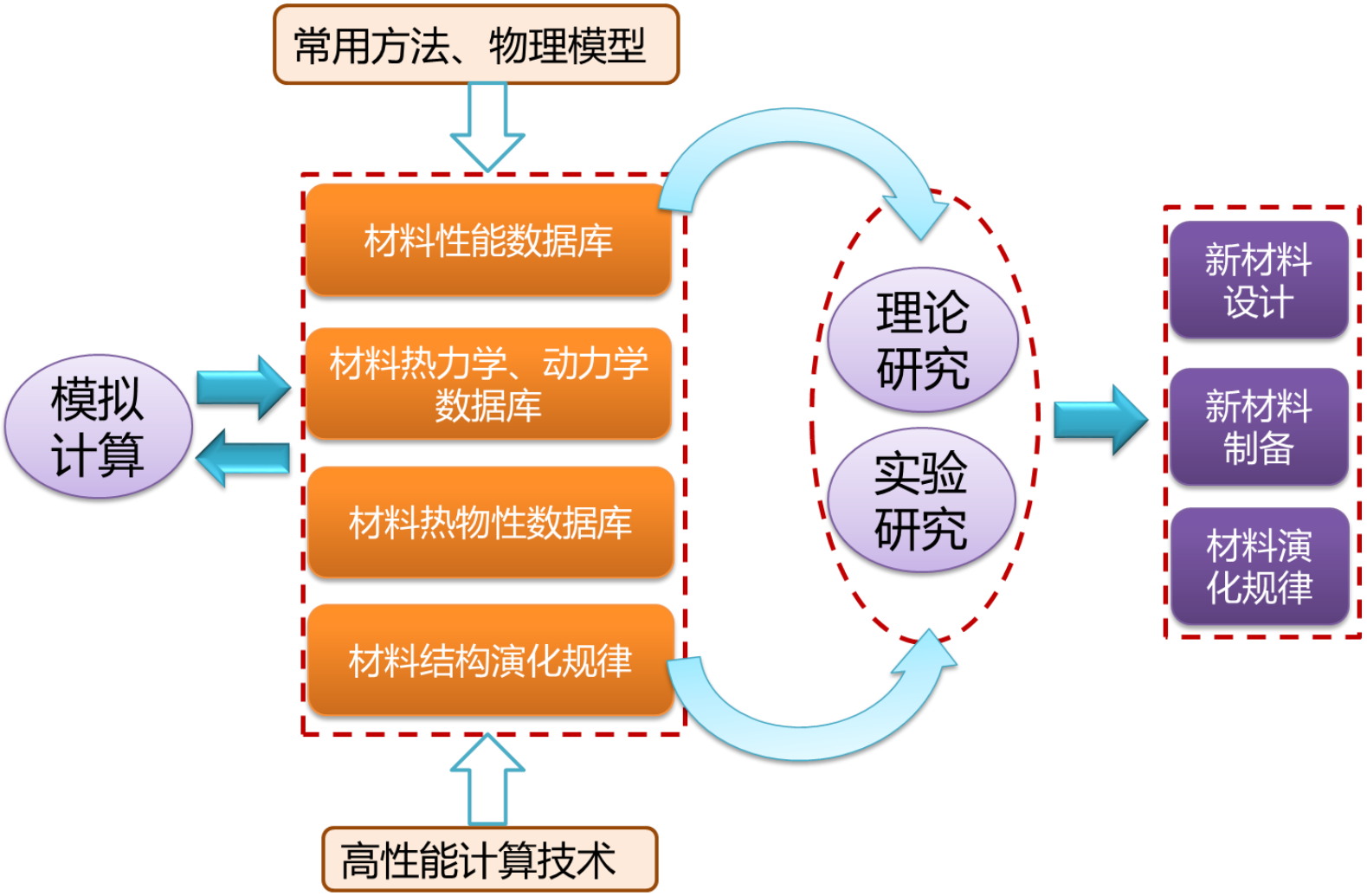
材料计算模拟是指采用数值方法求解相应的方程或者微分方程（组），获得微观组织的状态及其随时间演变的描述





材料计算模拟方法是沟通理论与实验、微观与宏观的桥梁

计算模拟可以做什么



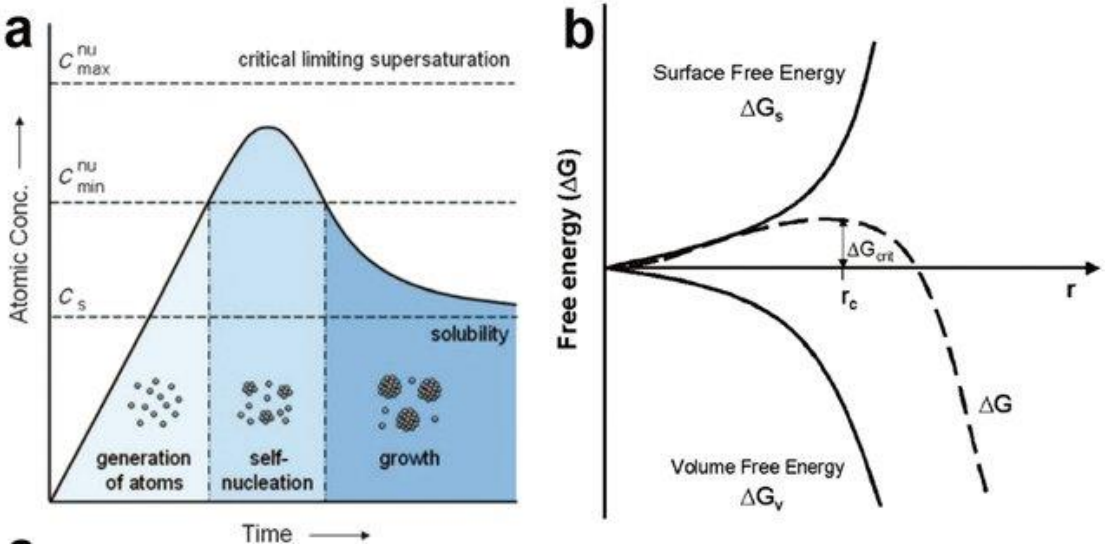
借助计算机技术的飞速发展，材料计算仿真在材料研究中的应用越来越广泛，在理论分析、性能预测、材料设计等方面起着关键作用

