异质固-液界面台阶自由能的计算研究

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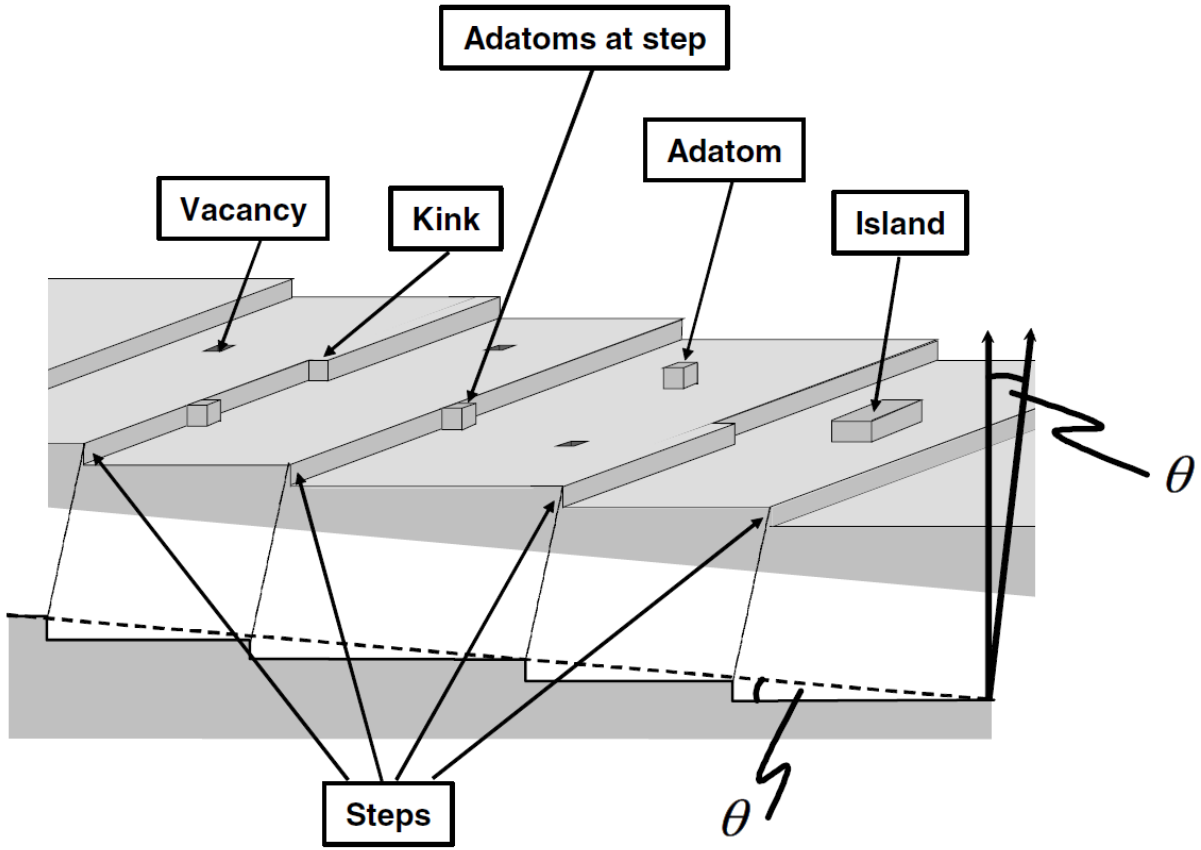
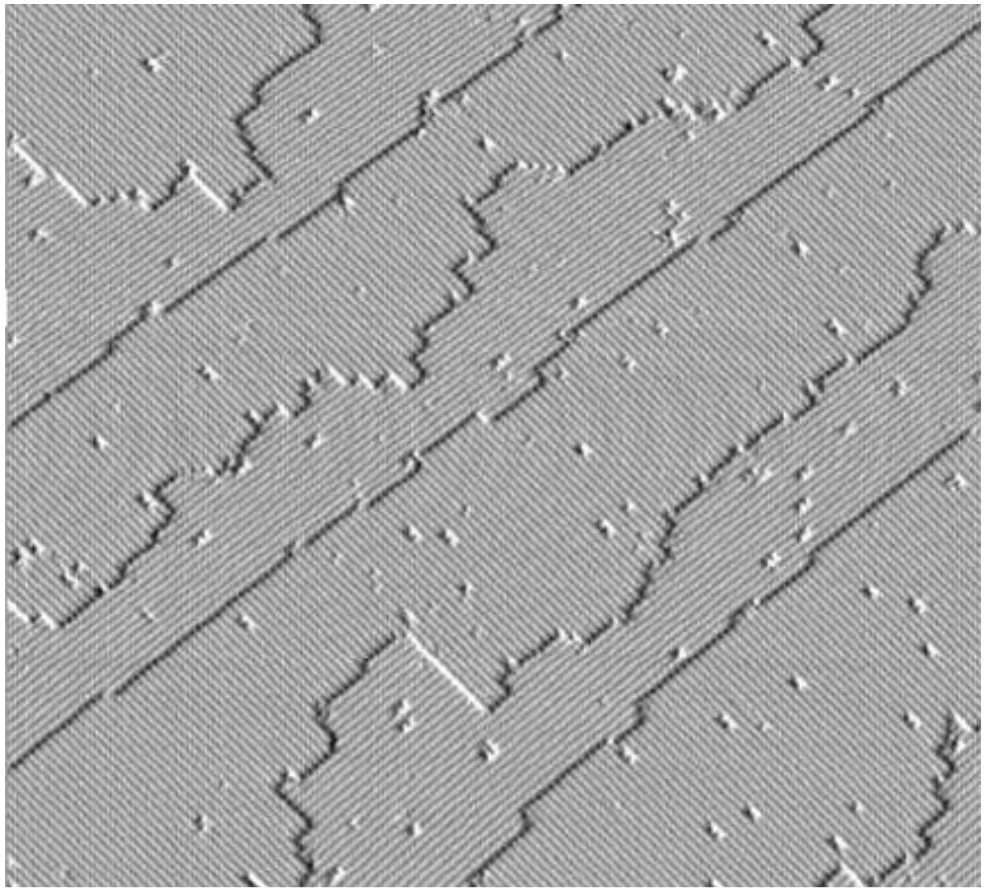
目录

