Schedule of The First Half of The Course (Hasegawa)

Lecture Slides (PDF files)
http://www-surface.phys.s.u-tokyo.ac.jp/KougiOHP/

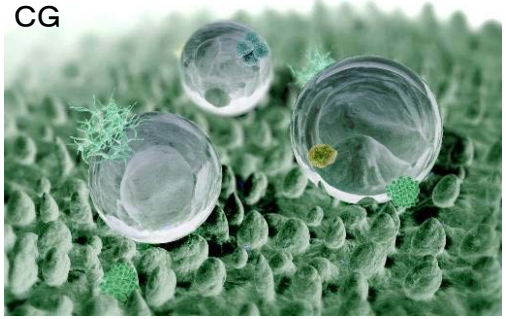
1. Nanoscience and Surface Physics ナノサイエンスと表面物理
   Nanoscience in Nobel Prize
2. Atomic Arrangements at Surfaces 表面原子配列構造
   Scanning Tunneling Microscopy, Electron Diffraction
   走査トンネル顕微鏡、電子回折
3. Surface Electronic States 表面電子状態
   Surface states 表面状態、 Rashba Effect ラシュバ効果
   Topological Surface States トポロジカル表面状態、
   Band Bending バンド湾曲
4. Surface Electronic Transport 表面電気伝導
   Space-Charge-Layer Transport and Surface-State Transport
   空間電荷層伝導と表面状態伝導
   2D Materials 2次元物質
   Atomic-Layer Superconductivity 原子層超伝導

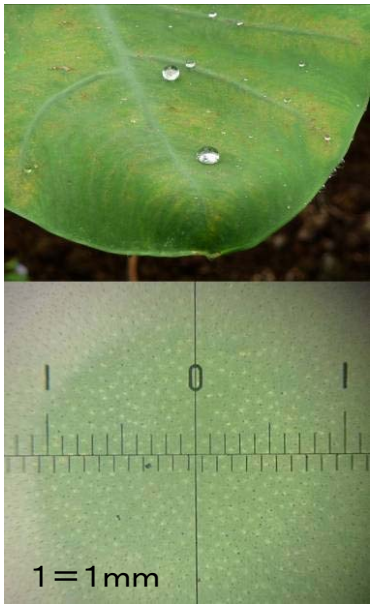
The Surface is Cool!

ロータス効果(Lotus effect, ハス効果)

天然の自浄機構（超撥水性 Ultrahydrophobicity）：
ハスの葉はその微細構造と表面の化学的特性により、濡れない。葉の表面についた水は表面張力によって丸まって水滴となり、泥や、小さい昆虫や、その他の異物を絡め取りながら転がり落ちる。（Wikipedia）

疎水性 hydrophobic
親水性 hydrophilic



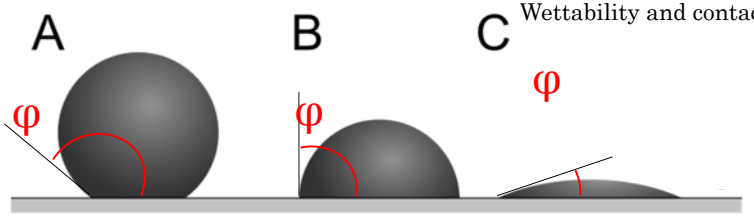


表面張力 Surface Tension (N/m)
表面の端の単位長さ当たりに生じる、縮もうとする力
Force, trying to shrink, per unit length at the edge of surface

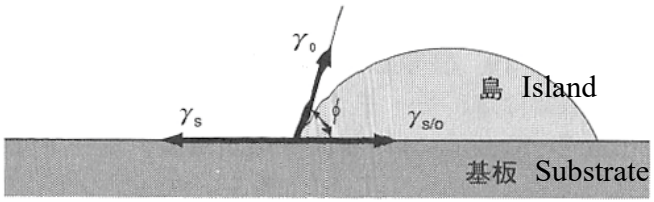
表面エネルギー Surface Energy (J/m^2)
単位面積の表面を作り出すのに必要なエネルギー
Energy necessary to create surface of unit area

←原子・分子間の引力 Attractive force among atoms and molecules

濡れと接触角
Wettability and contact angle



表面張力のつりあい Surface tension and Balance



Young(-Dupre) Formula $\gamma_s = \gamma_{s/o} + \gamma_0 \cos\phi$

γ_s :基板表面の表面エネルギー(張力) Surface energy (tension) of Substrate
γ_0 :吸着物の表面エネルギー(張力) Surface energy (tension) of adsorbate
$\gamma_{S/0}$:基板と吸着物の界面エネルギー Interface energy between Substrate and adsorbate