如何与实验研究相结合

- 与实验结果对比，相互检验
- 获得当前实验条件下难以获得的信息
- 模拟与实验研究相互支撑
- 根据计算模拟结果，指导实验研究

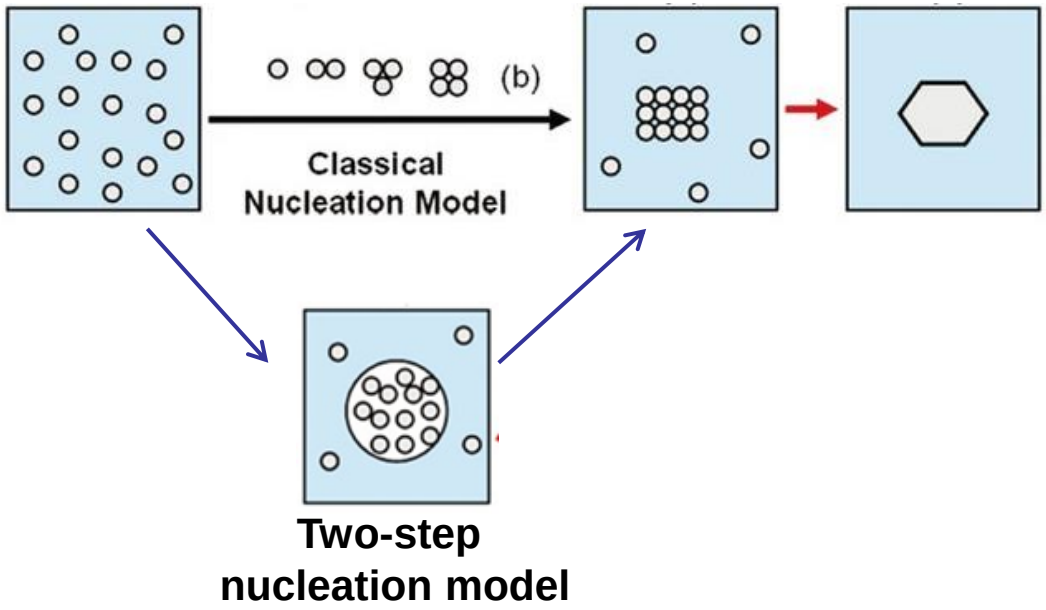
例一：金属凝固形核机理

经典形核理论



$$R = N_S Z j \exp\left(\frac{-\Delta G^*}{k_B T}\right)$$

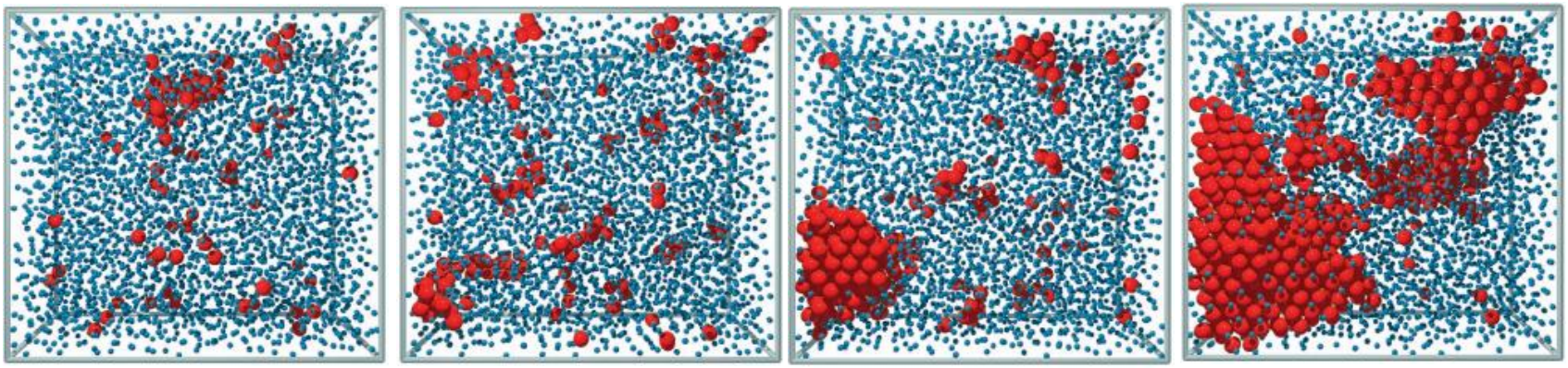
$$r_c = \frac{-2\sigma T_m}{\Delta H_f}\frac{1}{T_m - T}$$