1、研究背景：台阶，台阶自由能



固体表面示意图

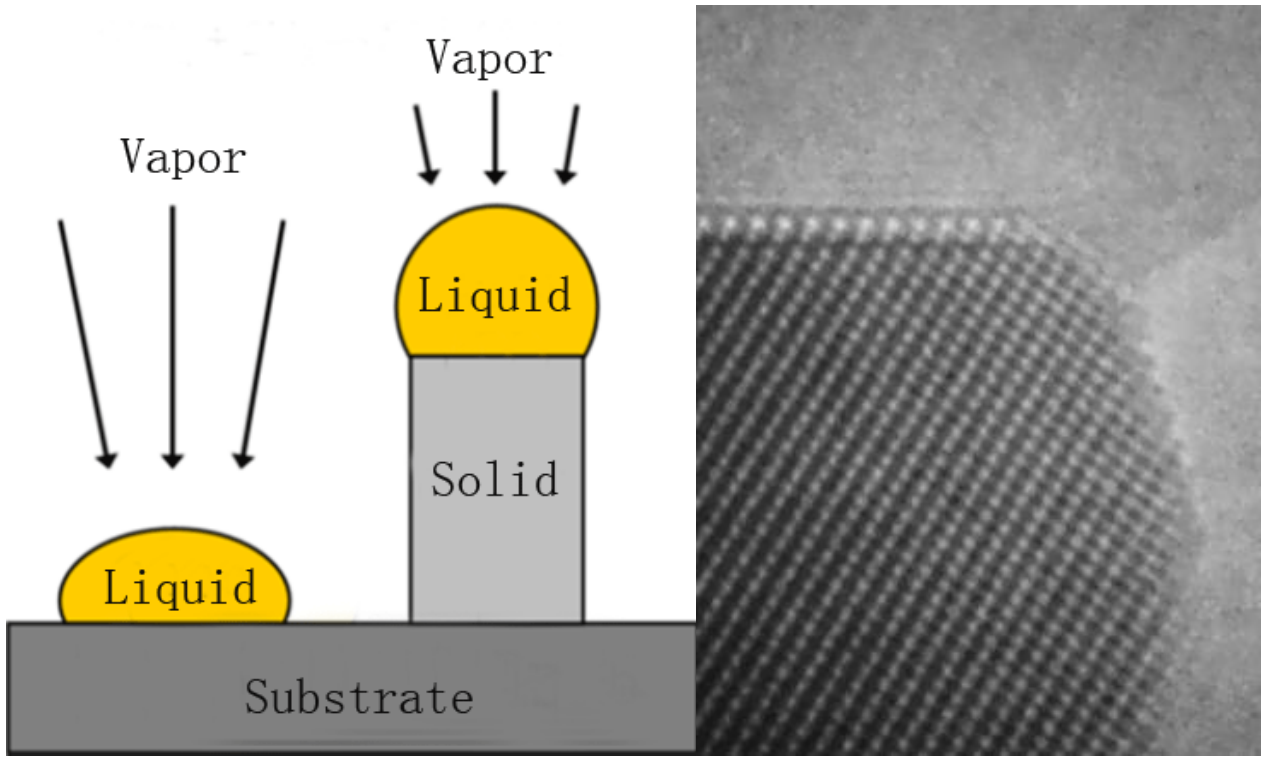


Si（100）表面STM图

台阶自由能是表征形成长度单位台阶难易程度的物理量。

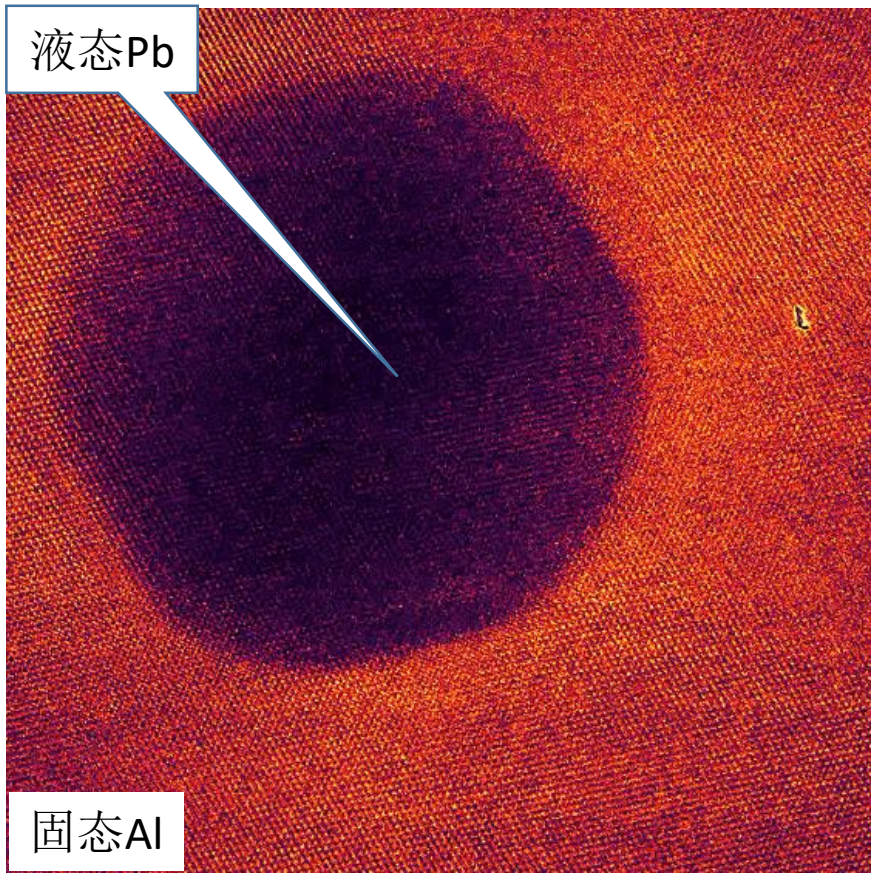
H. Ibach, Physics of Interfaces, Springer, Berlin, 2006

1、研究背景:台阶自由能的研究意义



纳米材料在纳米器件以及催化作用等方面具有很大的应用，其中在VLS一层一层生长晶须过程中，形成台阶是整个过程的第一步。

Sang Ho Oh el, Science. 489,93(2010)

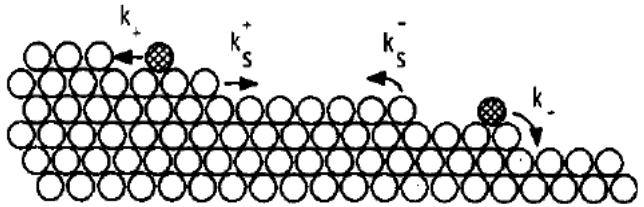