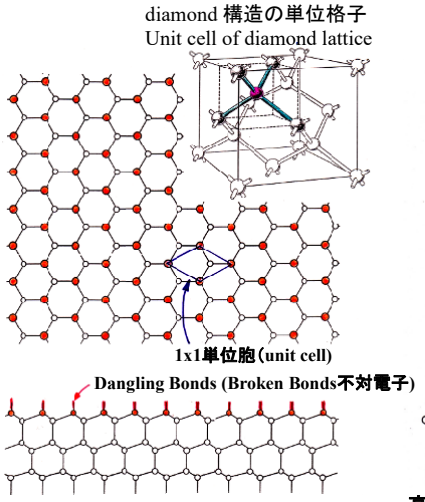
接触角 Contact angle φ

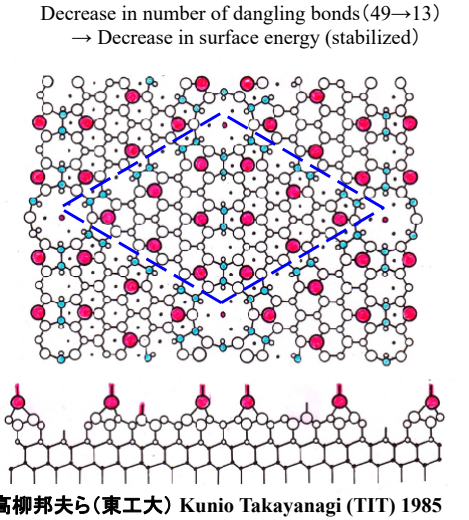
φ=0° :wetting　　φ～0° :親水性 hydrophilic
φ>0° :dewetting　　φ> 90° :疎水性 hydrophobic

Si(111)結晶表面 Crystal Surface

1×1切断(理想)表面
1×1 Truncated (Ideal) Surface

7×7表面超構造(最安定構造)
7×7 Surface Superstructure (most stable)