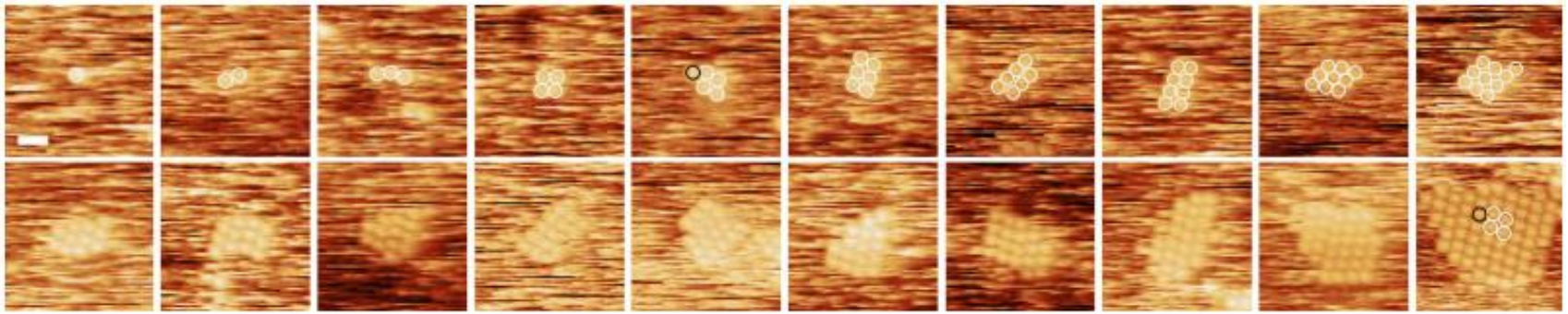
- 无法获得晶核的结构转变信息
- 难以预测或者描述形核路径

例一：金属凝固形核机理

实验研究



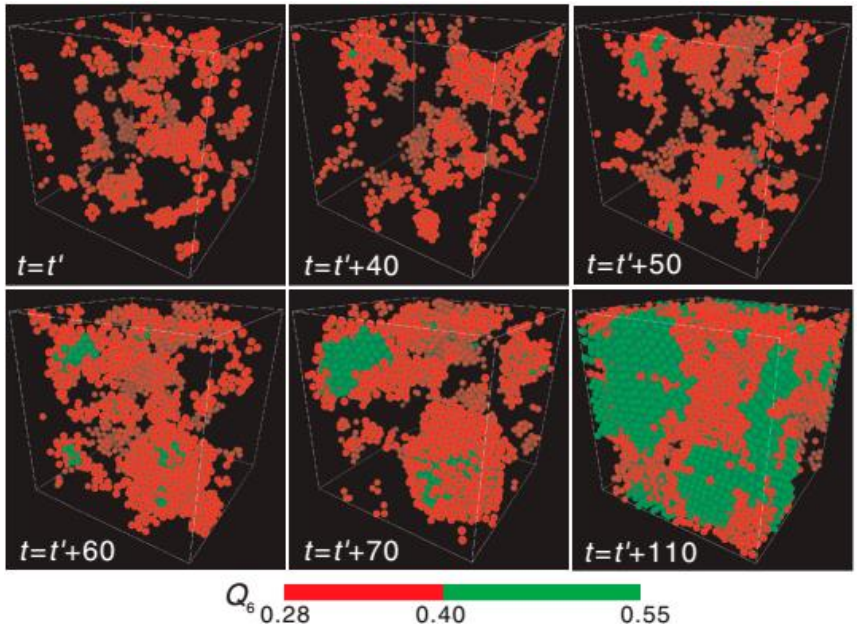
大分子胶体结晶的形核过程



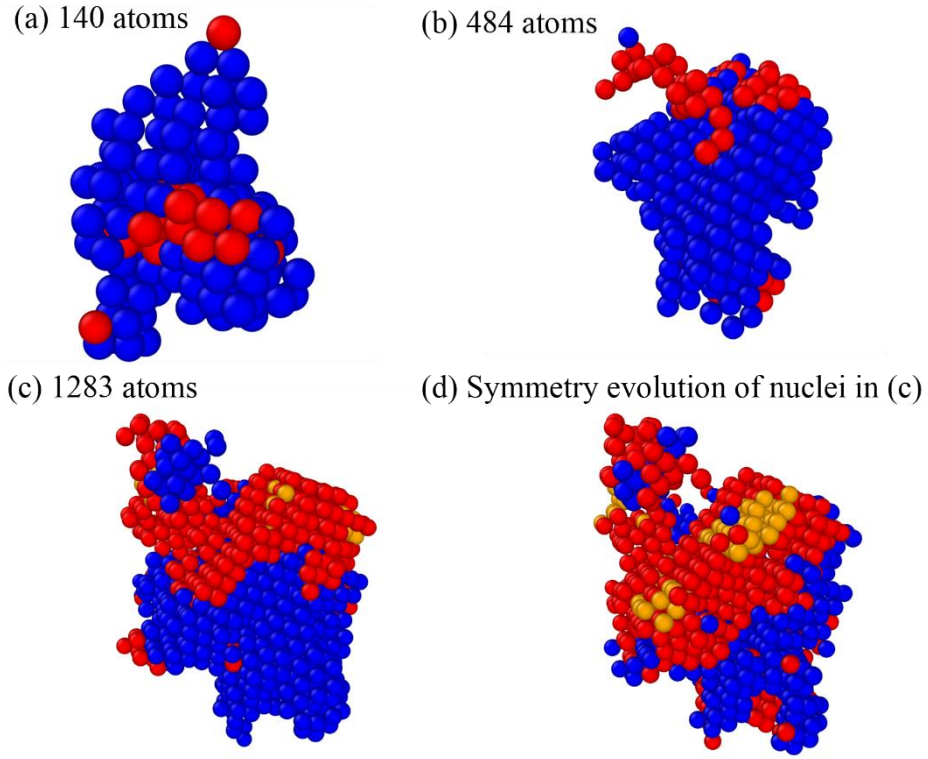
二维KCL晶体在衬底上的形核过程

金属凝固形核是在高温下发生的原子尺度结构转变过程，具有随机性，难以通过试验原位观察，迄今为止，还实验表征还难以获得凝固过程晶核的形成机理。

例一：金属凝固形核机理

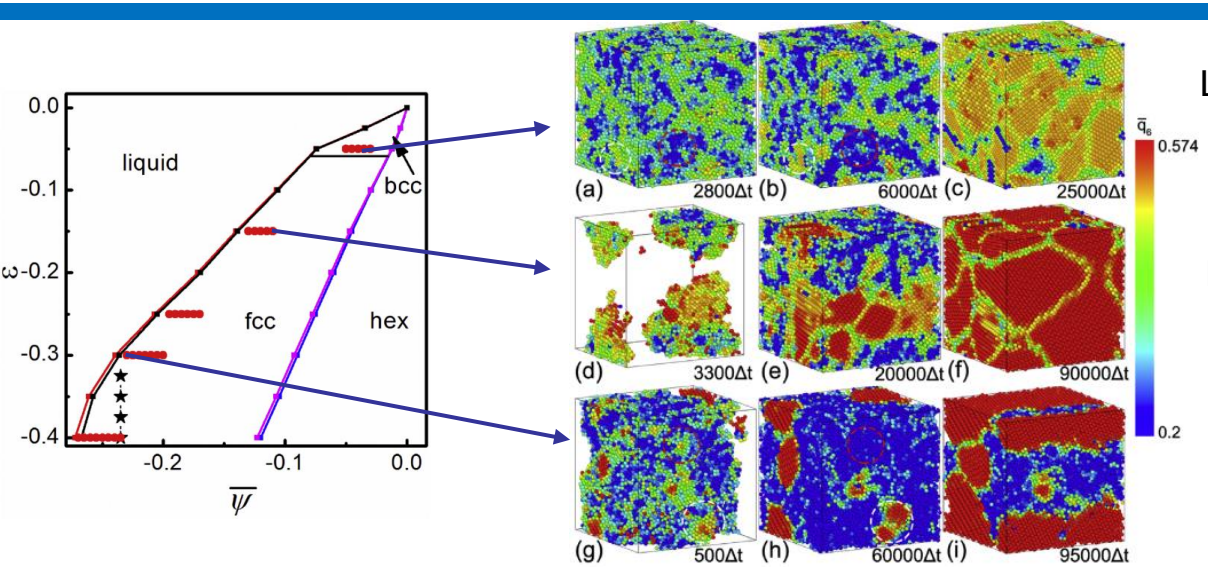