在异质固液界面成核理论中，台阶自由能的大小将影响成核的大小等。以及液态杂质在固体中的迁移速度等。

E. Johnson et al., J. Mater. Sci. (2005), and Privately provided by Uli Dahmen.

1、研究背景:台阶自由能的计算方法

70年代左右

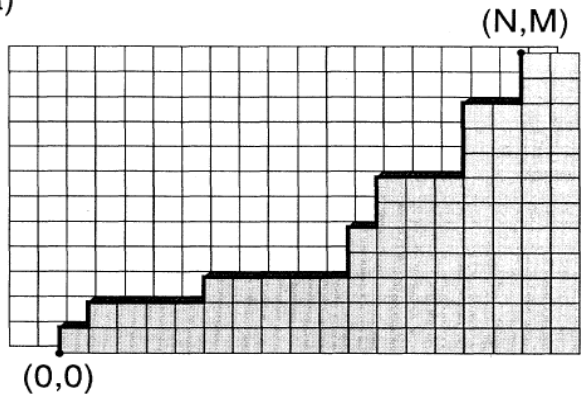


Richard L. Schwoebel, Journal of Applied Physics,49,2(1969)

solid-on-solid model

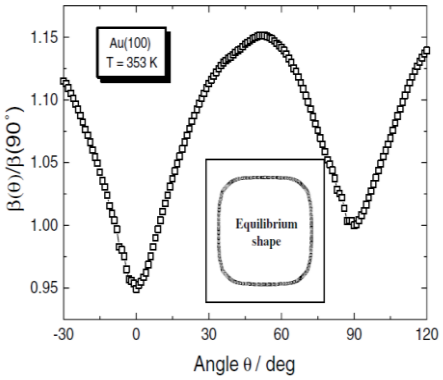
G Bilalbegovic, J. Phys. A: Math. Gen. 22,L833-L836 (1989)

