

中科院物理研究所, 研究生专业学位课程

# 基于扫描探针显微镜 的分析方法

Scanning probe microscopy:  
analytical methods

主讲: 吴克辉、陆兴华、孟胜、单欣岩

时间: 9月16日开始、共计40课时

每周二、四上午8:30-10:30

地点: D楼212

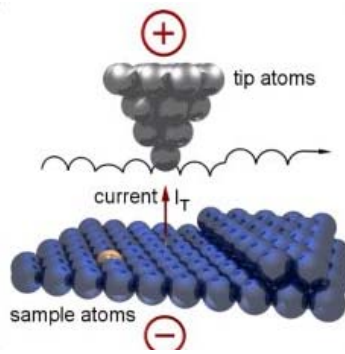
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## 第一章: 扫描探针显微镜概述 (4课时)

§ 1.1 显微镜发展简史	}	2课时
§ 1.2 STM的基本原理和应用		
§ 1.3 STM仪器设计及和制作		
§ 1.4 STM的基本理论	}	2课时
§ 1.5 STM的基本应用实例		

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### § 1.4 STM基本理论



### § 1.4 STM基本理论

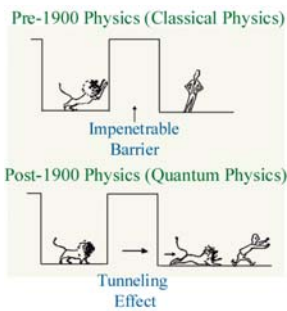
#### § 1.4.1 量子力学“一维势垒散射”

#### § 1.4.2 Barden公式

#### § 1.4.3 三维情况“Tersoff-Hamann”模型



凝聚态物理中有许多概念可以在经典物理中找到对应的图像，但“隧穿”这个概念是量子力学独有的，在经典物理中找不到对应的概念。



•隧穿现象在历史上许多重要的发现中扮演了重要的角色:

- H原子在强电场下自发电离（奥本海默，1928）
- 场致电子发射现象（Fowler and Nordheim, 1928）
- 重原子核的  $\alpha$  衰变（Gamov, 1928）

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**H原子在强电场下的电离**

**金属针尖表面的场致电子发射**

**金属-绝缘体-金属隧道结**

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**隧穿理论中的几个基本概念：**

1. 弹性隧穿和非弹性隧穿：在弹性隧穿中电子保持原有的能量；非弹性隧穿中电子则与固体中的一些元激发相作用，例如声子、磁子或等离子元，而损失能量。
2. 一维隧穿和三维隧穿：早期的隧穿实验使用平板型金属-绝缘体-金属夹层结构，故可适用一维隧穿模型。但在STM中针尖具有三维的形状，故考虑三维隧穿是必要的。
3. 方势垒与任意形状势垒：为简化问题可以从方势垒出发，并推广到任意形状势垒。
4. 含时或者不含时的处理方法：理论上可以由不含时的薛定谔方程出发，也可以由含时薛定谔方程出发，使用一级含时微扰的Fermi golden rule进行推导。

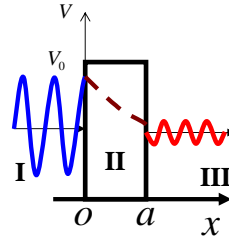
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§ 1.4.1：一维势垒散射问题

a.1 方势垒的穿透（隧道效应）

$$V(x) = 0, \quad x < 0, x > a$$

$$V(x) = V_0, \quad 0 \leq x \leq a$$



按经典力学观点，当一个粒子能量 $E < V_0$ 时，此粒子是不能越过此势垒的。 $E > V_0$ 时，此粒子全部越过势垒，不会部分被反射的。

按量子力学观点，无论一个粒子能量 $E < V_0$ 或 $E > V_0$ 时，此粒子都将有一定几率越过此势垒，也将有一定几率被反射回去。

§ 1.4.1：一维势垒散射问题

$$-\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} = E \varphi(x), \quad x \leq 0 \text{ 或 } x \geq a$$

I 区的解:  $\varphi_1(x) = e^{ikx} + R e^{-ikx}, \quad x \leq 0$

III 区的解:  $\varphi_3(x) = S e^{ikx}, \quad x \geq a$

以上考虑了粒子是从I区入射，在I区中有入射波、反射波；在III区只有透射波。

其中,  $e^{ikx}, R e^{-ikx}, S e^{ikx}$

分别代表入射波，反射波与透射波。

反射系数=

$$j_r / j_i = |R|^2$$

透射系数T=

$$j_t / j_i = |S|^2$$

§ 1.4.1：一维势垒散射问题

II区定态薛定谔方程为：

$$-\frac{\hbar^2}{2m} \frac{d^2 \varphi_2(x)}{dx^2} + V_0 \varphi_2(x) = E \varphi_2(x), \quad 0 \leq x \leq a$$

$$\frac{d^2 \varphi_2(x)}{dx^2} - k_2^2 \varphi_2(x) = 0, \quad (0 \leq x \leq a) \quad k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

得，  $\varphi_2 = Ae^{k_2 x} + Be^{-k_2 x}, (0 \leq x \leq a)$

与  $\varphi_1(x) = e^{ikx} + Re^{-ikx}, (x \leq 0)$

$\varphi_3(x) = Se^{ikx}, (x \geq a)$

在  $x=0, a$  处波函数与一阶导数要连续：



§ 1.4.1：一维势垒散射问题

根据连续条件，可求得4个系数R, S, A, B:

$$\varphi_1(0) = \varphi_2(0) \quad \frac{d\varphi_1(x)}{dx} \Big|_{x=0} = \frac{d\varphi_2(x)}{dx} \Big|_{x=0}$$

$$\varphi_2(a) = \varphi_3(a) \quad \frac{d\varphi_2(x)}{dx} \Big|_{x=a} = \frac{d\varphi_3(x)}{dx} \Big|_{x=a}$$

解之得，(11)、(12)式。

(11) 式:  $A = \frac{1}{2} \left[ \left(1 + \frac{ik}{k_2}\right) + R \left(1 - \frac{ik}{k_2}\right) \right] \quad B = \frac{1}{2} \left[ \left(1 - \frac{ik}{k_2}\right) + R \left(1 + \frac{ik}{k_2}\right) \right]$

(12) 式:  $A = \frac{S}{2} \left[ 1 + \frac{ik}{k_2} \right] e^{ika - k_2 a} \quad B = \frac{S}{2} \left[ 1 - \frac{ik}{k_2} \right] e^{ika + k_2 a}$



§ 1.4.1：一维势垒散射问题

由 (11) 与 (12)，消去A、B，得 (13)

$$(13) \text{ 式: } \begin{cases} (1 + \frac{ik}{k_2}) + R(1 - \frac{ik}{k_2}) = S(1 + \frac{ik}{k_2})e^{ika - k_2 a} \\ (1 - \frac{ik}{k_2}) + R(1 + \frac{ik}{k_2}) = S(1 - \frac{ik}{k_2})e^{ika + k_2 a} \end{cases}$$

由 (13) 式，消去R，得S， (15) 式:

$$(15) \text{ 式: } Se^{ika} = \frac{-2ik/k_2}{[1 - (k/k_2)^2]shk_2 a - 2i\frac{k}{k_2}chk_2 a}$$



§ 1.4.1：一维势垒散射问题

由 (15) 式得透射系数:  $T = \frac{1}{1 + (k_1^2 + k_2^2)/4k_1^2 k_2^2 \sinh^2 k_2 a}, (16)$

由 (13) 式消去S，得R，得反射系数:  $|R|^2 = \frac{(k^2 + k_2^2)^2 sh^2 k_2 a}{(k^2 + k_2^2)^2 sh^2 k_2 a + 4k^2 k_2^2}, (17)$

$$|R|^2 + |S|^2 = 1$$

由 (12) 式与S，

得A、B，从而得波函数:  $\phi_1, \phi_2, \phi_3$ 。



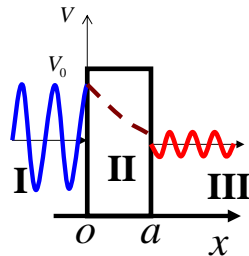
§ 1.4.1: 一维势垒散射问题

$$T = \frac{1}{1 + (k_1^2 + k_2^2) / 4k_1^2 k_2^2 \sinh^2 k_2 a}, \quad (16)$$

估算. 设  $\kappa a \gg 1$ , 此时  $\sinh \kappa a \approx \frac{1}{2} e^{\kappa a} \gg 1$

$$T \approx \frac{16k^2 \kappa^2}{(k^2 + \kappa^2)^2} e^{-2\kappa a}$$

$$= \frac{16E(V_0 - E)}{V_0^2} \exp\left[-\frac{2a}{\hbar} \sqrt{2m(V_0 - E)}\right]$$



§ 1.4.1: 一维势垒散射问题

对任意形状的势垒(见图), 势垒贯穿几率公式推广 (WKB近似) 为:

$$D = D_0 e^{-\frac{2}{\hbar} \int_a^b \sqrt{2m[U(x) - E]} dx}$$

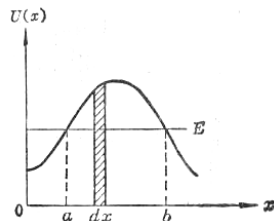


图 17 任意形状的势垒

上述推导:

1. 隧道结两边没有施加电压
2. 没有考虑隧道结两边的电子态密度

## § 1.4.2 Bardeen 公式

1960年Bardeen利用多体理论发展了时间相关微扰理论，可以计算电子从一个电极（针尖 $E_p, \psi_i$ ）转移到另外一个电极（样品 $E_s, \psi_f$ ）的速率，由电子转移速率由费米黄金定则来确定（参见曾谨言《量子力学》（第四版）卷 I P393）。

费米黄金定则：

$\rho_f(E)$ 表示体系（ $H_0$ ）的末态的态密度，从初态 $\varphi_i(E_i)$ 到末态 $\varphi_f(E_f)$ 附近的一系列可能的末态的跃迁速率之和为：