纯铝凝固形核过程Brown dynamic动力学模拟



Al-Cu合金凝固形核过程分子动力学模拟

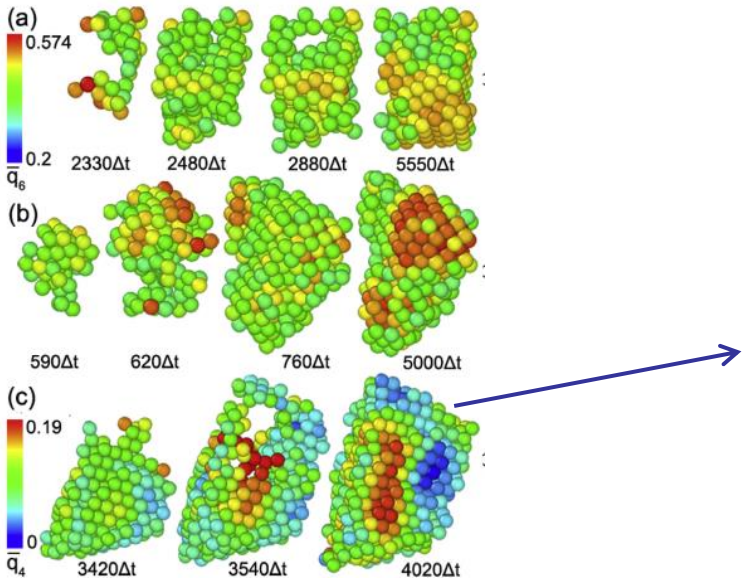
例一：金属凝固形核机理

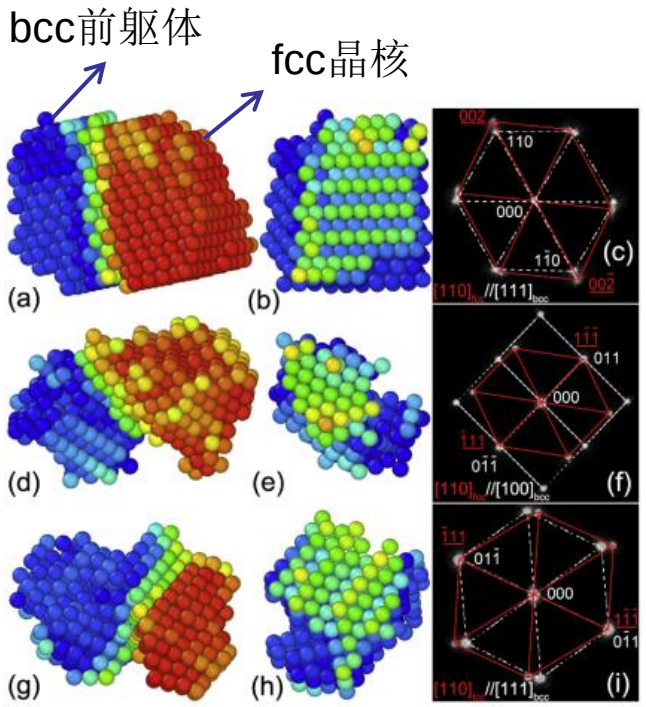


Liquid→ amorphous precursor → bcc

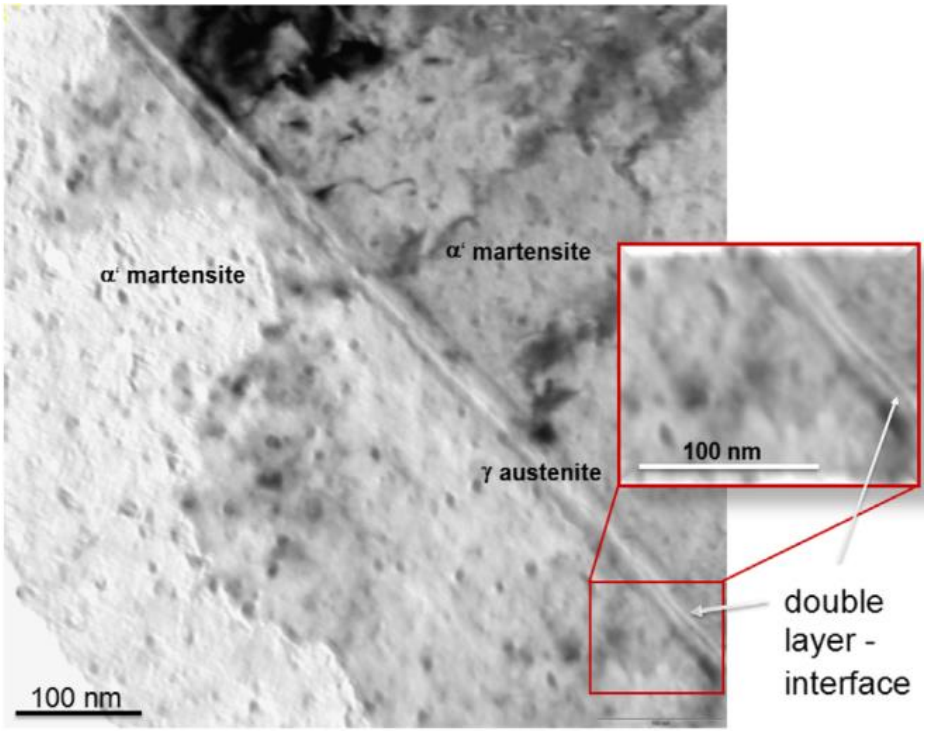
Liquid→ amorphous precursor → bcc→fcc

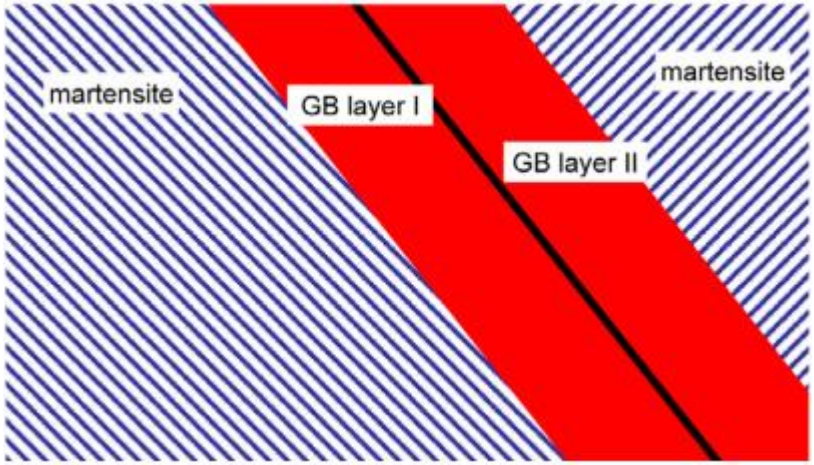
Liquid→ amorphous precursor → fcc