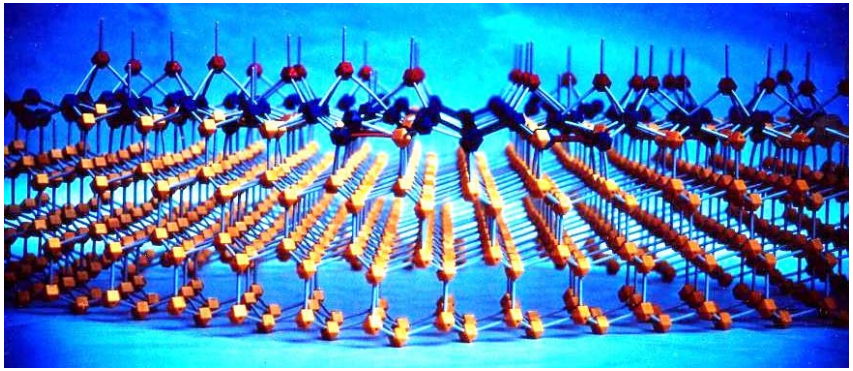




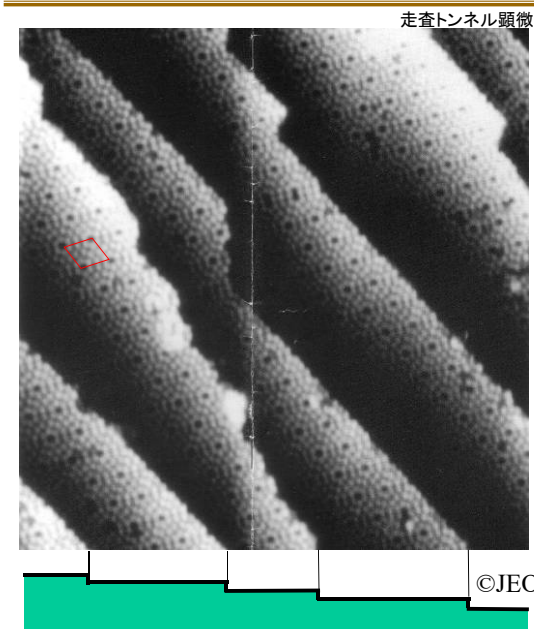
高柳邦夫ら(東工大) Kunio Takayanagi (TIT) 1985

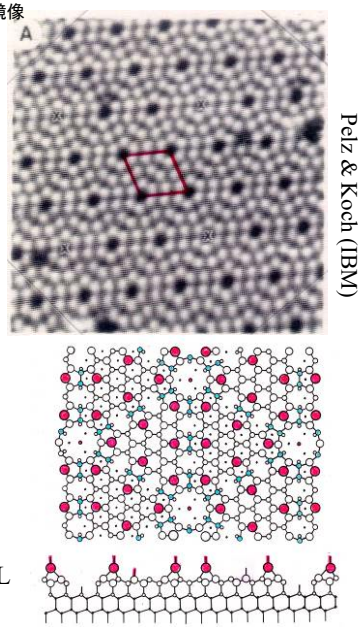
Si(111)-7×7清浄表面構造の模型

Ball-and-Stick Model of Si(111)-7×7 Clean Surface



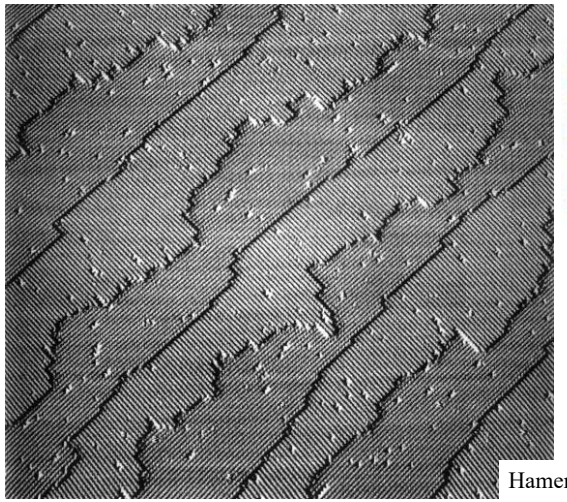
STM Image of Si(111)-7×7 Clean Surface

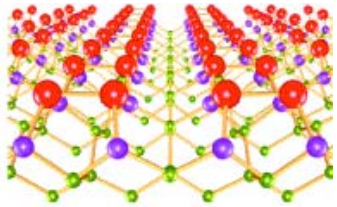




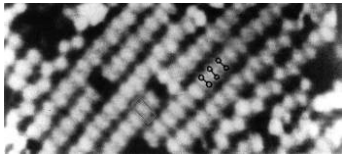
STM Image of Si(001)-2×1 清浄表面 Clean Surface