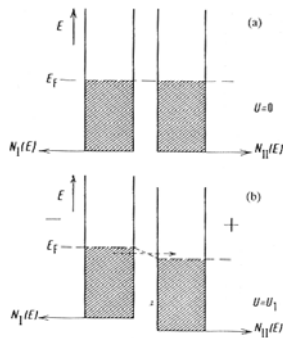
$$\omega = \int dE_f \rho(E_f) \omega_{if} = \frac{2\pi}{\hbar} \rho(E_f) |H'_{if}|^2$$

$$\text{其中 } \omega_{if} = \frac{2\pi}{\hbar} |H'_{if}|^2 \delta(E_f - E_i)$$

$H'_{if} = \langle f | H' | i \rangle$  为微扰 $H'$ 在初态和末态之间的矩阵元。

### Bardeen 公式

如果将STM的针尖和样品简化为两个平面金属隧道结，可以应用费米黄金定则，从左边的某个量子态隧穿到右边某个态的几率为：



$$j_t = \left(\frac{2\pi}{\hbar}\right) |M_{rl}|^2 n_r (1 - f_r)$$

隧穿矩阵元      Fermi 分布函数  
 右边电极的态密度

仅在针尖和样品距离较远，针尖对样品的电子态的影响可以忽略不计时适用。



§ 1.4.3

三维模型

Tersoff and Hamann  
 PRB 31, 805(1984)

**Tersoff-Hamann模型**

$$I = \frac{\hbar \pi e}{\eta} \sum_{\mu\nu} f(E_\mu) |1 - f(E_\nu + eV)| |M_{\mu\nu}|^2 \delta(E_\mu - E_\nu)$$

式中,  $\hbar$  隧穿矩阵元

$$|M|_{\mu\nu} = \frac{\hbar^2}{2m} \int_s (\psi_\mu^* \nabla \psi_\nu - \psi_\nu \nabla \psi_\mu^*) \cdot d\vec{s}$$

$\psi_\mu, \psi_\nu$  分别为样品和针尖的波函数。

在低温和小偏压条件下,

$$I = \frac{2\pi e^2 V}{\hbar \eta} \sum_{\mu\nu} |M_{\mu\nu}|^2 \delta(E_\mu - E_F) \delta(E_\nu - E_F)$$

样品波函数

$$\psi_\mu = \frac{1}{\sqrt{\Omega_s}} \sum_G a_G \exp\{-\kappa^2 + |\vec{K}_G|^2\}^{1/2} z\} \exp(i\vec{K}_G \cdot \vec{x})$$

式中,  $\Omega_s$  为样品体积,  $\kappa = \sqrt{2m\phi_s}/\hbar$  为衰减常数,  
 而,  $\vec{K}_G = \vec{K}_\parallel + \vec{G}$ ,  $\vec{K}_\parallel$  为表面波矢,  $\vec{G}$  为倒格矢。

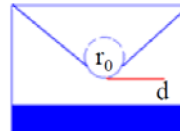
针尖波函数

$$\psi_\nu = \frac{1}{\sqrt{\Omega_t}} \times \frac{\exp(-\kappa |\vec{r} - \vec{r}_0|)}{\kappa |\vec{r} - \vec{r}_0|} \times c, \kappa \text{Re}^{\kappa R}$$

式中,  $\Omega_t$  为针尖体积,  $R$  为针尖曲率半径,

$\kappa = \sqrt{2m\phi_t}/\hbar$  为衰减常数

s-wave近似 (球形渐近波)



$$\frac{e^{-\kappa r}}{\kappa r} = \int d^2 q b(q) \exp[-(\kappa^2 + q^2)^{1/2} |z|] \exp(i\vec{q} \cdot \vec{x})$$

$$b(q) = \frac{1}{2\pi} \frac{1}{\kappa^2} \left(1 + \frac{q^2}{\kappa^2}\right)^{-1/2}$$



代入隧穿矩阵元的计算公式，有

$$M_{\mu\nu} = \frac{\eta^2}{\hbar^2 m} 4\pi\kappa^{-1} \Omega^{-\frac{1}{2}} \times \kappa \operatorname{Re} e^{\kappa R} \psi_{\mu}(\vec{r}_0)$$

隧道电流

$$I = 32\pi^3 \eta^{-1} e^2 V \phi_s \phi_t D_t(E_F) R^2 \kappa^{-4} e^{2\kappa R} \times \sum_{\mu} |\psi_{\mu}(\vec{r}_0)|^2 \delta(E_{\mu} - E_F)$$

$$\sigma = \frac{I}{V} \sim 0.1 R^2 e^{2\kappa R} \rho_s(\vec{r}_0, E_F)$$

局域态密度 (LDOS)

$$\rho_s(\vec{r}_0, E_F) = \sum_{\mu} |\psi_{\mu}(\vec{r}_0)|^2 \delta(E_{\mu} - E_F)$$

$$\rho_s(\vec{r}_0, E_F) \sim \exp[-2\kappa(R+d)], \sigma \sim e^{-2\kappa d}$$

低偏压下STM图对应样品在费米能级附近的LDOS曲面



## § 1.4.2 STM 基本应用实例

### 1. 清洁/吸附表面的重构

弛豫与重构  
Si(111)表面  
Si(100)表面  
Moiré pattern

### 2. 表面动态过程

TiO<sub>2</sub>表面吸水  
Si(111)-7x7表面吸附



## 1. 弛豫与重构

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### 金属表面: 典型的弛豫机制

#### Contractive relaxation of low index metal surfaces

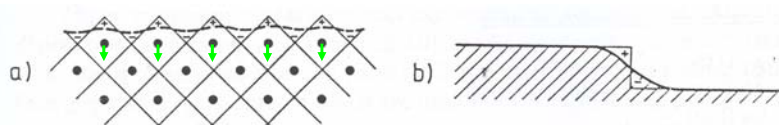
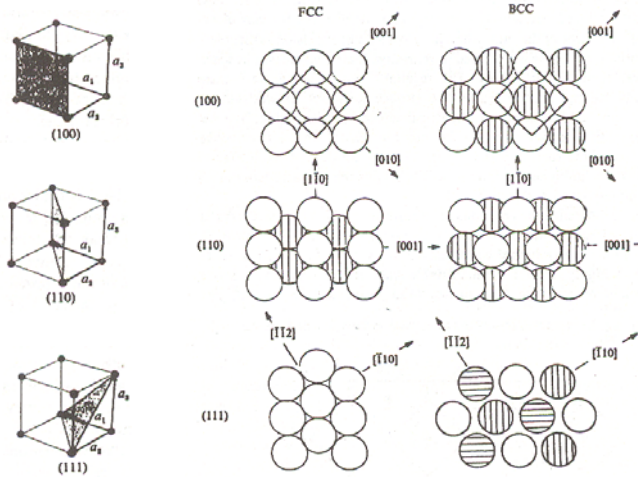


Fig.3.7. Schematic representation of the formation of electronic surface dipoles at metal surfaces (a) by smearing out of the electronic charge distribution of the Wigner Seitz cells at the surface (*rectangles*), and (b) by smearing out of the electronic charge distribution at a step

金属: 电子公有化, jellium模型, 没有方向性.

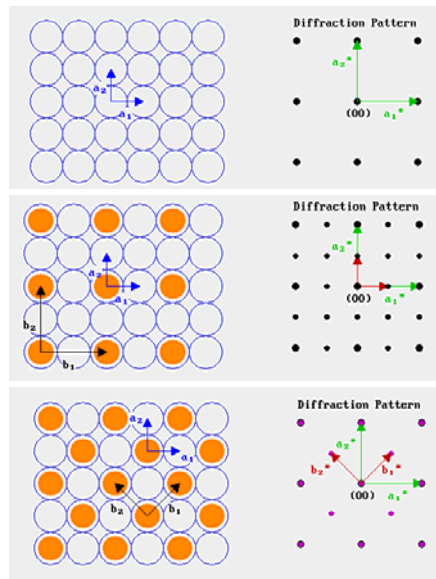
表面物理与材料科学

### Low-index surfaces of cubic lattice



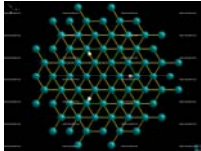
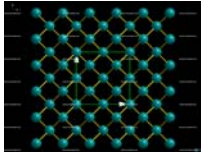
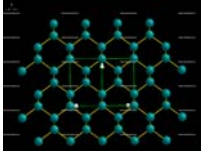
Vertical and horizontal markings indicate the second and third layers, respectively.