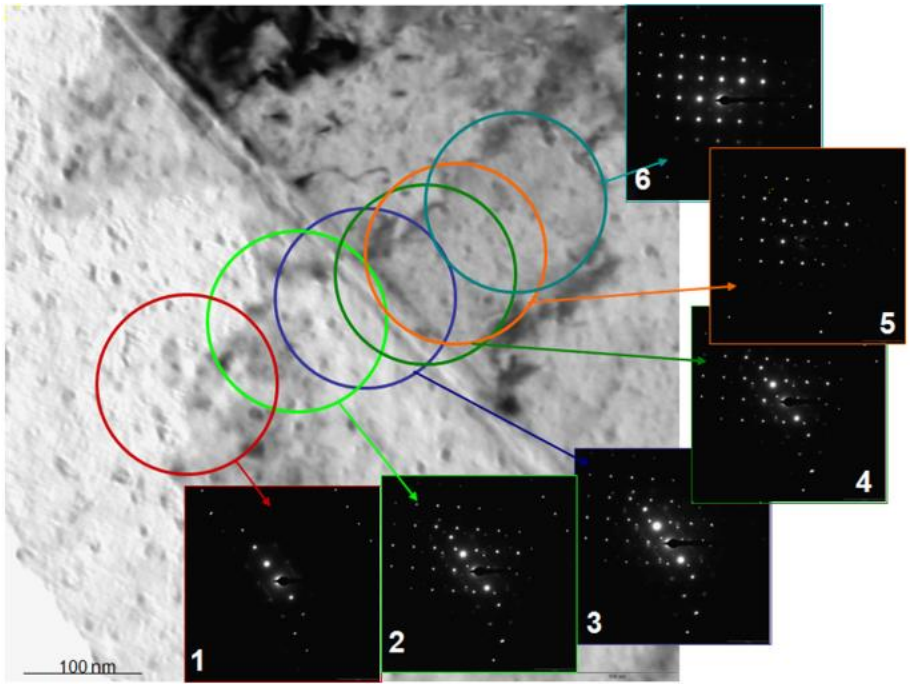
例二：晶界沉淀析出相模拟

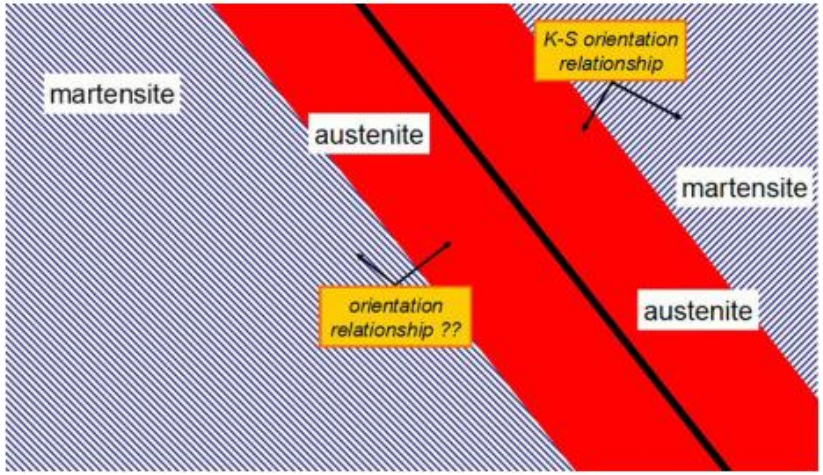




Fe9Mn1.9Ni-X (at.%)合金中发现沿马氏体晶界析出的双层奥氏体相

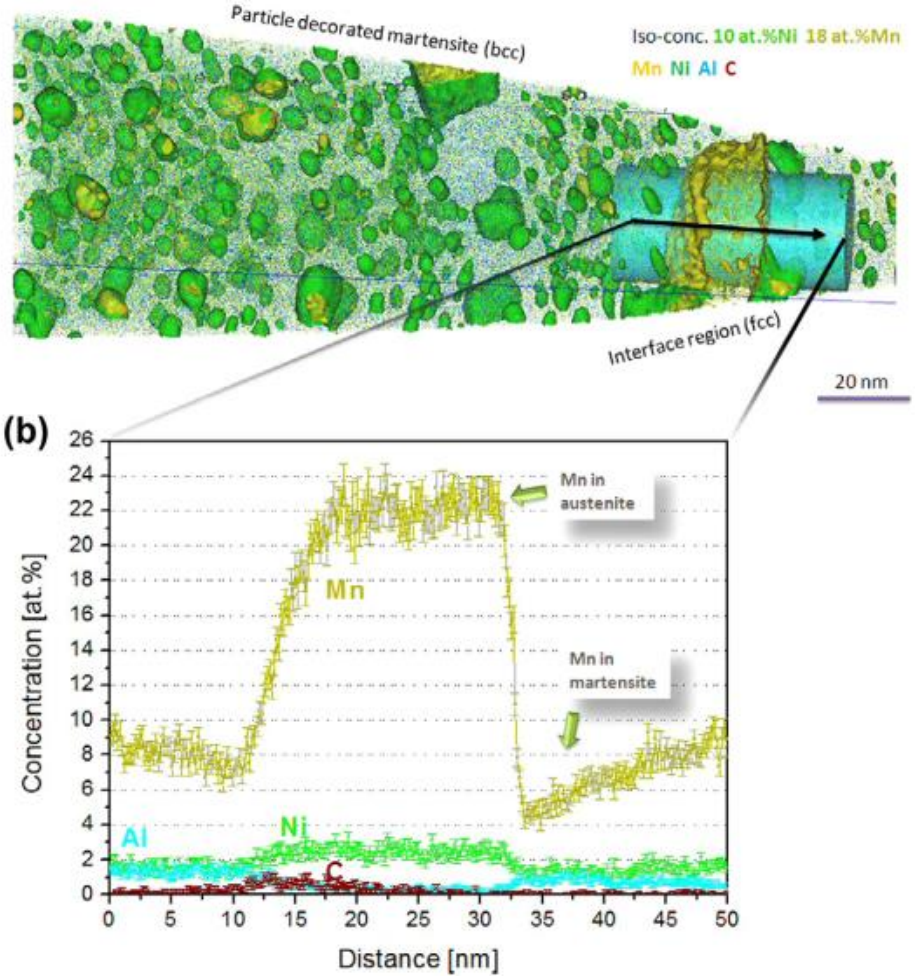
例二：晶界沉淀析出相模拟





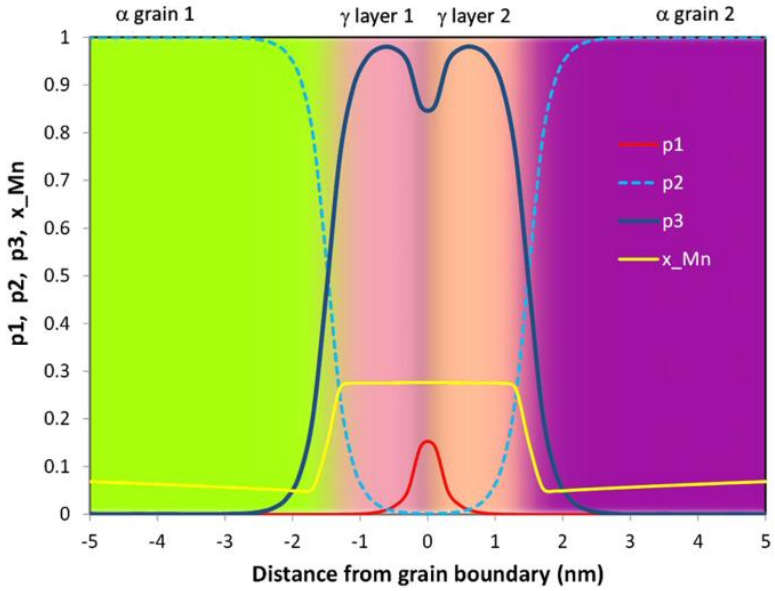
通过结构表征，发现其中一层奥氏体与马氏体成KS取向关系，另一层的关系不确定

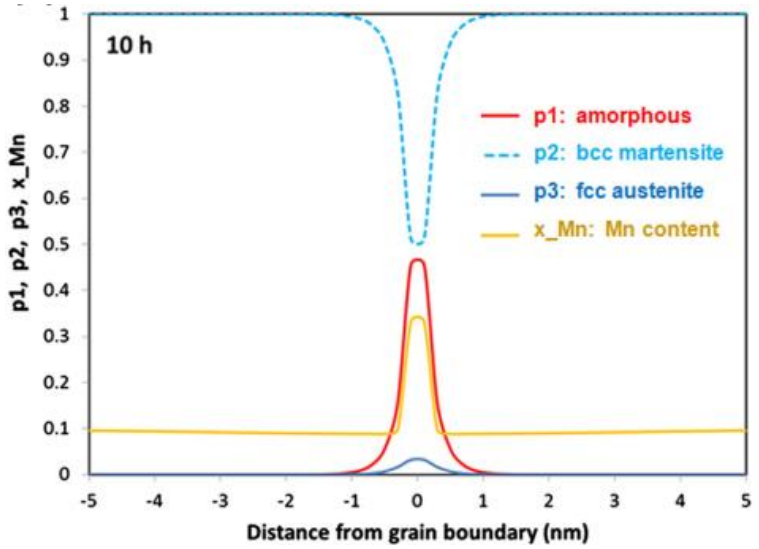
例二：晶界沉淀析出相模拟