Swartzentruber, et al., Phys. Rev. Lett. 65 (1988) 1973



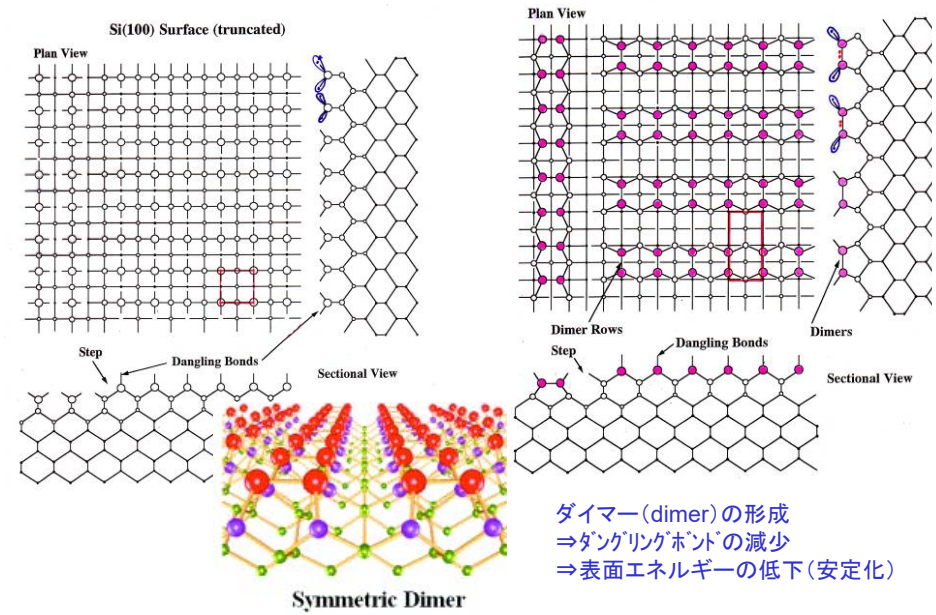


Symmetric Dimer

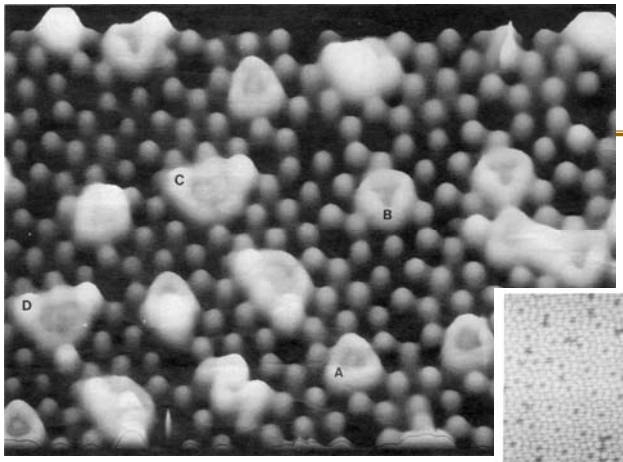


Hamers, et al., Phys. Rev. B34 (1986) 5343

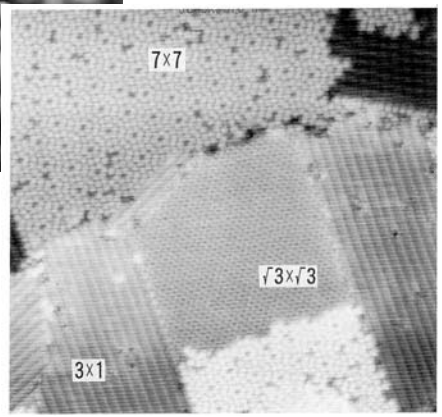
Atomic Structure of Si(001)-2×1 Clean Surface



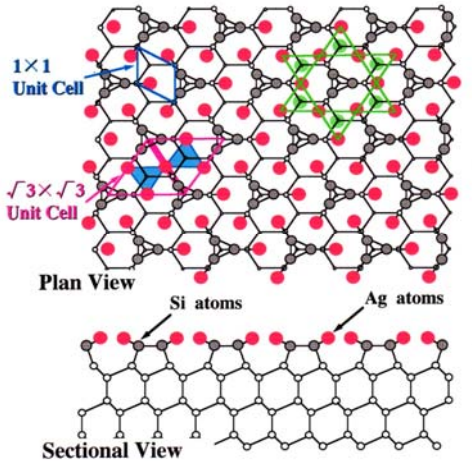
ダイマー(dimer)の形成
⇒ﾀﾞﾝｸﾞﾘﾝｸﾞﾎﾞﾝﾄﾞの減少
⇒表面エネルギーの低下(安定化)

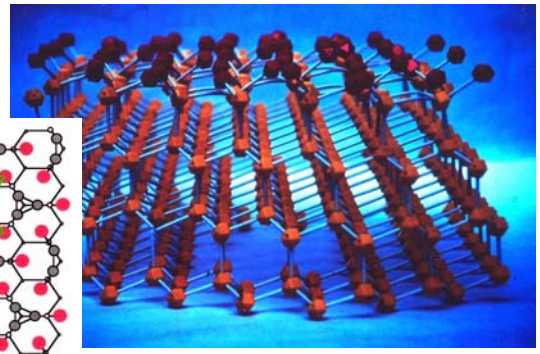


Ag Adsorption on Si(111)-7×7 Surface



Si(111)-√3×√3-Ag 表面超構造 Surface Superstructure



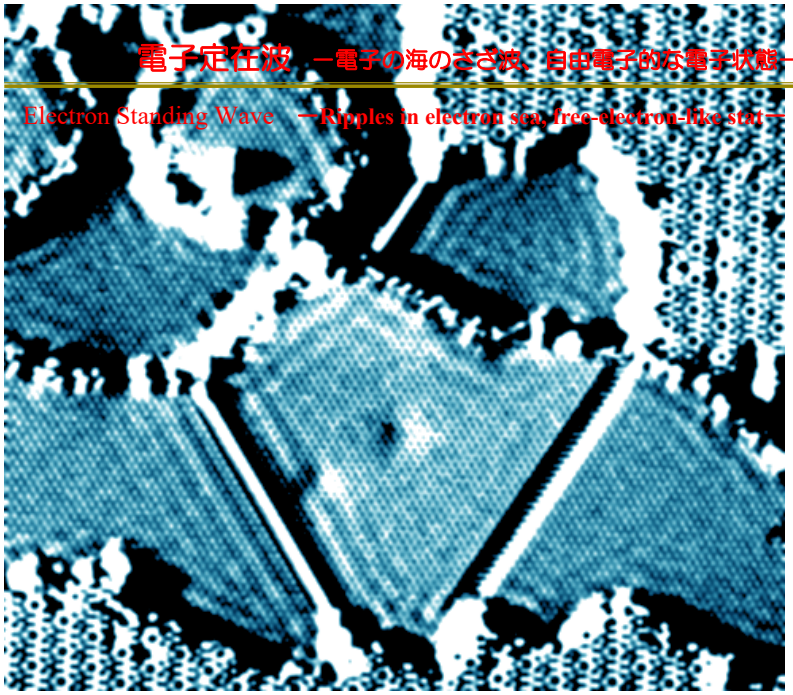


Honeycomb-Chained Triangle (HCT) Structre
高橋敏男ら(物性研) Toshio Takahashi (ISSP)

- ダングリング・ボンド無し No dangling bonds
- 原子的に平坦 Atomically flat
- 2次元金属　Two-dimensional metal