### 重构：周期重排



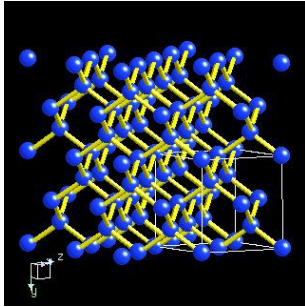
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清洁硅表面

- Si(111): 
- Si(100): 
- Si(110): 




Space group: Fd-3m (Space group number: 227)  
 Structure: diamond  
 Cell parameters:  
 a: 543.09 pm  
 b: 543.09 pm

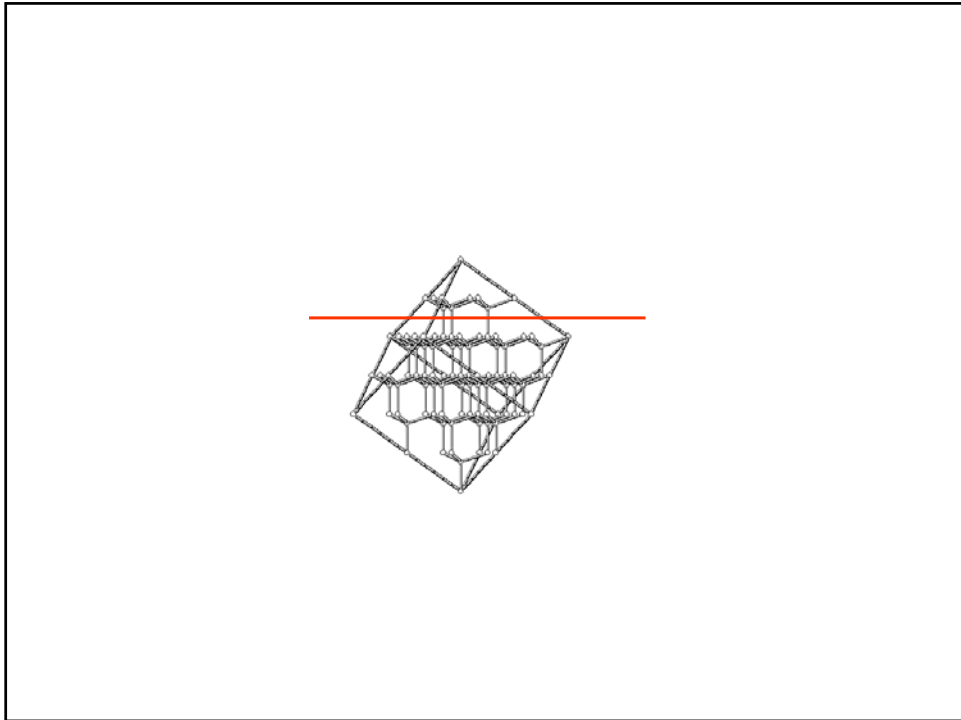




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Si(111)





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## Si(111)2X1

Sp<sup>2</sup>杂化-π链模型

(111)-2<sub>1</sub>

from Pandy Phys. Rev. Let 47(1981)1913

### Famous Si(111)7x7

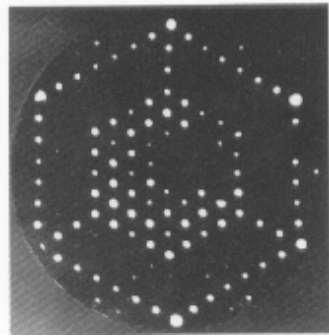


Fig.2 Low-energy electron diffraction (LEED) pattern of the Si(111)7x7 reconstruction [3].

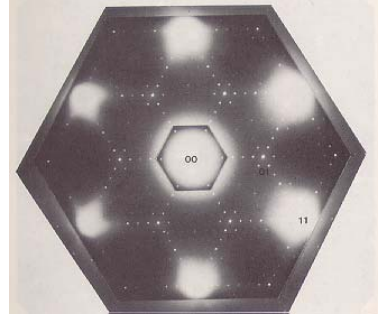


Fig.3 Transmission electron diffraction (TED) pattern of the Si(111)7x7 [4].

Schlier, R.E. and Fransworth, H.E., *J.Chem.Phys.* 30, 917 (1959).

Takayangi, K., Tanishiro, Y., Takahashi, S. and Takahashi, M., "Structure analysis of Si(111)-7x7 reconstructed surface by transmission electron diffraction", *Surf. Sci.* 164, 367 (1985).



### Si(111)7X7

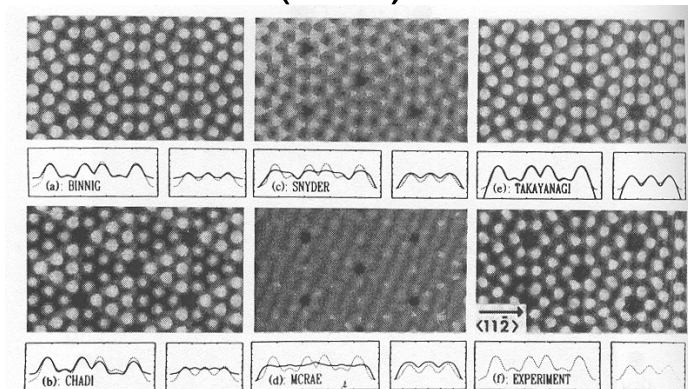
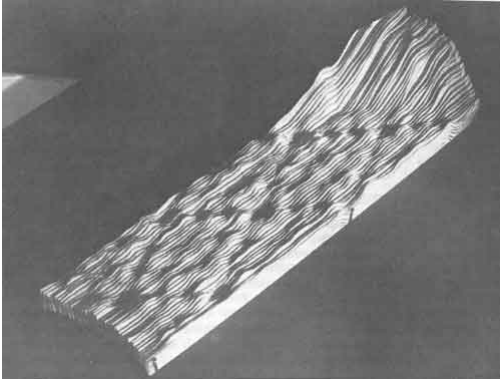


Fig. 4.3. (a)–(e) STM images calculated for (a) Binnig's model, (b) Chadi's model, (c) Snyder's model, (d) McRae's model, and (e) Takayanagi's model. (f) Measured STM image. The line scans run from corner hole to corner hole along the long (left) and short (right) diagonal of the (7×7) unit cell. The vertical range in these line scans is 4 Å. Solid lines are calculations, dashed lines represent the experimental results (Tromp *et al.*, 1986).



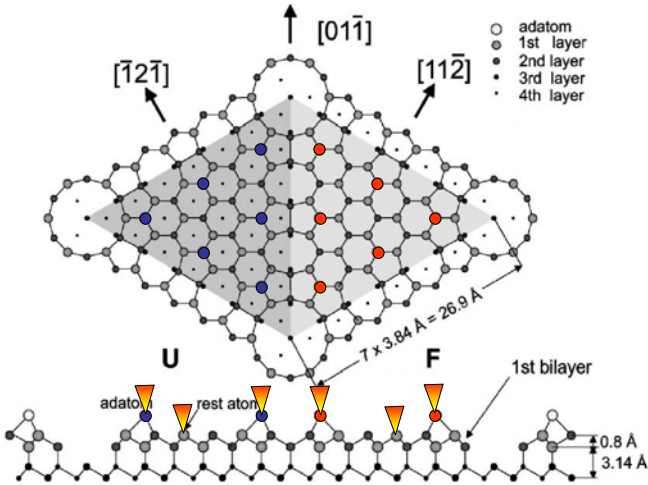
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The "relief" of 7x7 silicon (111), produced by Gerd Binnig in 1982 (courtesy of IBM research center Zürich)

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○ adatom  
 ● 1st layer  
 ● 2nd layer  
 ● 3rd layer  
 ● 4th layer

$[11\bar{2}]$   $[1\bar{2}1]$   $[011]$

$7 \times 3.84 \text{ \AA} = 26.9 \text{ \AA}$

U rest atom F 1st bilayer

0.8 Å 3.14 Å

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adatom  
 dimer  
 rest atoms  
 (1x1) bulk

Si(111)-(7x7) DAS model (Takayanagi/Tong) BAI,SAC p14

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“有位错”与“无位错”半原胞

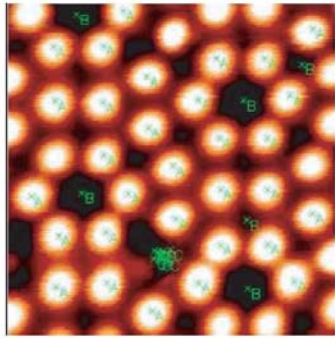
(a) (b) (c)

UNFAULTED HALF FAULTED HALF

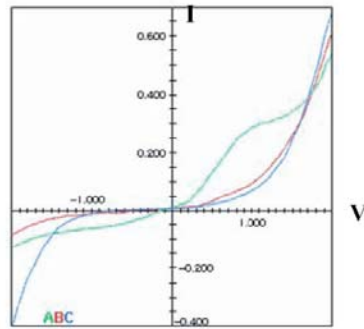
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# Scanning Tunneling Spectroscopy

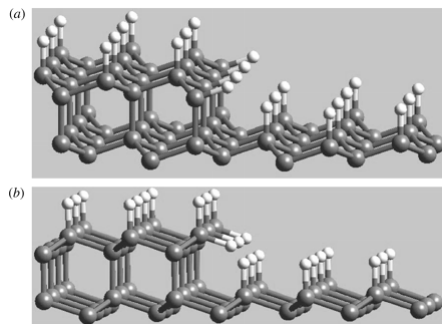
Si(111)-(7x7)



Tunneling I(V) curves at the specified points A,B,C



We can study LDOS as a function of energy by varying voltage on tip




Images of a ball and stick representation of steps on hydrogen-terminated {111} diamond surfaces: (a) a step edge with a local {110} like structure requiring a two-atom addition event to continue growth and (b) a step edge with a local {100} dihydride structure requiring only one-atom addition events to continue growth.