(a)

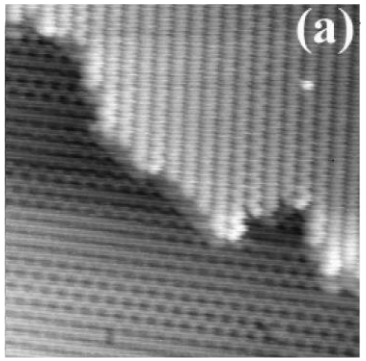


Mark Holzer and Michael Wortis, PRB,40,11044(1989)

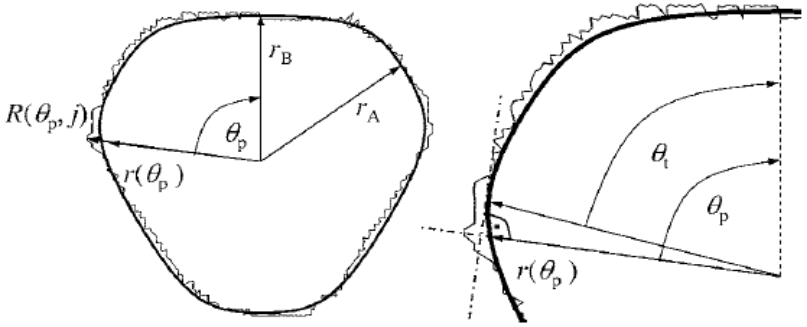
2000年左右



Ch. Bombis and H. Ibach, Surface Science 564, 201-210(2004)

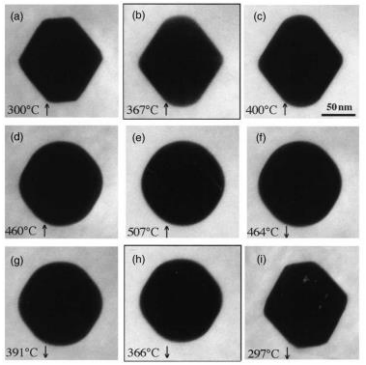


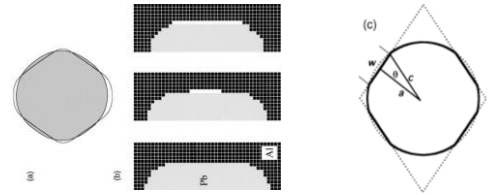
H. J. W. Zandvliet, PHYSICAL REVIEW B 75, 9972(2000)



Julian Ikonomov, Kirilka Starbova, and Harald Ibach, PHYSICAL REVIEW B 75, 245411(2007)

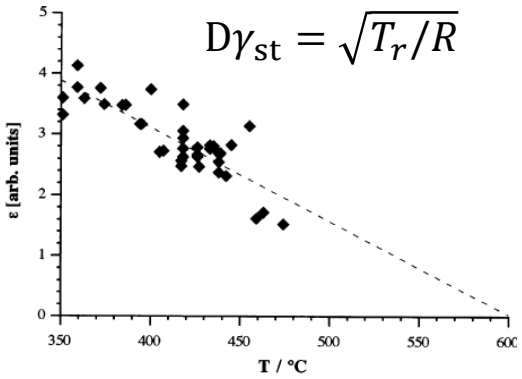
近期研究—固液界面





$$\Delta G(r) = 2\pi r\gamma_{st} - \pi r^2 h\Delta G_{vol}$$

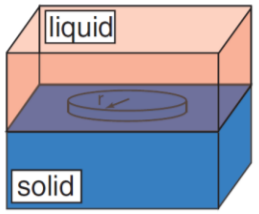
$$D\gamma_{st} = \sqrt{T_r/R}$$

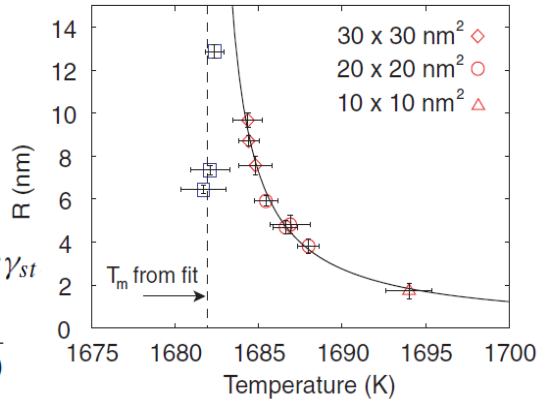


$$\frac{\gamma_{st}}{\gamma_{Al/Pb}} = h\sqrt{1-\frac{a^2}{c^2}}$$

$$T = 623K;$$
$$\gamma_{st} = 0.19 \times 10^{-10} J/m$$

H.Gabrisch, L.Kjeldgaard, E.Johnson and U. Dahmen, Acta mater. 49.4259(2001)