電子定在波 ―電子の海のさざ波、自由電子的な電子状態―

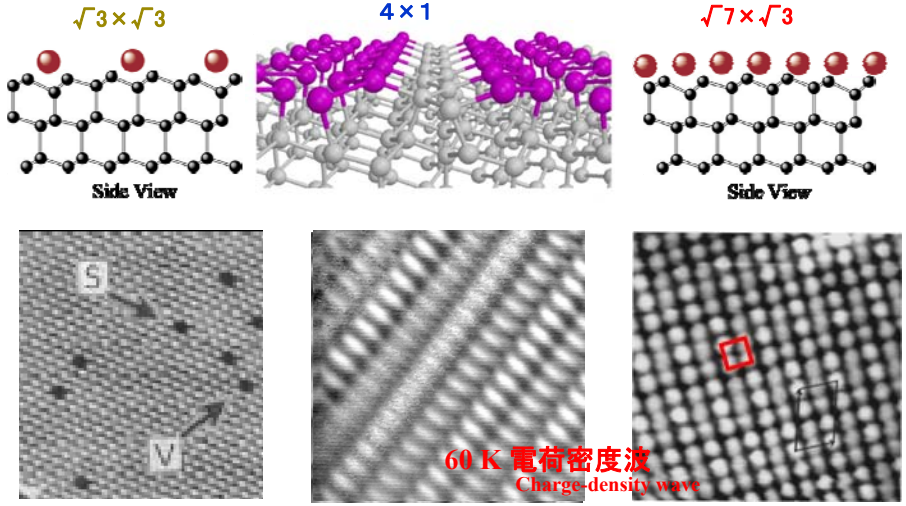
Electron Standing Wave ―Ripples in electron sea, free-electron-like state―



N. Sato, et al., Phys. Rev. B 59, 2035 (1999).

インジウム吸着Si(111) 表面 Indium-adsorbed Si(111) surfaces

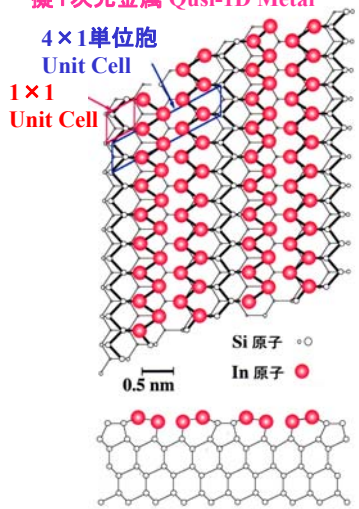
絶縁体 Insulator　　擬1次元金属 Quasi-1D Metal　　2次元金属 2D Metal



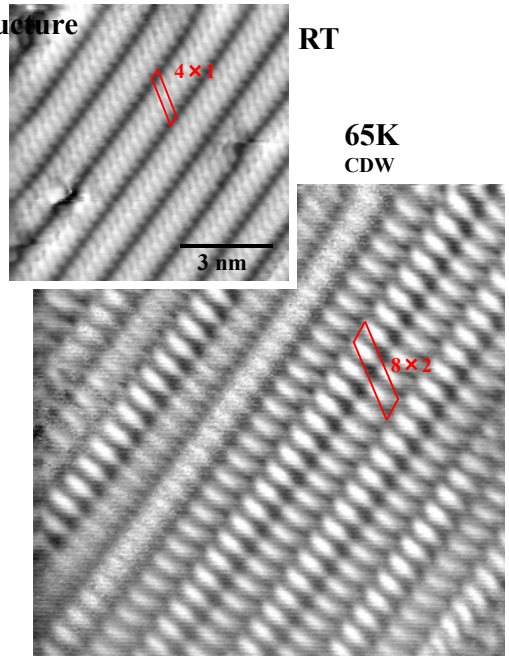
A. A. Sarranin, et. al.　　H. Y. Yeom, et al., PRL **82**, 4898 (1999)　　S. L. Surnev, et. al.