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# Si(100)

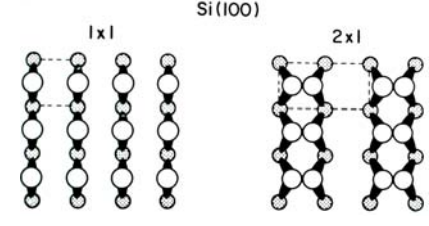


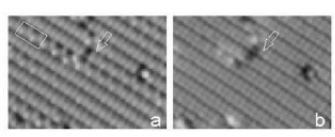
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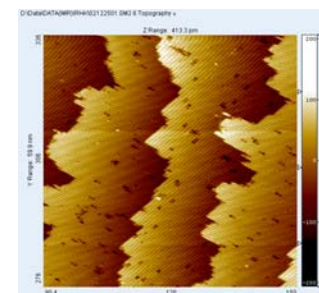
## Structure model of the Si(100)-2x1

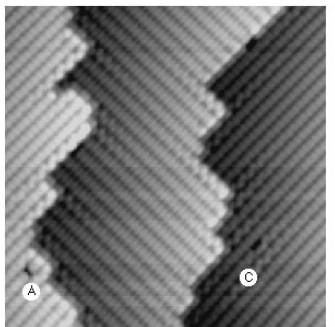
*Tromp et al., PRL 1985*


Si(100)

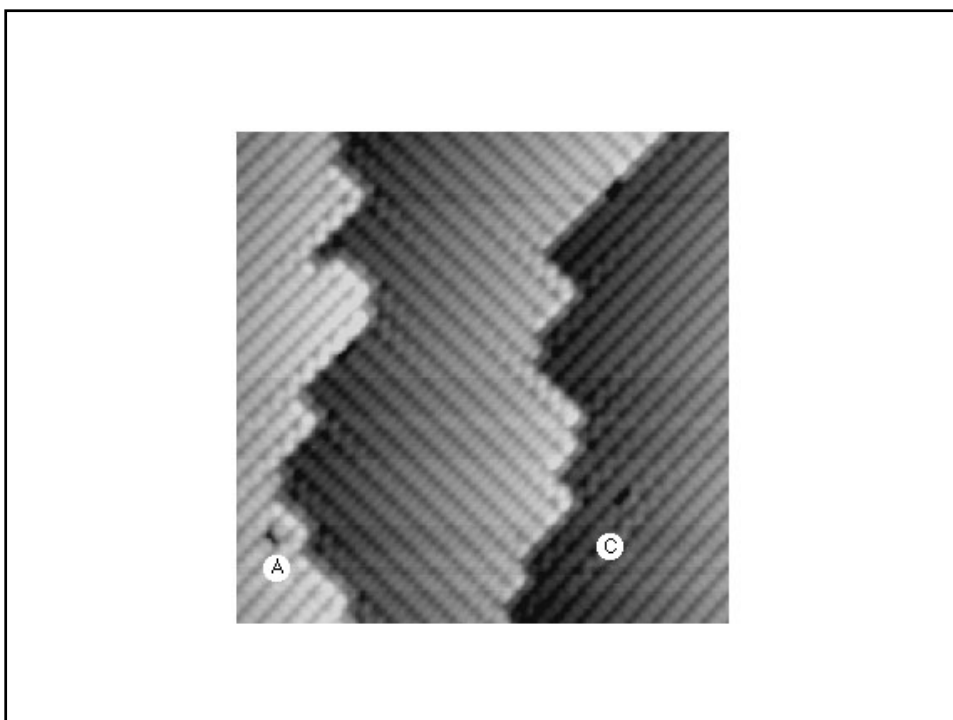
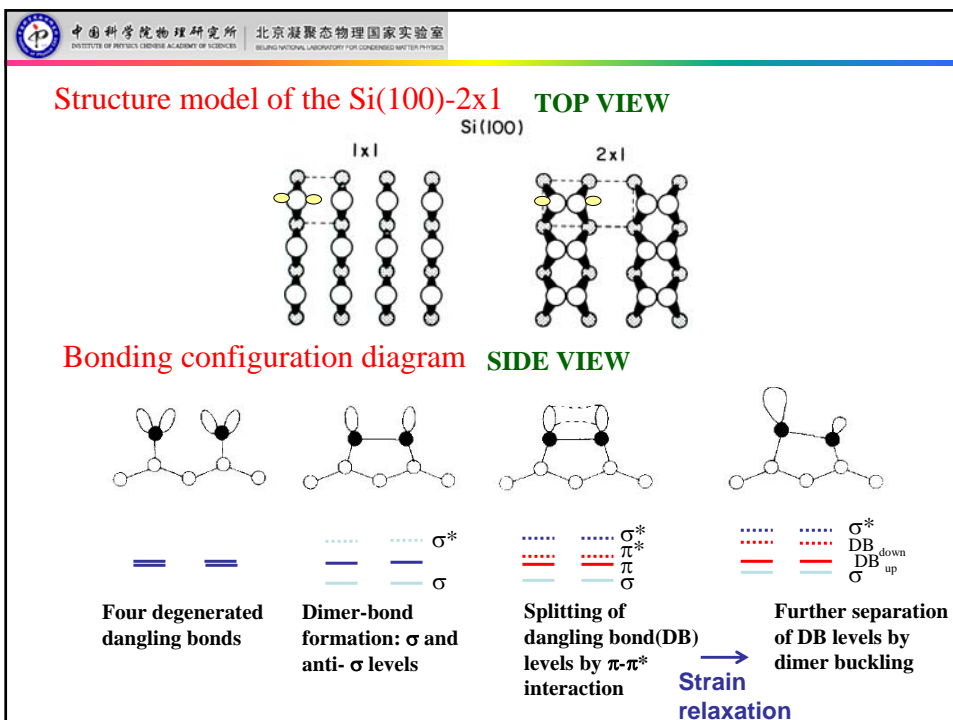












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Si(100)-2x1  $\rightarrow$  c(4x2)

filled states (-1.0 V) empty states (1.0 V) at 63K.

Takashi Yokoyama\* et al. PRB 61,6

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## STM observations below 50 k

(a) 29K (b) 43K (c) 50K

(d) 43K topographic (e) 43K current (f) change in the component ratio

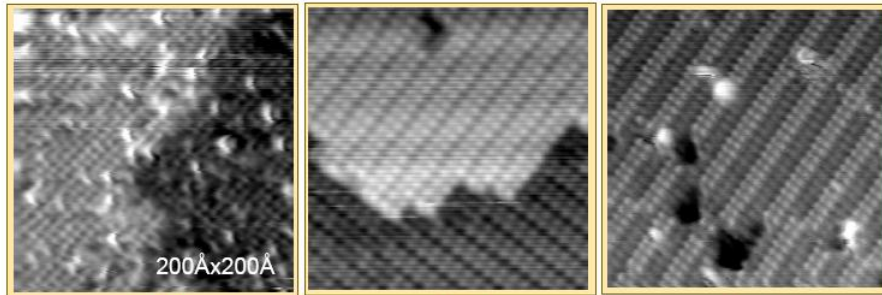
ratio %

Temperature (K)

From T. Uda et al/ surface science 76(2004) 147-162

### Hydrogen-terminated Si(100)-2x1 Surface

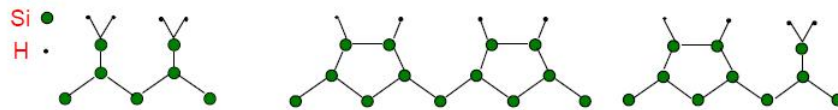
Dimer buckling is killed by hydrogen-termination – strain increases



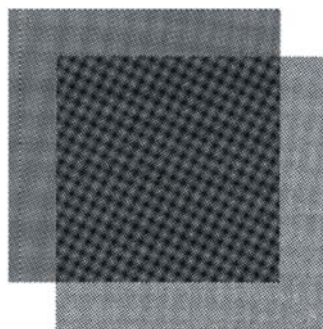
1x1  
Dihydride

2 x 1  
Monohydride

3 x 1  
Monohydride + Dihydride



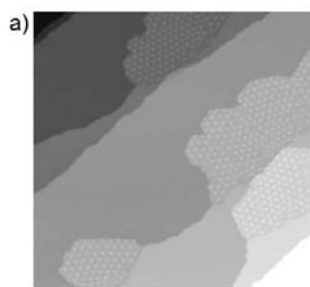
莫尔条纹  
Moiré pattern



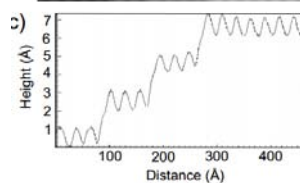
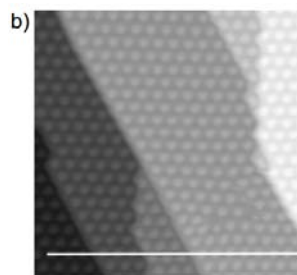
**莫尔条纹**是18世纪法国人莫尔首先发现的一种光学现象。两套(或多套)周期网格之间以恒定的角度和频率发生干涉, 当人眼无法分辨这两条线或两个物体时, 只能看到干涉的花纹, 即莫尔条纹。