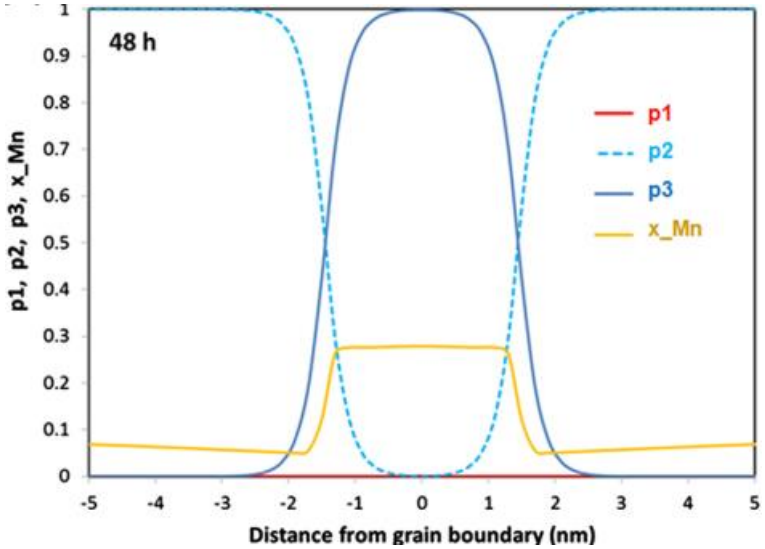


三维原子探针对成分表征显示，双层奥氏体新相的形成是由Mn在晶界偏析导致的

例二：晶界沉淀析出相模拟

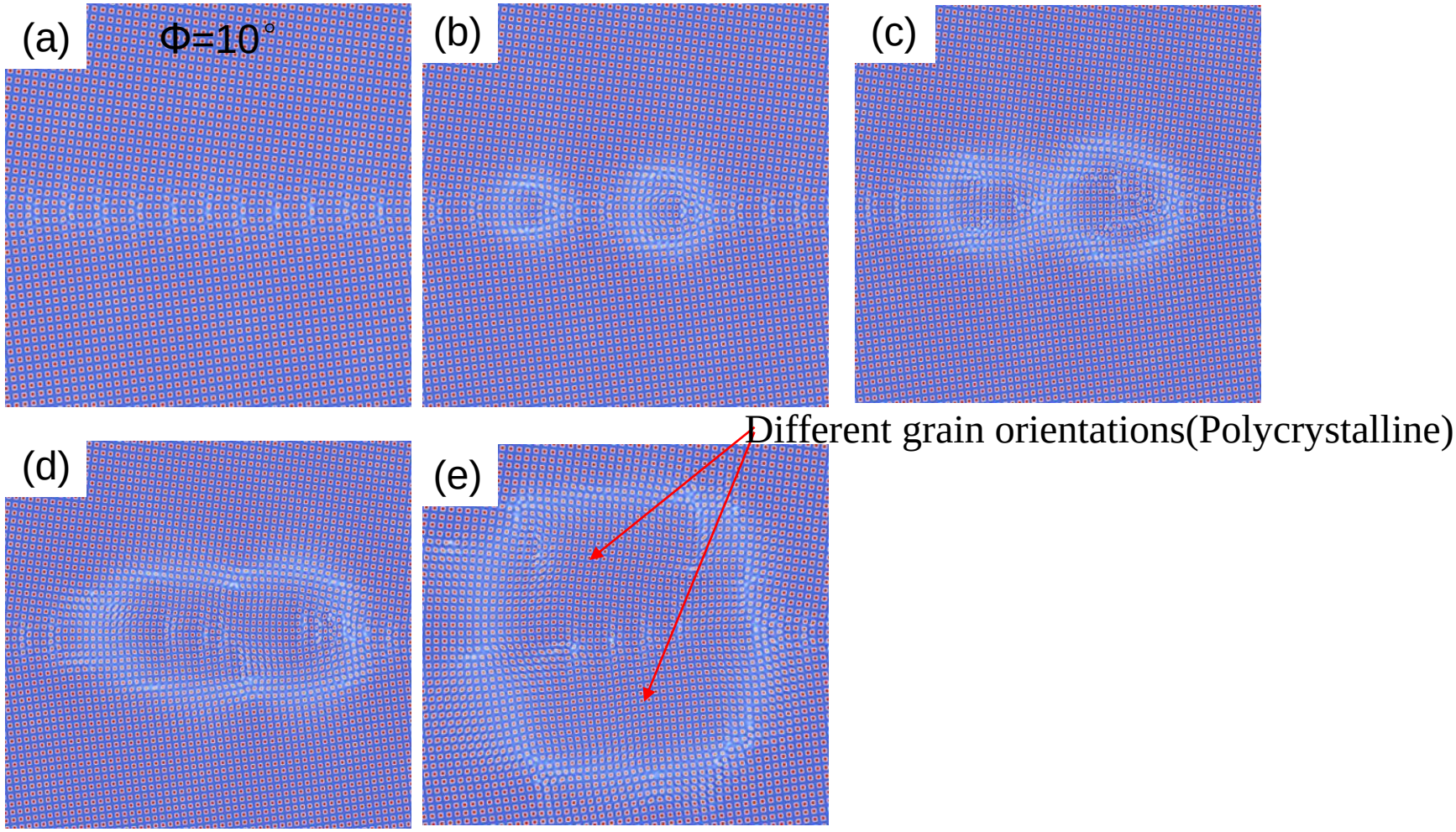






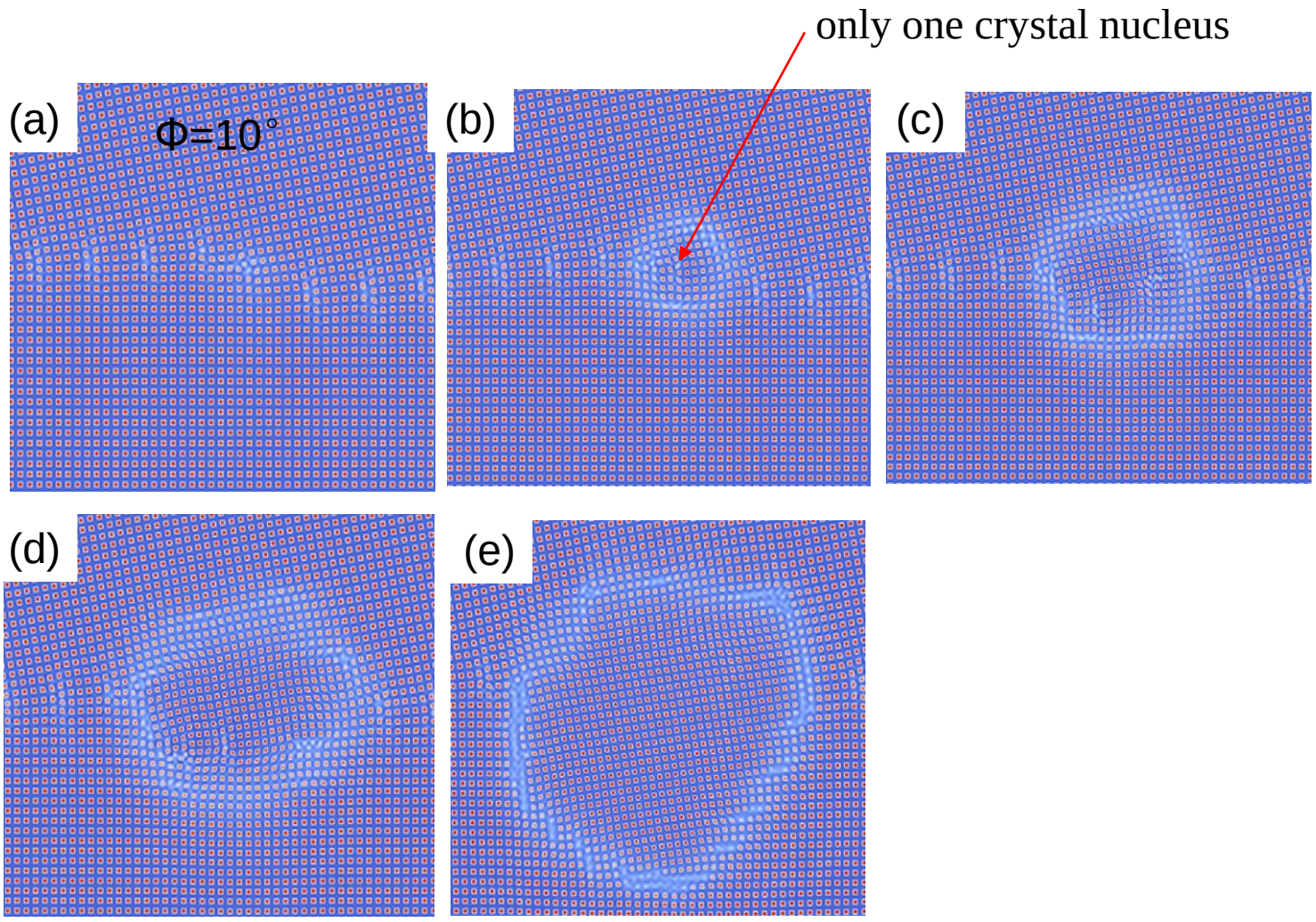
相场模拟研究表明，只有当角度小于15°才有可能形成双层奥氏体析出层

例二：晶界沉淀析出相模拟



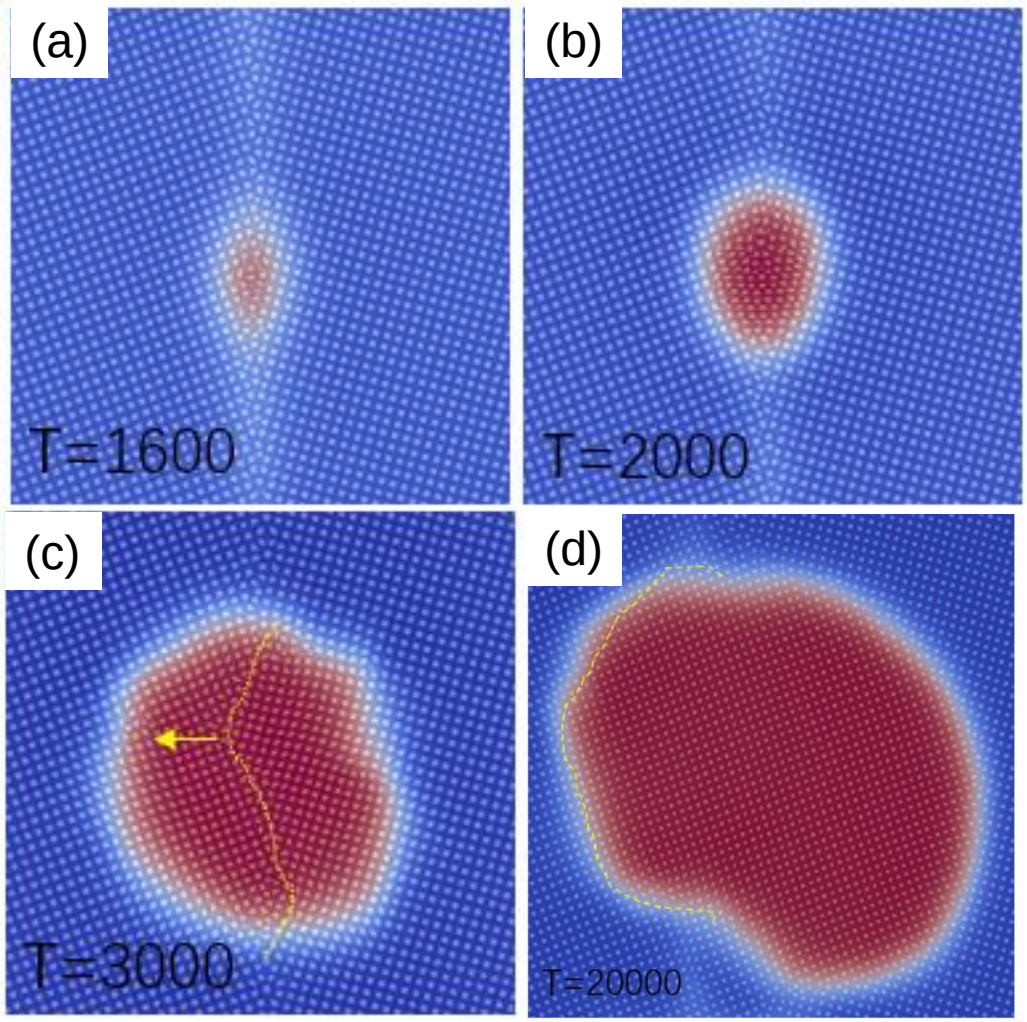
晶体相场模型研究表明对称倾斜小角度晶界可出现双层析出相，析出相的形成是由于晶界两侧晶粒同时发生形核，进而演变为对称的两个晶核