Si(111)-4×1-In Surf. Superstructure

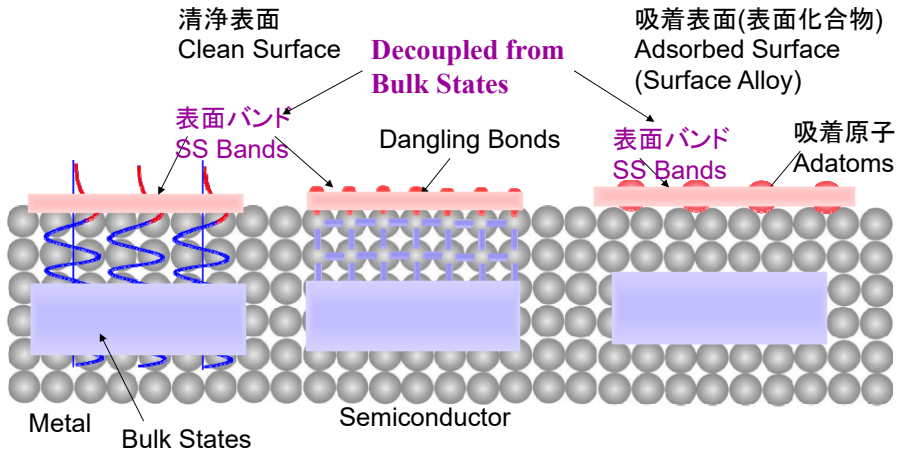
擬1次元金属 Qusi-1D Metal



H.-W. Yeom, et al.,
Phys. Rev. Lett. 82 (1999) 4898

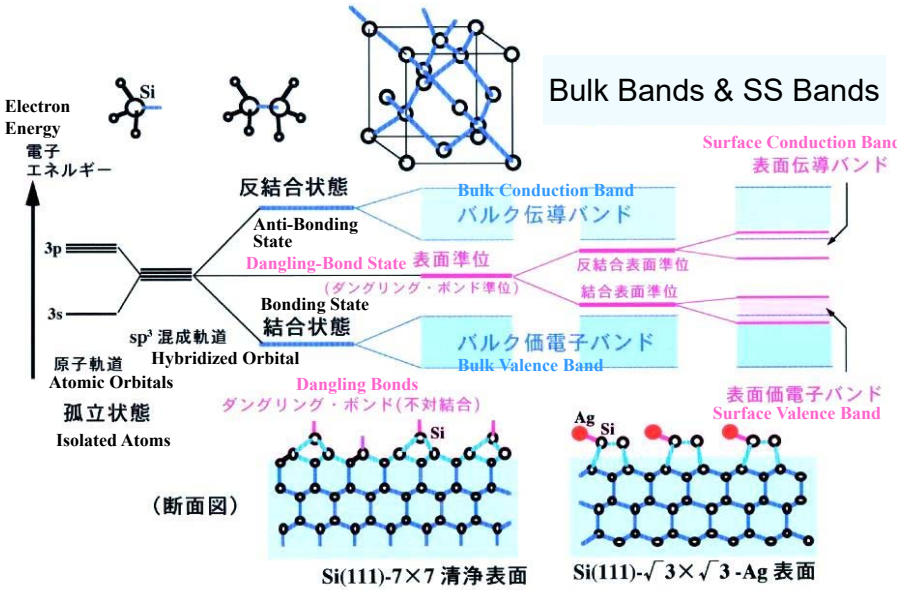


Surface Electronic States are Different from States in Bulk Crystal.

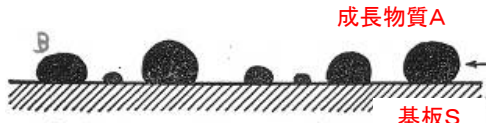


低次元電子系 Low-D Electronic Systems
(反転)対称性の破れ Inversion-Symmetry-Broken Systems
構造と電子物性　Atomistic structures and electronic properties

From Energy Levels to Band Formation ⇒ Chap 3



原子層・薄膜の成長モード Growth Modes

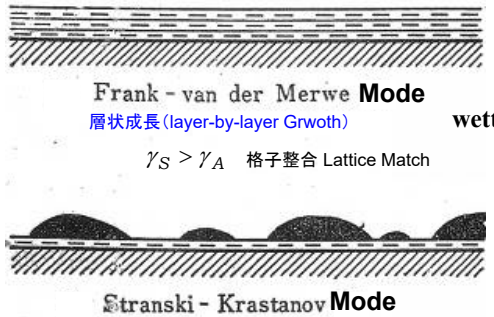


島状成長(3次元核成長、island (3D Nucli) Growth

γ_S : **Surface Energy of Substrate**
γ_A : **Surface Energy of Adsorbate**

$\gamma_S < \gamma_A$ 格子不整合 Lattice Mismatch

Governing Factor
- 表面(界面)エネルギー
  Surface(Interface) Energy
- 格子不整合による歪みエネルギー
  Strain Energy due to Lattice Mismatch



層状成長(layer-by-layer Grwoth)

$\gamma_S > \gamma_A$ 格子整合 Lattice Match

混合成長 格子不整合
Mixed Growth Lattice Mismatch

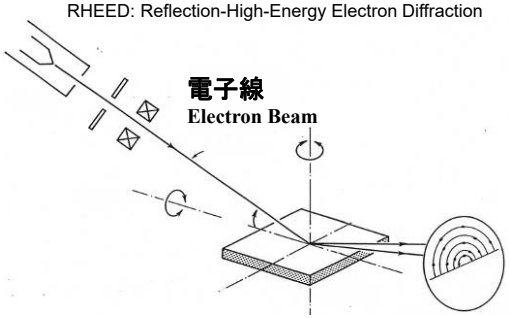
$\gamma_S > \gamma_A \Rightarrow \gamma_S' < \gamma_A$