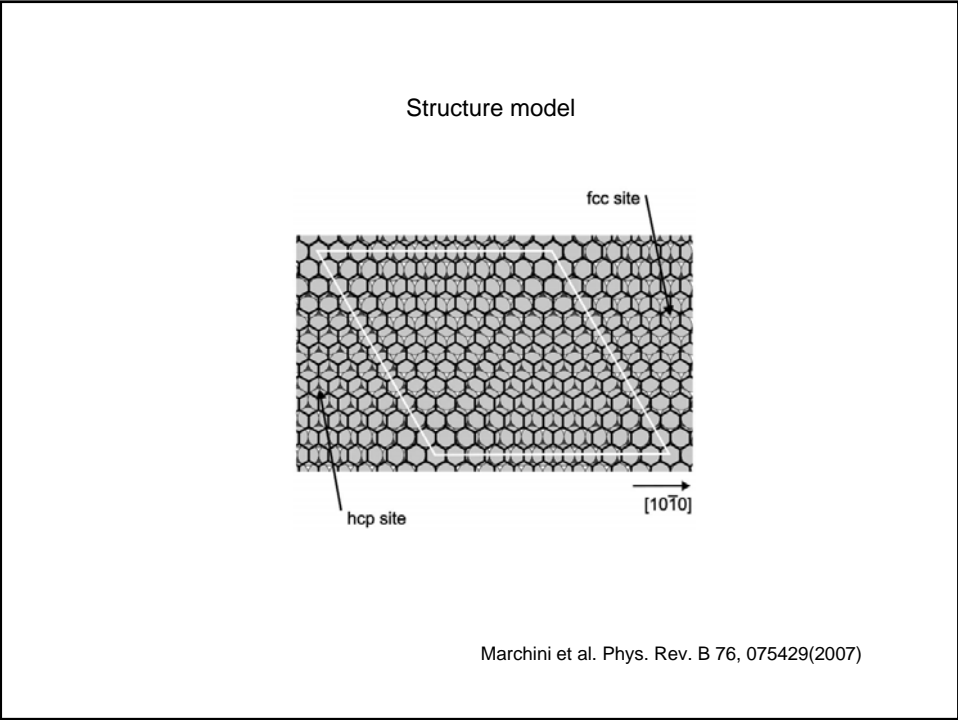
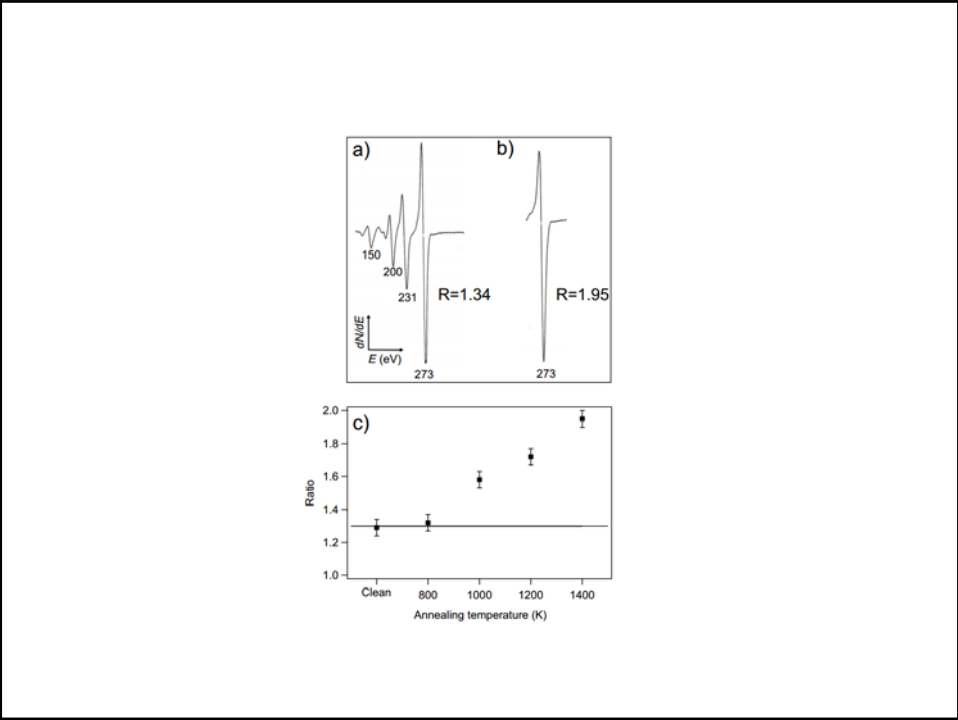
在清洁表面上蒸发单层薄膜, 表面晶格和薄膜的晶格之间的干涉, 造成周期性的调制结构, 也称为莫尔条纹, 从莫尔条纹中能够获得很多薄膜结构的信息。

### Graphene on Ru(0001)



制备方法: 高温退火清洁 Ru表面





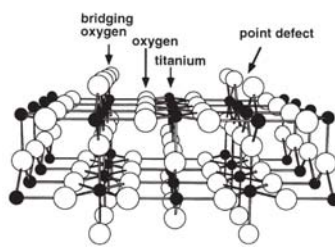
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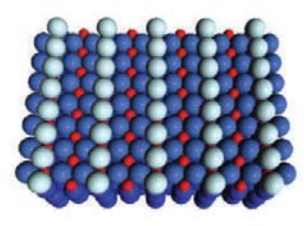
### 3. TiO<sub>2</sub>表面吸水过程

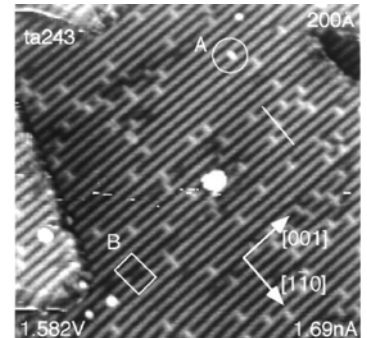
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### TiO<sub>2</sub> (110) 的表面原子结构





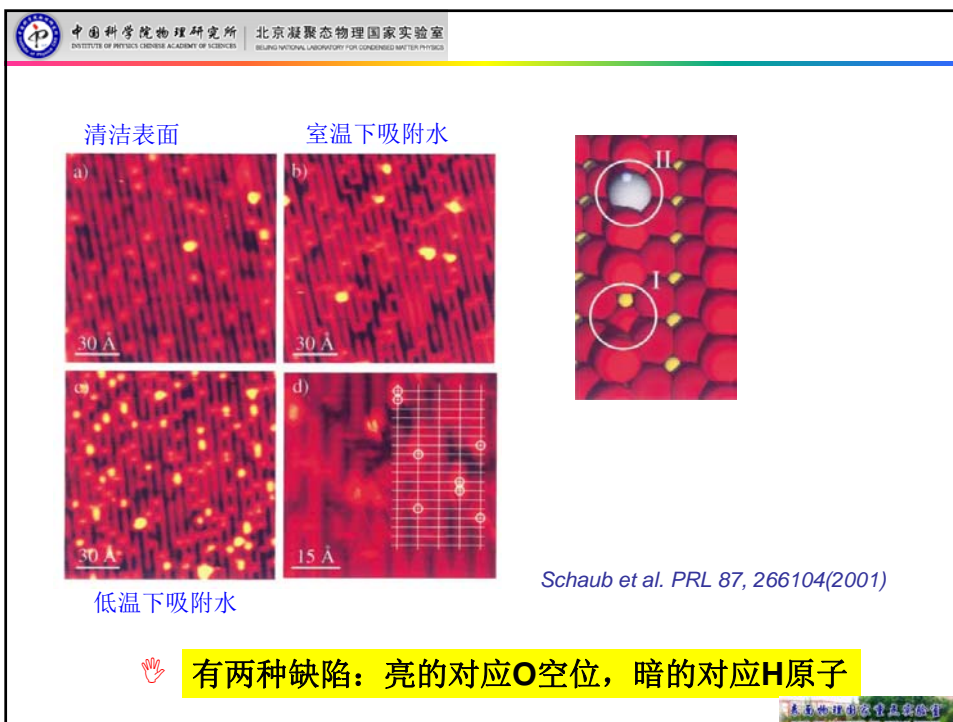
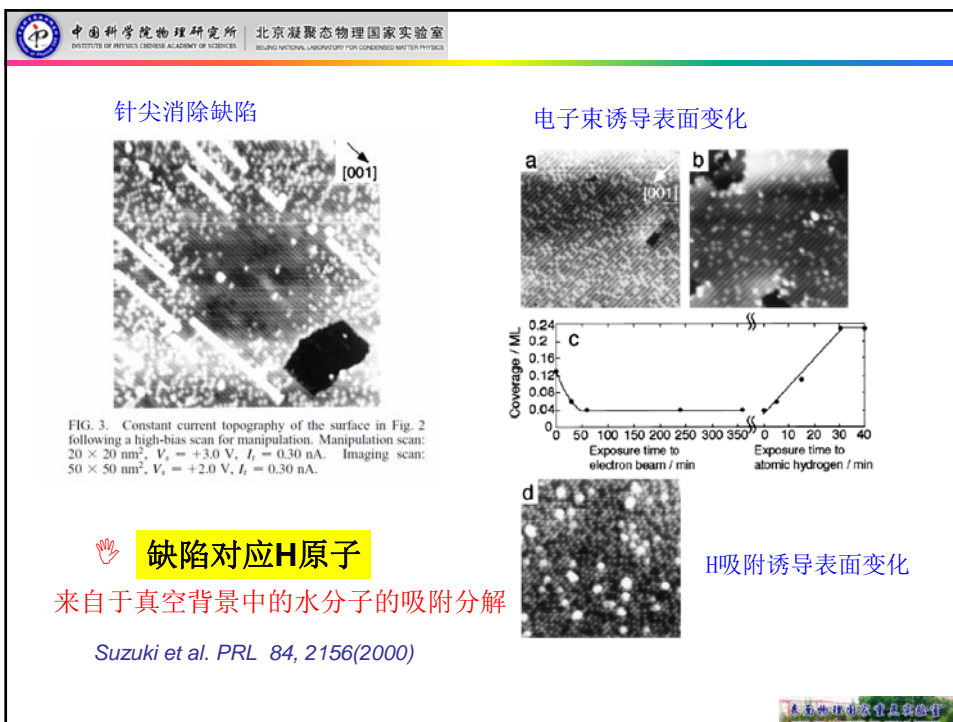


**STM 图像**  
 注意：暗线对应氧链

**缺陷对应氧空位**

*Diebold et al. Surf. Sci. 411, 137(1998)*

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氧分子中介的氧空位移动??

困惑??