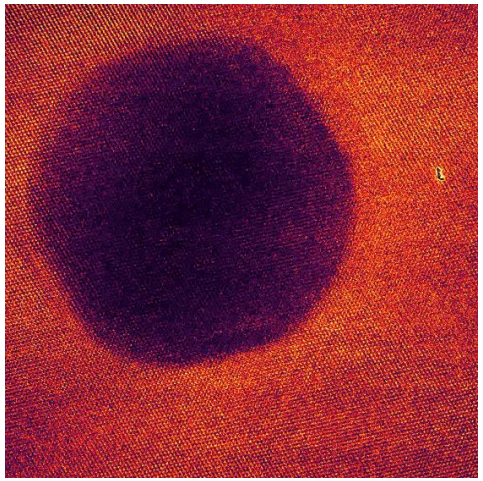
$$G = -\Delta\mu\rho_A\pi r^2 + 2\pi r\gamma_{st}$$

$$R = \frac{\gamma_{st} T_m}{\rho_A H_m (T_m - T)}$$

$$\gamma_{st} = 0.103 \pm 0.005 \times 10^{-10} J/m$$

T. Frolov and M. Asta, J.Chem.Phys. 137,214108(2012)

2、研究动机和理论基础



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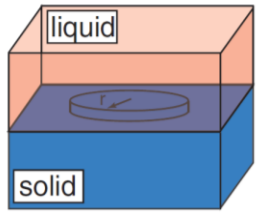

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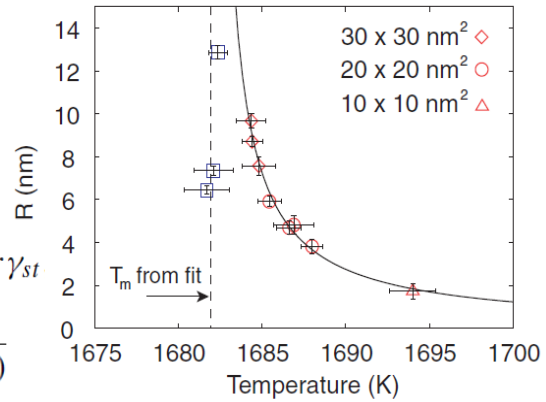

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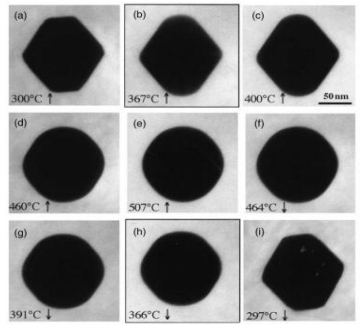
T. Frolov and M. Asta, J.Chem.Phys. 137,214108(2012)



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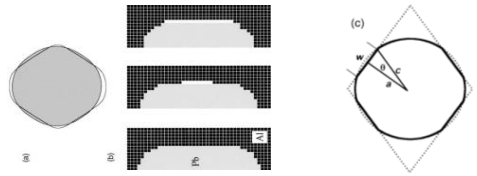

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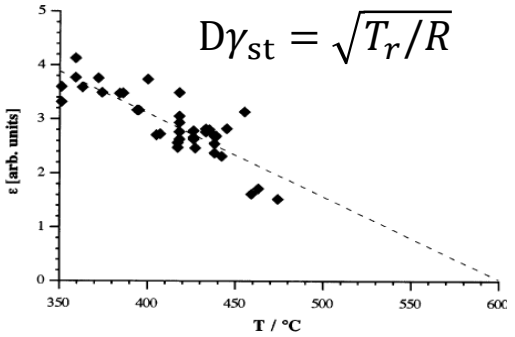
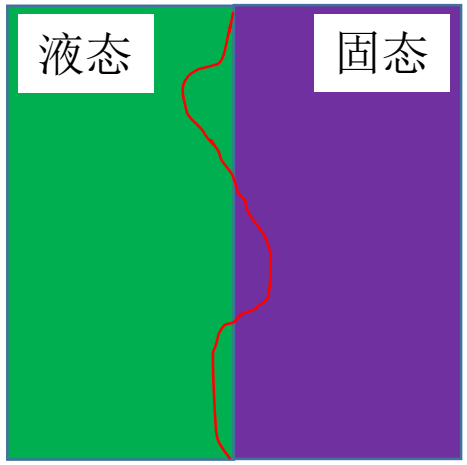