γ_S' : **吸着層の表面エネルギー**
Surface Energy of Adlayer

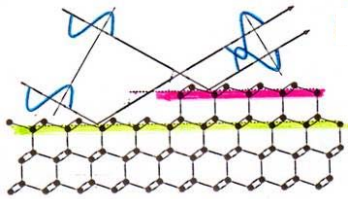
Atomic-Layer Growth and RHEED Intensity Oscillation

Harris, Joyce, Dobson 1981

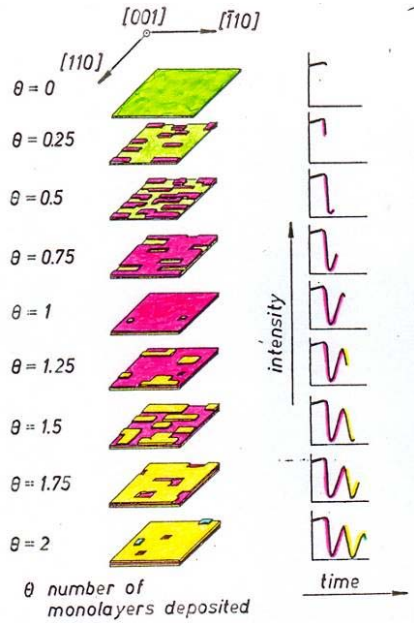
RHEED: Reflection-High-Energy Electron Diffraction



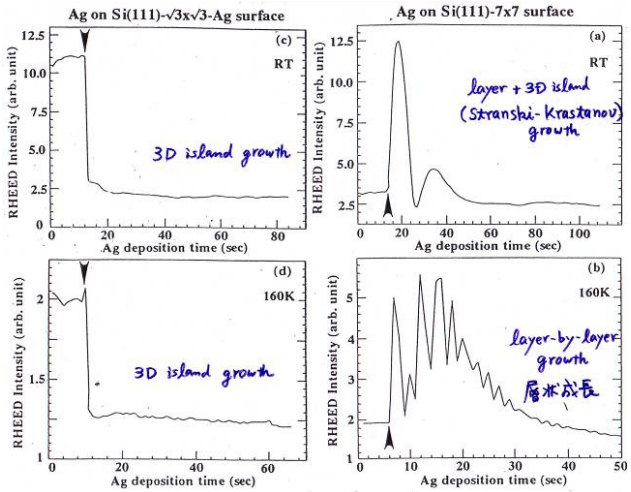
Off-Bragg Condition (Out-of-Phase Condition)

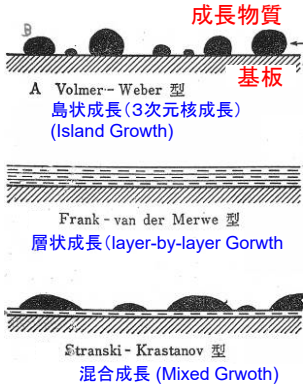


Layer-by-layer Growth



Atomic-Layer Growth and RHEED Intensity Oscillation

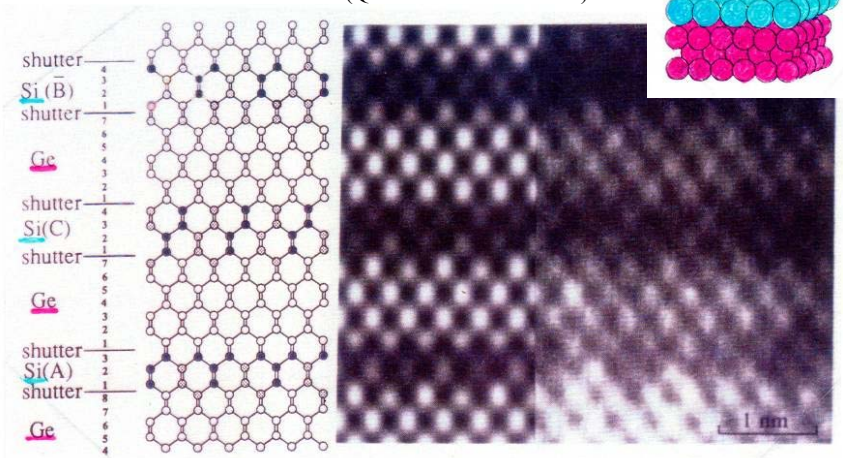




超格子構造 – 人工結晶
Superlattice Structures—Man-made Crystal

異なる原子を積み重ねる
→ 自然には存在しない人工物質
（量子井戸）

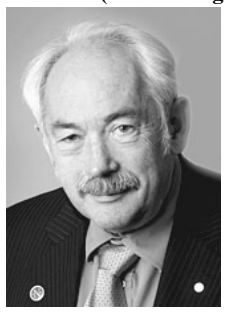
Stack up different atoms layer-by-layer
⇒ Artificial materials which do not exist in nature.
(Quantum well structures)