*Thompson et al. Chem. Phys. Lett. 393, 28(2004)*

*Rasmussen et al. J. Chem. Phys. 120, 988(2004)*

*Wu et al. PRB 68, 241402(2003)*

● Ti surface atom  
● O surface atom  
● adsorbed atom

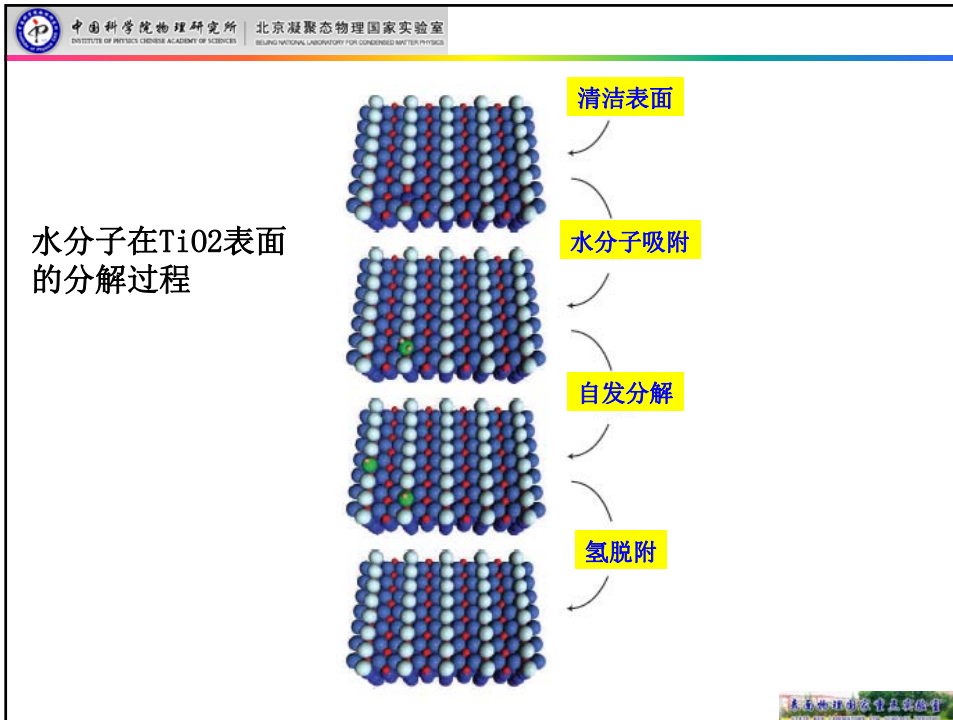
*Schaub et al. Science 299, 377(2003)*

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清洁表面      针尖移除亮点      吸水

亮的对应H原子，暗的对应O空位

*Bikondoa et al. Nature Mater. 5, 189(2006)*



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## 水分子在TiO<sub>2</sub>表面的分解过程

一对OH基团在氧空位上的形成及其迁移过程

● BBO   ● Ti   ● H<sub>2</sub>O

*Li et al. J. Am. Chem. Soc. 130, 9080-9088 (2008)*

中国科学院物理研究所

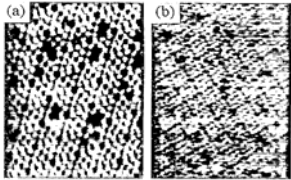
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## 碱金属在Si (111) 7x7表面的吸附

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**Na on Si(111)-(7x7): Previous STM observations**



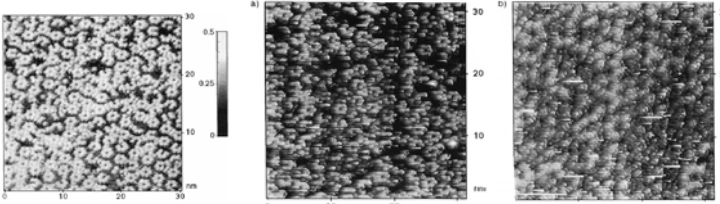
(a) (b)

D. Jeon et al. Appl. Surf. Sci. 94, 493(1996)

**DIFFICULTIES:**

- ☞ **Extremely-High Vacuum (XHV) is needed**
- ☞ **AM Coverage determination**
- Not by STM alone

---



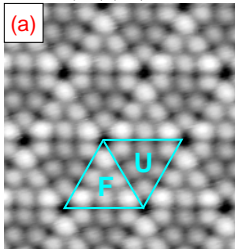
J. J. Paggel et al. Surf. Sci. 414,221(1998)

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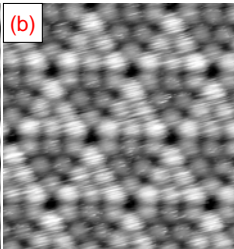
中国科学院物理研究所 北京凝聚态物理国家实验室  
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☞ Filled state STM images, -1.2 V, 20pA, **Na /Si(111)-(7x7):  $\theta < 0.08$  ML**

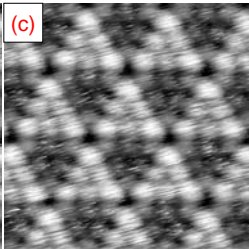
Clean Si(111)-(7x7)      1 atom/UC (0.02 ML)      2 atom/UC(0.04 ML)



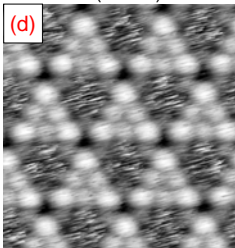
(a)



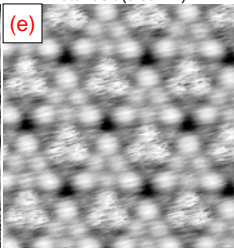
(b)



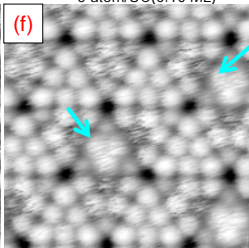
(c)



(d)

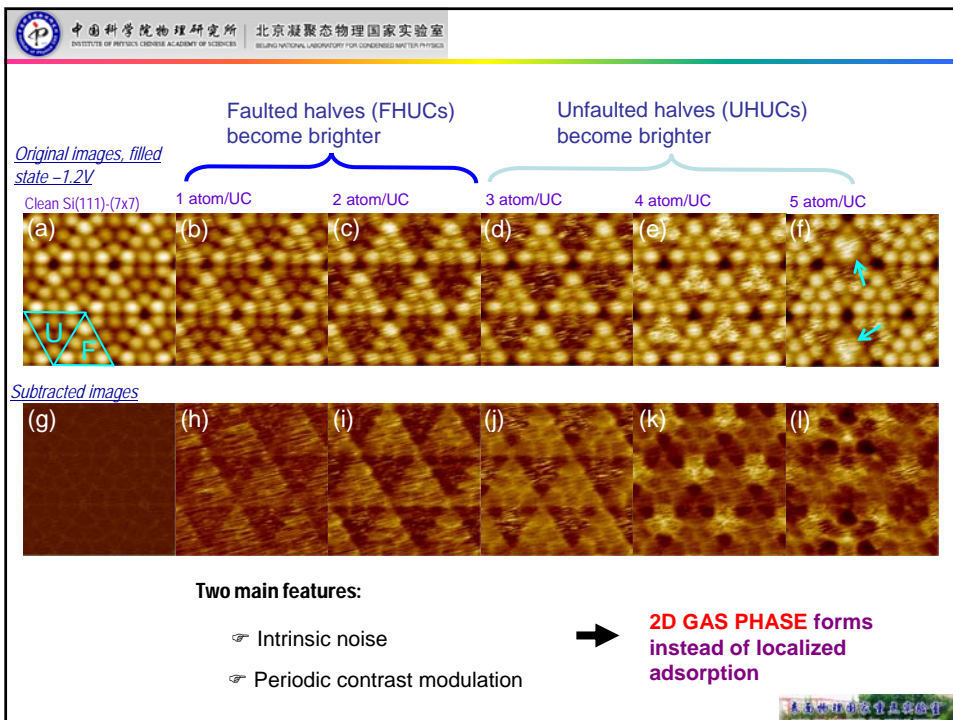
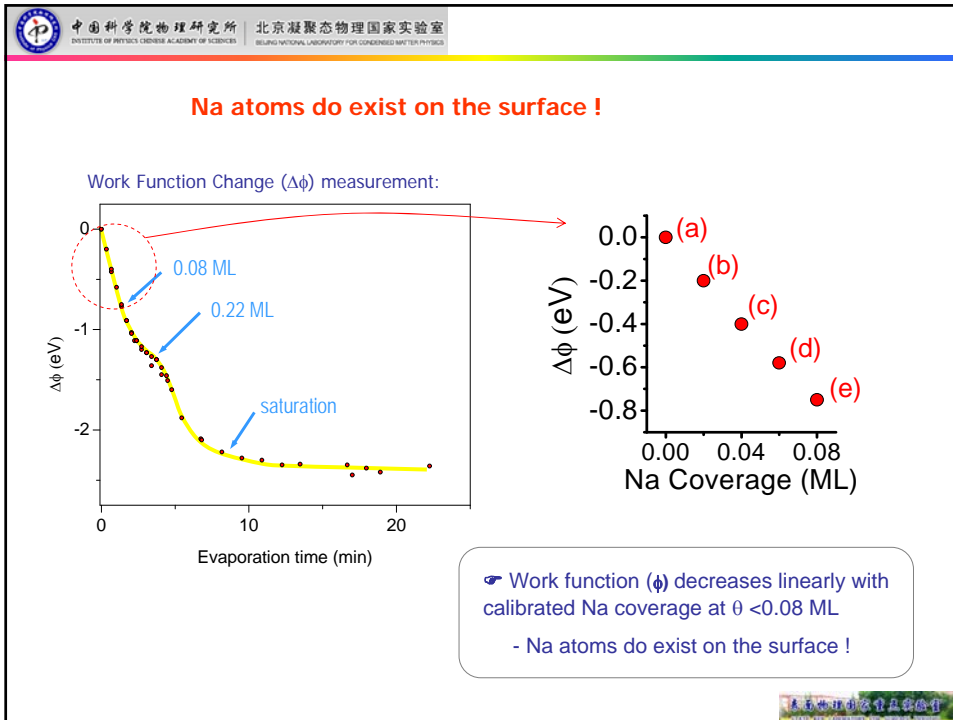


(e)



(f) Na cluster

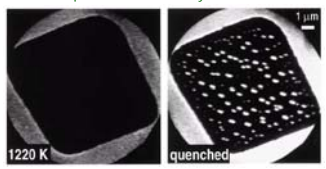
☞ No visible adsorption site (dangling bond adsorption) at  $\theta < 0.08$  ML



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**eg.1: Clean Si(100) surface at HT:**  
 - Increased adatom mobility at HT

R. M. Tromp and M. Mankos, Phys. Rev. Lett. 81, 1050(1998)

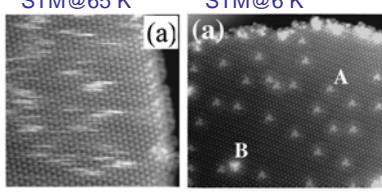


1220 K      quenched

Low energy electron microscopy (LEEM) observation

**eg. 2. Ag adatoms on Ag/Si(111)-√3x√3**  
 - Surface with small corrugation

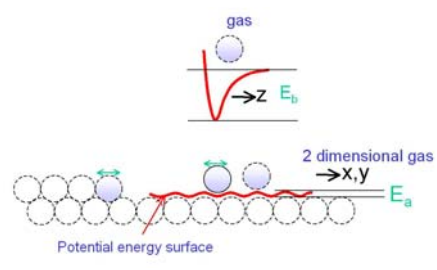
STM@65 K      STM@6 K



(a) (a)