H.Gabrisch, L.Kjeldgaard, E.Johnson and U. Dahmen, Acta mater. 49,4259(2001)

目标：使用分子动力学模拟结合一种直接测量方法计算Al-Pb体系固液界面台阶自由能。



$$H = \gamma_{\mathrm{st}} \int \left[\sqrt{1 + (\nabla\xi_{(x)})^2} - 1\right] dx$$

$$H = \frac{1}{2}\gamma_{\mathrm{st}} L_x \sum_{q\neq 0} q^2 \left|\widehat{\xi_q}\right|^2$$

$$\xi_{(x)} = \sum_{q\neq 0} \widehat{\xi_q} \exp(iqx)$$

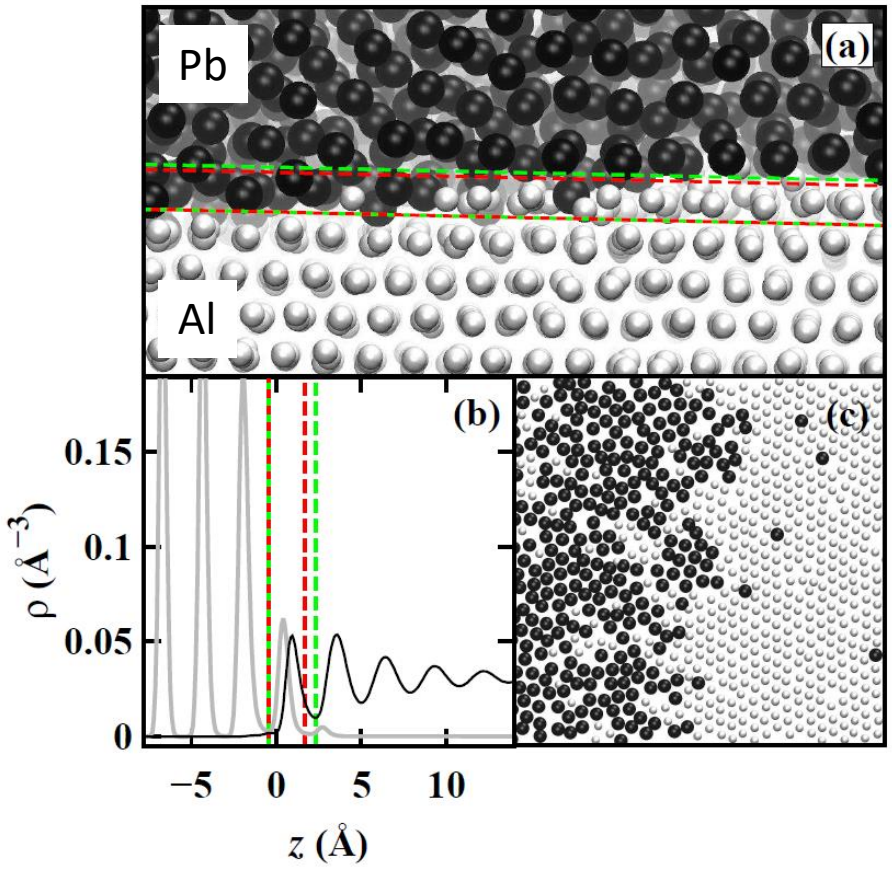
$$\left\langle \left|\widehat{\xi_q}\right|^2 \right\rangle = \frac{k_B T}{L_x \gamma_{\mathrm{st}} q^2}$$