例二：晶界沉淀析出相模拟



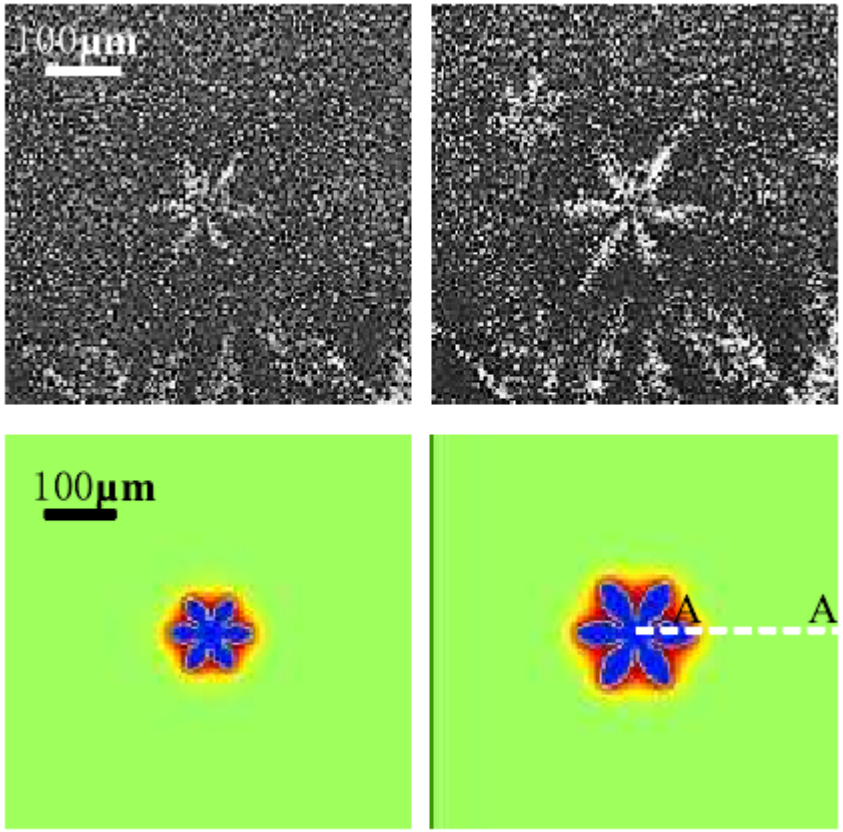
非对称倾斜小角度晶界，形核点两侧不对称，只在晶界一侧形核，并演化为单个析出相

例二：晶界沉淀析出相模拟



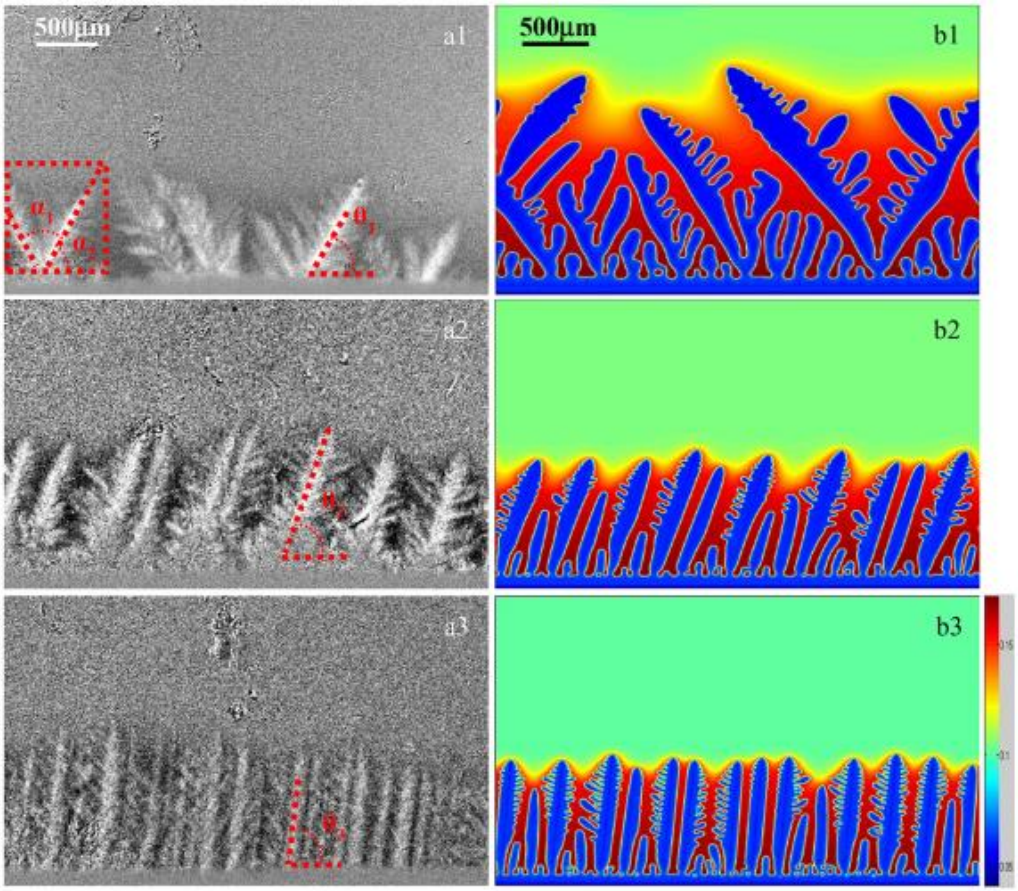
大角度晶界虽然在初期有两个晶粒形核，但其中一个晶粒会被另外一个吞噬，只留下一个晶粒。