N. Sato, et al. Phys. Rev. B60, 16083(1999)

**Examples of 2D Gas**



gas  
 $V \rightarrow z$   $E_b$

2 dimensional gas  
 $\rightarrow x, y$   $E_a$

Potential energy surface

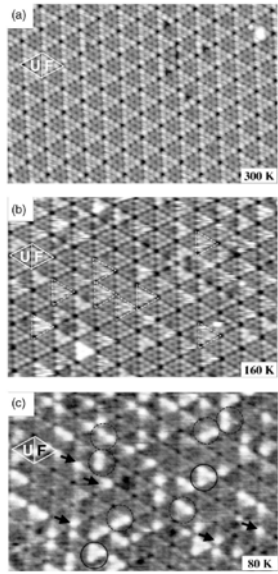
Diffusion probability:

$$n = A e^{-E_a/kT}$$

To form 2D gas, a system either has small potential barrier or is heated up

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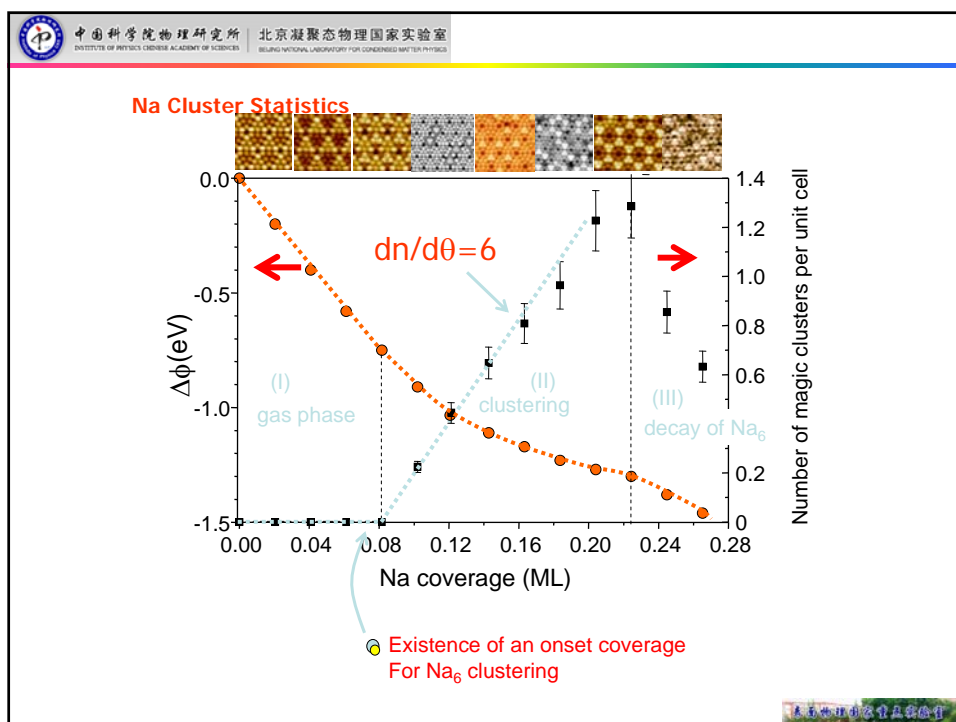
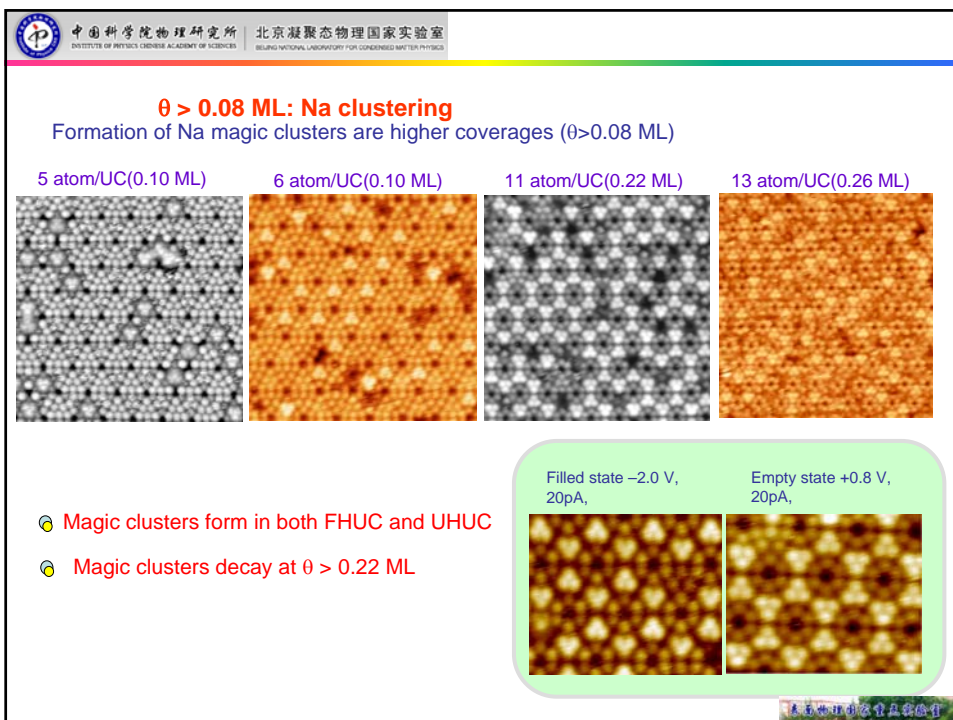
**Direct evidence of diffusing Na atoms: Cooling**



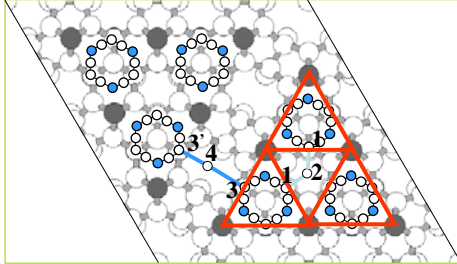
(a) 300 K

(b) 160 K

(c) 80 K



### Case 1: Single Na Adsorption



#### Results:

- Na atom on top of Si adatoms or rest atoms is unstable
- The most stable sites are within three "attraction basins" inside each half 7x7 unit cell

#### Binding energies:

- Inside a basin:

FHUC:  $E_b = 2.26 \pm 0.01$  eV

UHUC:  $E_b = 2.20 \pm 0.01$  eV

- Diffusion barriers ( $E_a$ ):

$$n = A e^{-E_a/kT}$$

Inside a basin :  $E_a = 0.14$  eV ( $10^{10}$  successful hopping/ s)

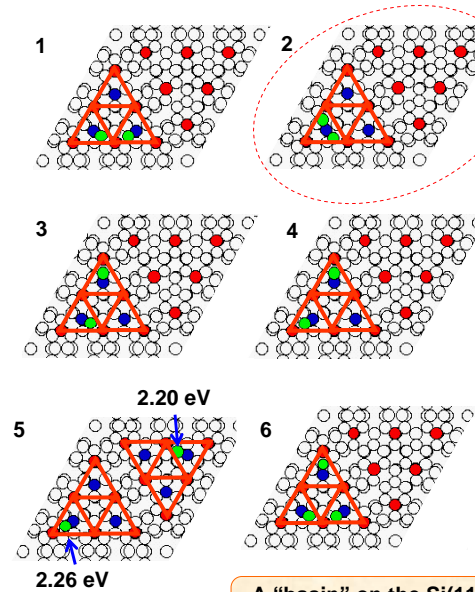
1-2-1 path:  $E_a = 0.36$  eV ( $10^7$  successful hopping/ s)

3-4-3' path:  $E_a = 0.42$  eV ( $10^6$  successful hopping/ s)

Results: The potential energy surface is flat along certain pathways !