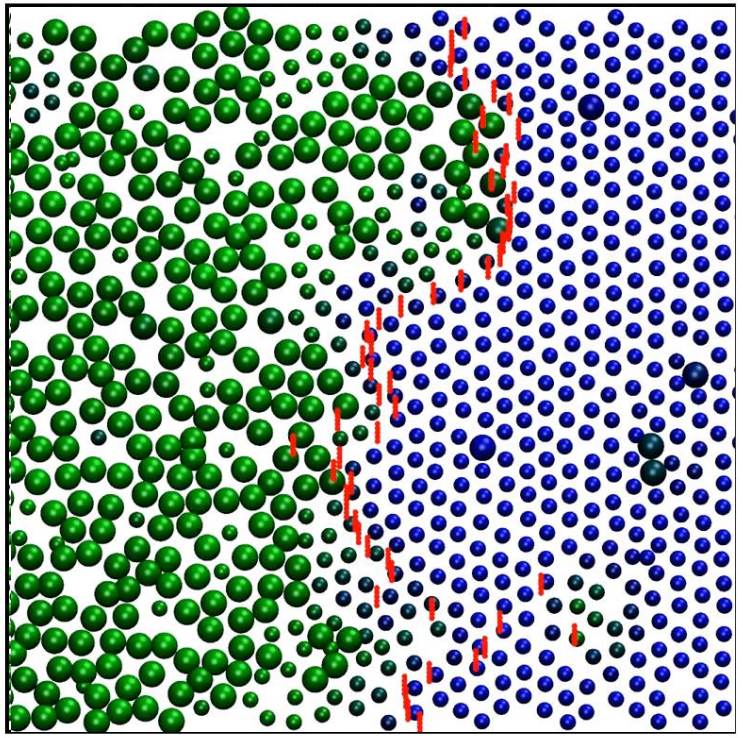
试图将毛细波理论方法拓展到固液界面台阶体系中。

5、研究方法和模拟细节

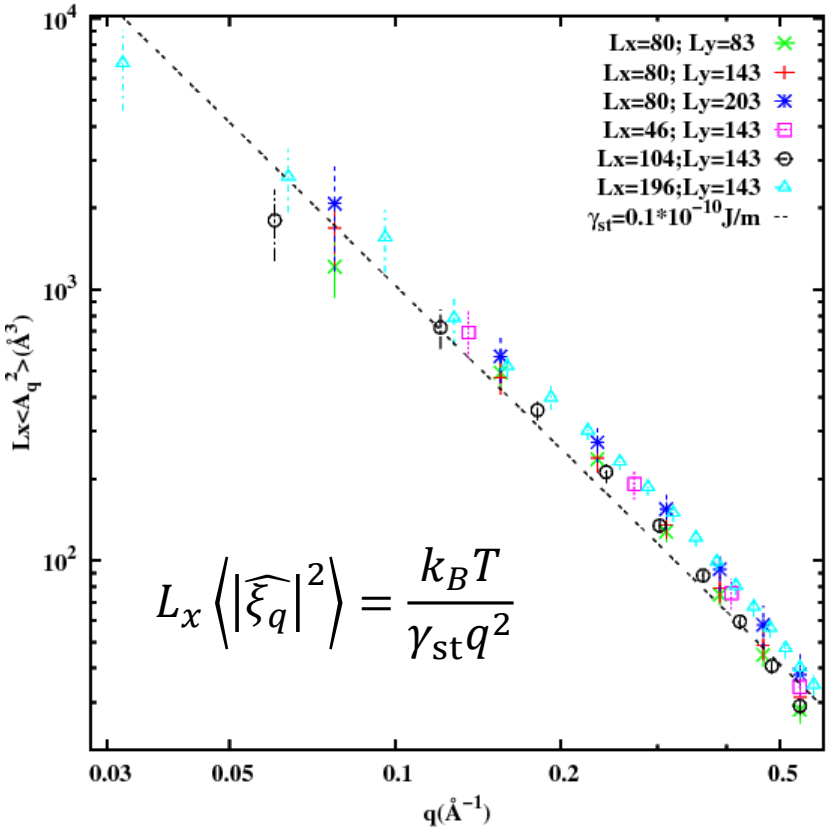
使用LAMMPS模拟；时间步长：2fs；模拟时长：50ns；相互作用势：EAM；温度：750K；