模拟与实验对比：枝晶生长同步辐射与相场模拟

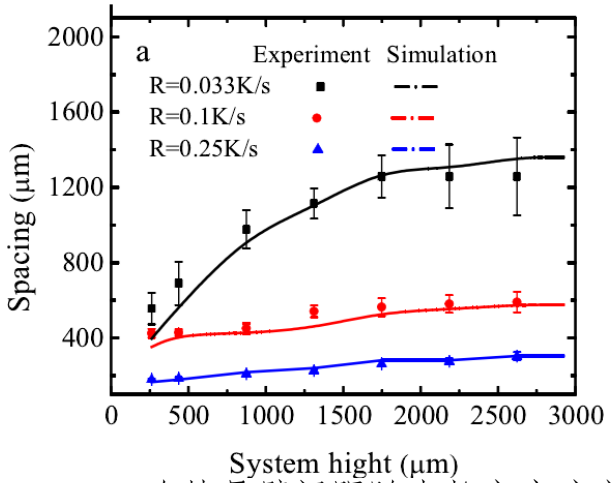


Mg-Gd二元合金凝固枝晶的同步辐射表征和相场法模拟

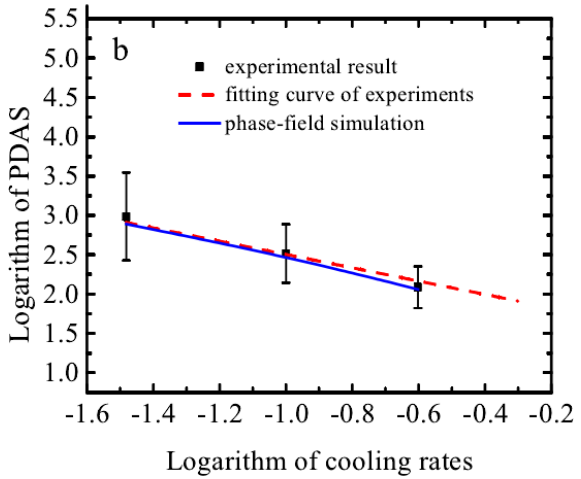
模拟与实验对比：枝晶生长同步辐射与相场模拟



不同冷速下Mg-Gd二元合金定向凝固枝晶的同步辐射表征和相场法模拟

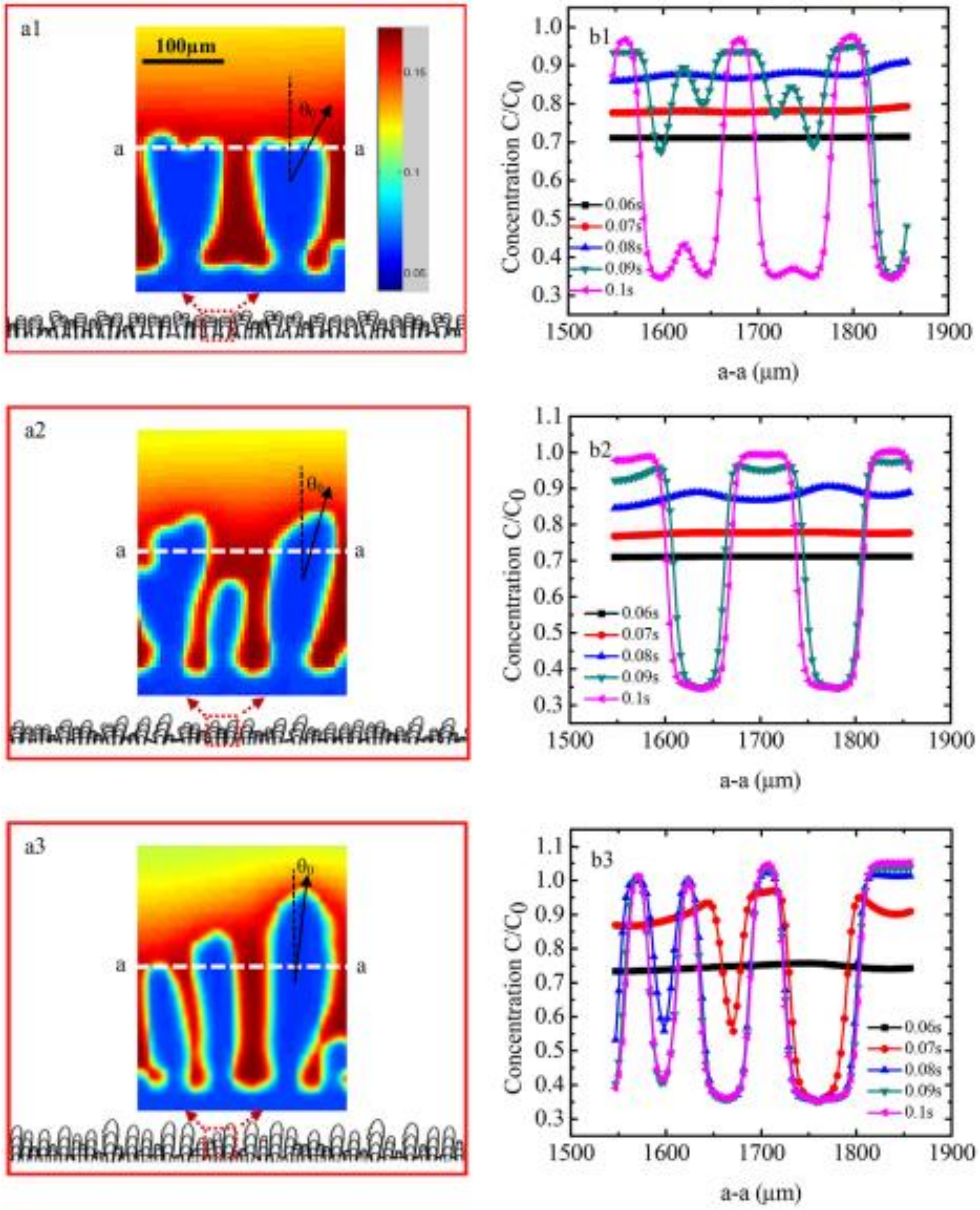


一次枝晶臂间距随生长高度演变



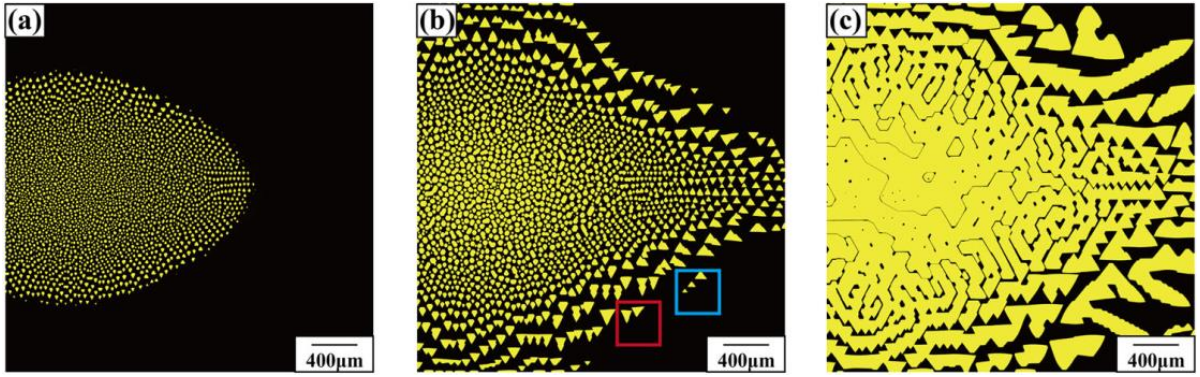
一次枝晶臂间距vs.过冷度

模拟与实验对比：枝晶生长同步辐射与相场模拟

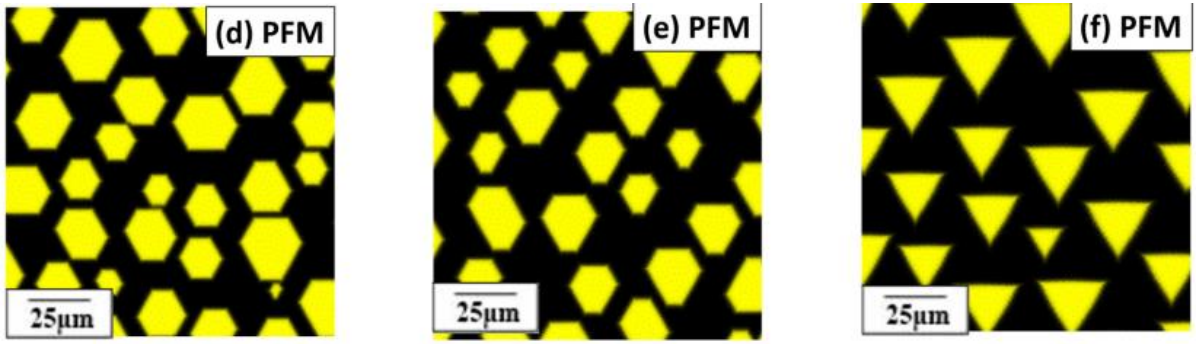


利用相场法可获得凝固前沿的浓度分布信息，分析枝晶形貌演变微观机制

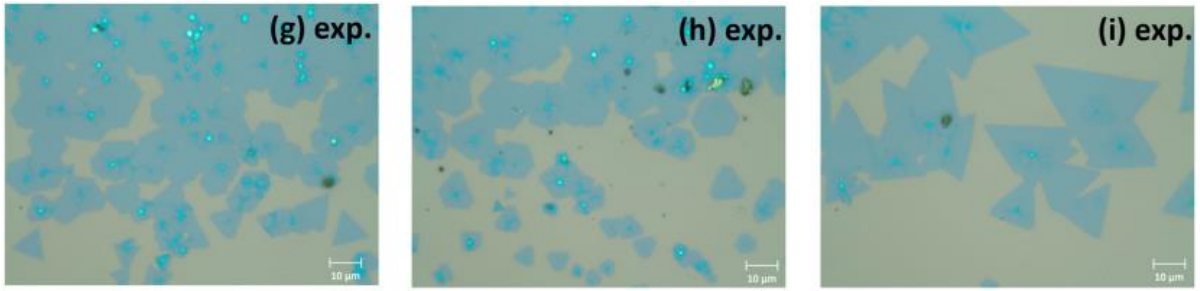
数值模拟指导实验研究：相场模拟指导下的MoS_2外延生长形貌演变



800°下单原子层MoS2外延生长晶核随时间生长及其分布的相场模拟



不同界面能和温度下MoS2外延生长晶核形貌演变的相场模拟



基于相场模拟指导下的实验结果

Thanks for your attention!