### Coverage-dependent calculation : multiple Na atoms



Model	$E_b/\text{Na}$ (eV)
1	2.262
2	2.117
3	2.259
4	2.253
5	2.238
6	2.262

#### Single atom calculation:

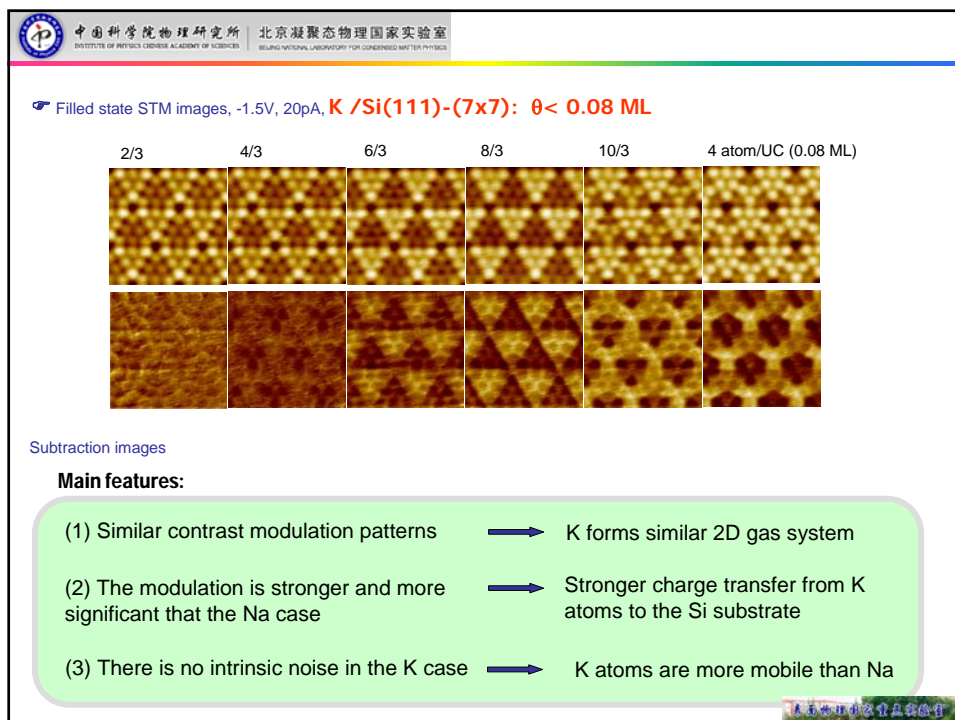
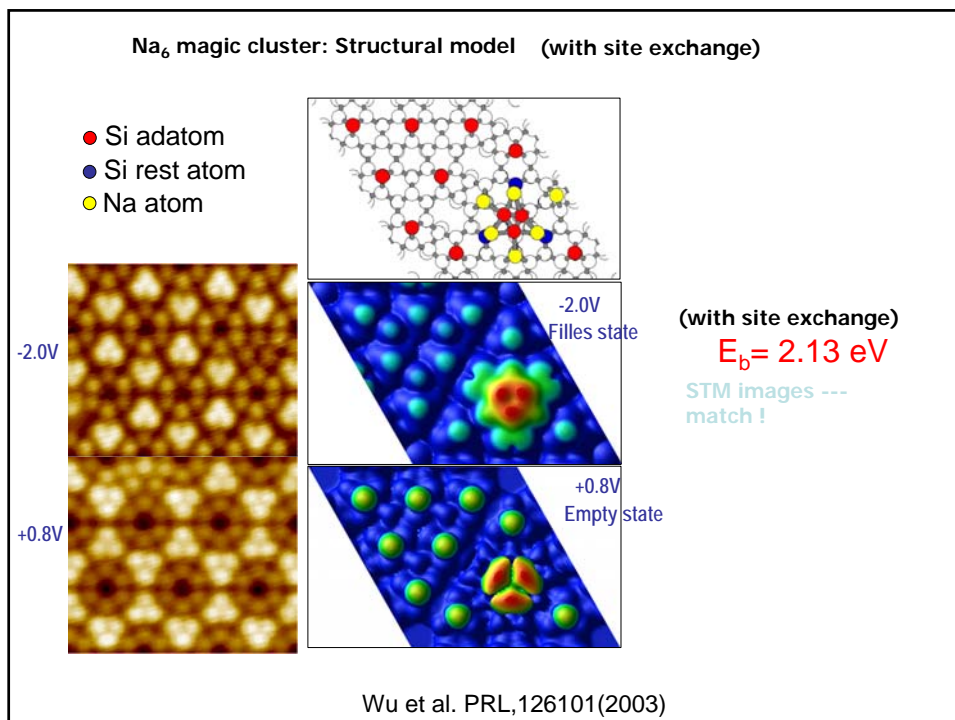
FHUC:  $E_b = 2.26 \pm 0.01$  eV

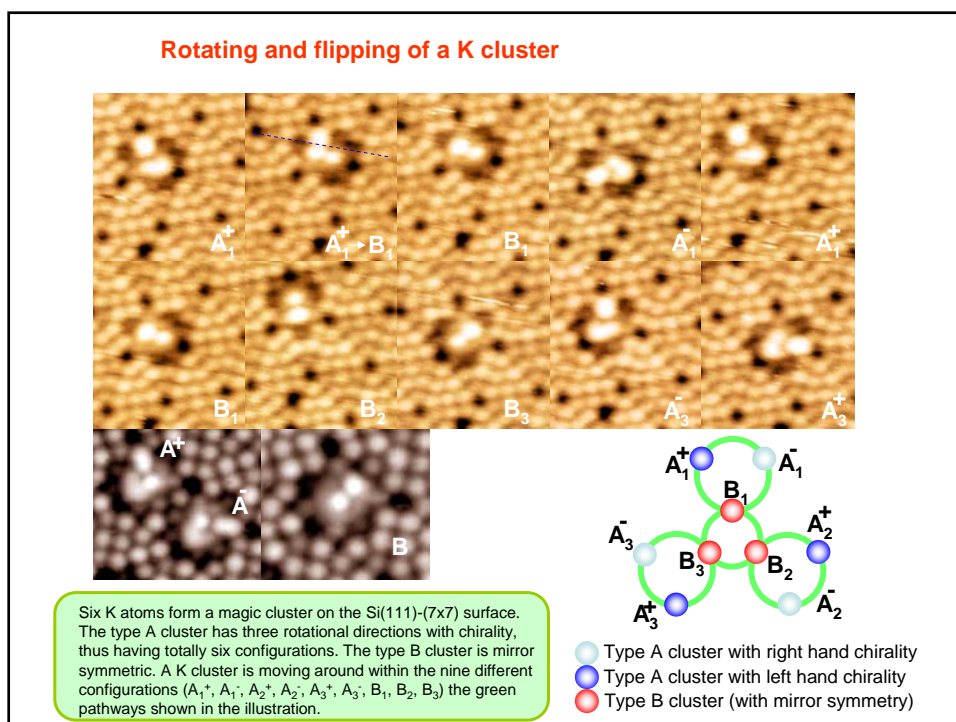
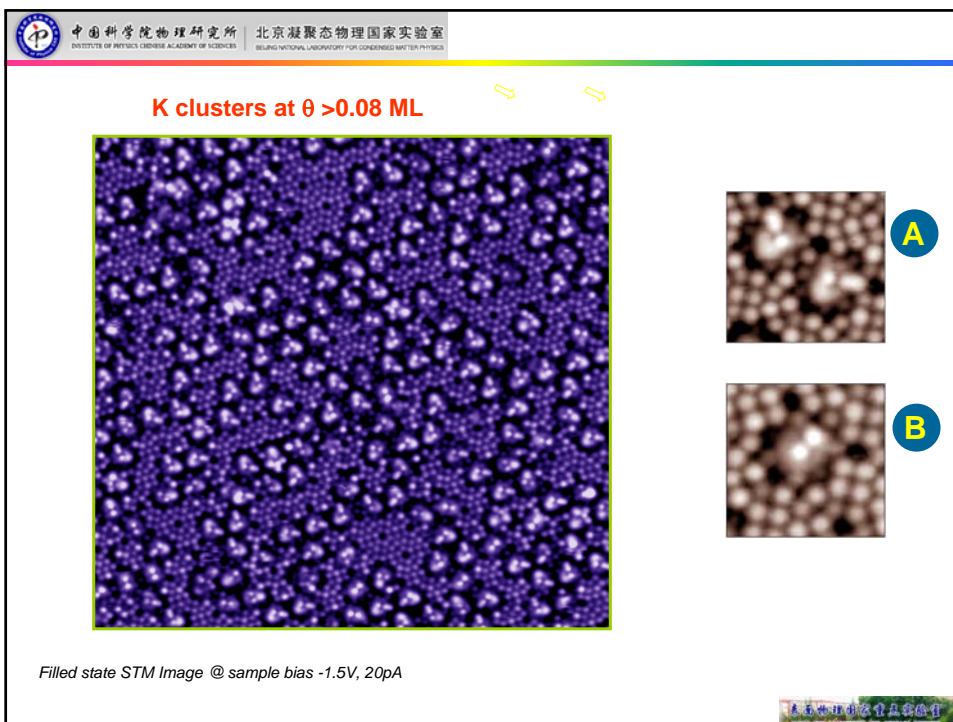
UHUC:  $E_b = 2.20 \pm 0.01$  eV

- Na atoms in different "basins" have negligible interaction

- Na atoms strongly repel each other when they go in the same basin

A "basin" on the Si(111)-(7x7) surface is exclusively occupied by one Na atom





## Adsorption of Ag atom on Si-7x7

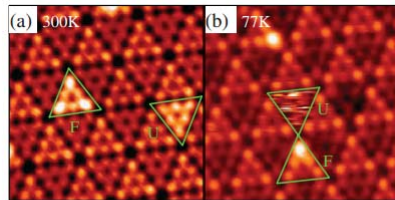


FIG. 1 (color). STM images of single Ag atoms on Si(111)-(7 × 7) at (a) 300 K and (b) 77 K, taken at a tunneling current of 50 pA and a sample bias of -2.0 V. The FUHC and UHUC with Ag atoms are labeled.

K. Wang et al. PRL 101, 266107 (2008)

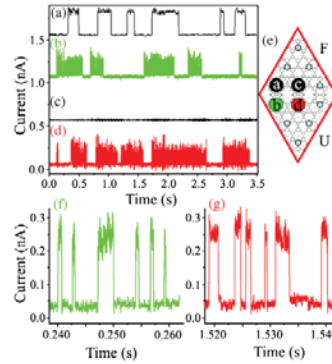


FIG. 2 (color). (a) and (c) Typical time-dependent tunneling spectra taken at 144 K for an STM tip above the corner and center Si-adatom, respectively, in a FUHC containing a moving Ag atom. (b) and (d) Typical time-dependent tunneling spectra at 106 K for an STM tip above the corresponding sites in a UHUC with a moving Ag atom. (e) Schematics for the STM tip positions to acquire the spectra in (a) to (d). (f) and (g) Zoom-in of the dense noisy spectra in (b) and (d), respectively.

## 总结

### § 1.4 STM基本理论

#### § 1.4.1 量子力学“一维势垒散射”

#### § 1.4.2 Barden公式

#### § 1.4.3 三维情况“Tersoff-Hamann”模型

### § 1.5 STM对表面原子结构研究的例子

#### § 1.5.1 清洁硅表面及其吸附结构

Si(111)表面

Si(100)表面

#### § 1.5.2 Morie Patterns

#### § 1.5.3 表面吸附问题

TiO<sub>2</sub>表面吸附水

Si(111)表面吸附碱金属