建立Al-Pb固液界面平衡态 → 确定界面层位置 → 使用序参量方法确定台阶位置 → 分析台阶震动谱，使用毛细波理论得出台阶自由能



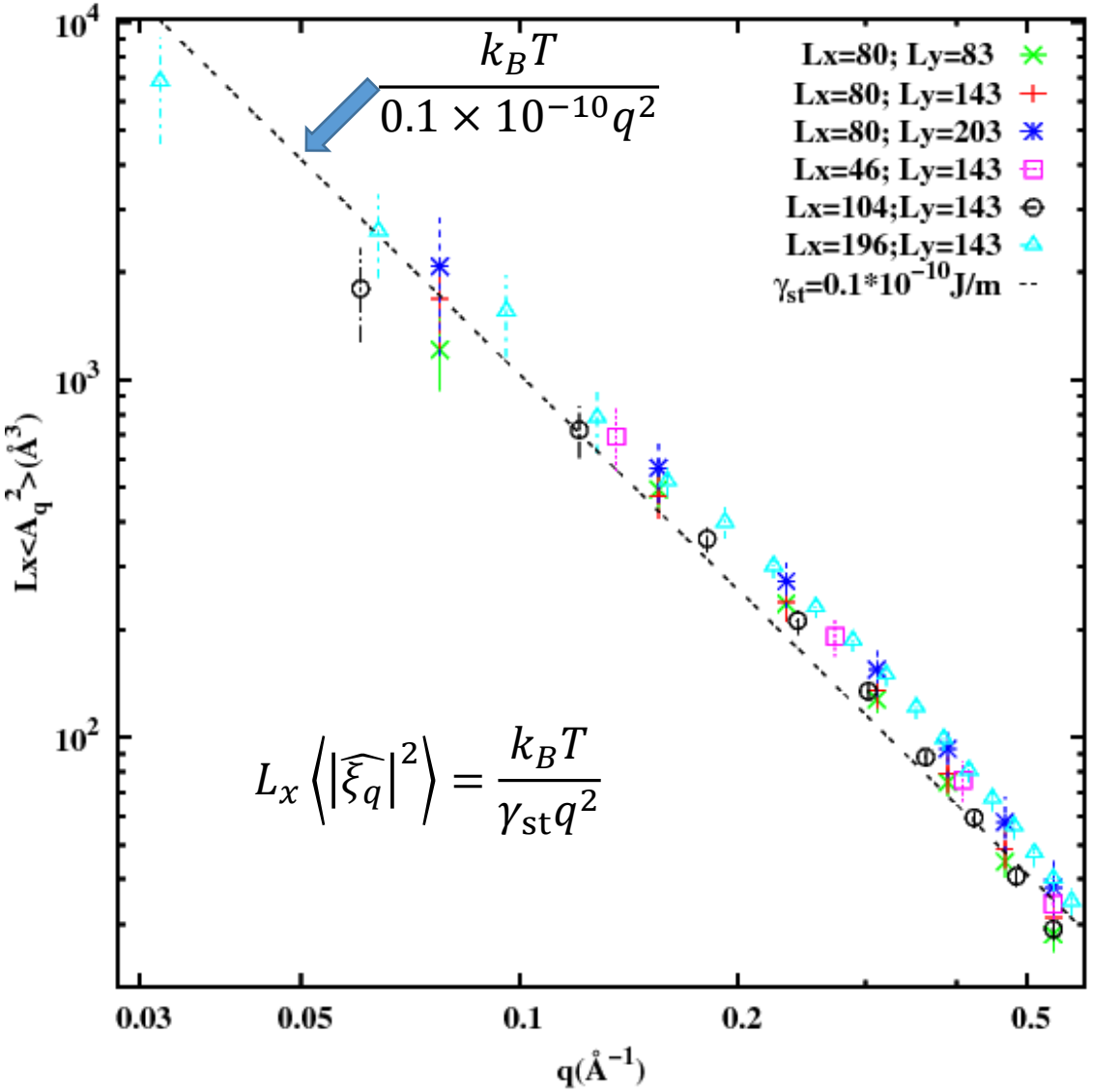


$$\varphi = \left| \frac{1}{N_b} \frac{1}{Z} \sum_r \sum_b \exp(i\vec{b} \cdot \vec{r}) \right|^2$$

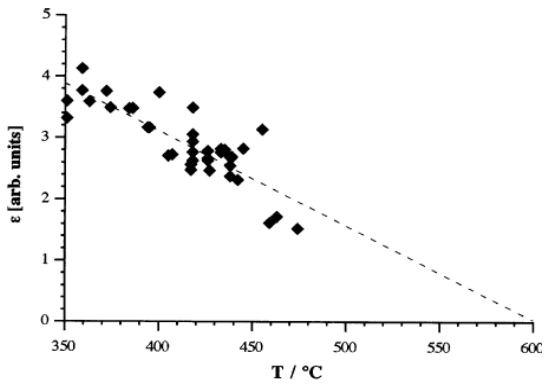


$$L_x \left\langle \left| \widehat{\xi_q} \right|^2 \right\rangle = \frac{k_B T}{\gamma_{st} q^2}$$

6、模拟结果



体系	原子数	Lx(Å)	Ly(Å)	γ_{st} $(10^{-10}J/m)$
A	42581	80	83	0.10(1)
B	73266	80	143	0.10 (2)
C	103906	80	203	0.09(2)
D	41883	46	143	0.08(1)
E	115168	127	143	0.11 (1)
F	177921	196	143	0.09 (1)
G	94205	104	143	0.10(1)
H	252899	277	143	0.11(2)



$T=623\text{K};\gamma_{st}=0.19\times10^{-10}J/m$

$T=873\text{K};\gamma_{st}=0.0J/m$

$T=750\text{K};\gamma_{st}=0.094\times10^{-10}J/m$

H.Gabrisch, L.Kjeldgaard, E.Johnson and U. Dahmen, Acta mater. 49,4259(2001)

5、总结

- 本次报告首先介绍了台阶和台阶自由能，以及很多关于台阶自由能的研究。针对目前研究情况，我们研究了固液界面台阶体系。

- 由于实验技术的限制，我们采用分子动力学模拟，结合毛细波涨落方法成功的得到了Al-Pb体系固液界面的台阶自由能。

- 我们拓展了CFM的适用范围，验证了该方法适用于计算固液界面内的台阶自由能。该方法同样也适用于其它体系。

Thank You ! ! !