GeSi超格子の電子顕微鏡写真 TEM image of GeSi superlattice

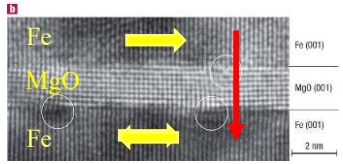
The Nobel Prize in Physics 2007

巨大磁気抵抗効果の発見
for the discovery of Giant Magnetoresistance"
→ 磁気ヘッド（ハードディスクの小型化・高密度化）
Magnetic head (down sizing and high-density magnetic hard disk)



Albert Fert
France
南パリ大学
b. 1938

Peter Grünberg
Germany
Julich研究所
b. 1939



S. Yuasa, et al., Nature Materials 3, 868 (2004).

トンネル磁気抵抗効果(TMR)
Tunnel magnetoresistance
Parallel M ⇒ Low resistance
Anti-parallel M ⇒High resistance

The Nobel Prize in Physics 2014

明るく省エネの白色光源を可能にした、
効率的な青色発光ダイオードの発明
for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources

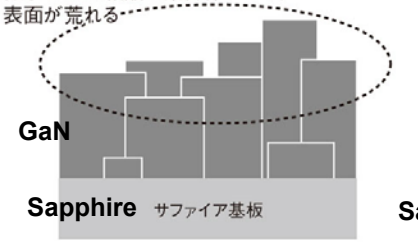
赤﨑 勇終身教授
（名城大学）
85歳

天野 浩教授
（名古屋大学）
54歳

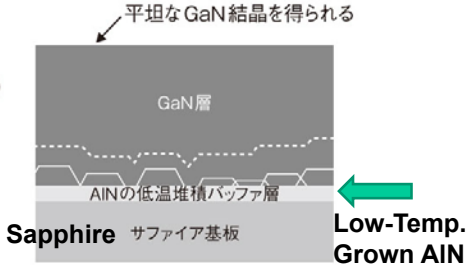
中村 修二教授
（カリフォルニア大学）
60歳

Growth of GaN Crystal : Low-Temp. Buffer Layer
GaN 窒化ガリウム

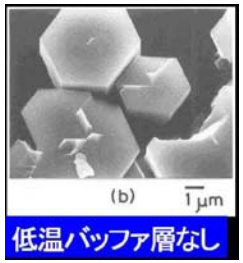
Without Buffer Layer
(a)バッファ層を導入しない場合
微小なGaN結晶の集合体になり、
表面が荒れる



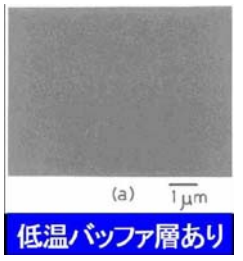
With Buffer Layer
(b)バッファ層を導入した場合
平坦なGaN結晶を得られる



Low-Temp. Grown AlN Layer



低温バッファ層なし



低温バッファ層あり

Release Strain in GaN

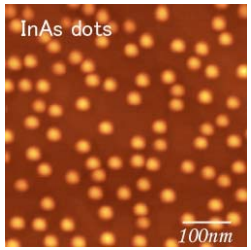
（財）武田計測先端知財団
2005／7／21

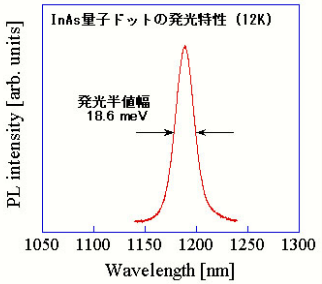
SK成長を利用した量子ドットの自己組織的形成

Self-Organization of Quantum Dots due to Stranski-Krastanov Growth

電気通信大学 ECU　山口浩一研究室 Prof. K. Yamaguchi

InAs/GaAs





Photoluminescence Spectrum

格子不整合（格子不整合量, 7.2%）のため、FvMモードからVWモードへ
20 nm程度の小さいピラミッド状のInAs微小結晶粒が約1兆個/cm^2
電子（または正孔）がInAsドット内に閉じ込められ、量子サイズ効果
ドットサイズを制御⇒発光波長を制御できる（量子ドットレーザ）

電子回折

Electron Diffraction

電子の脱出（侵入）深さ　Escape (Penetration) Depth of electrons

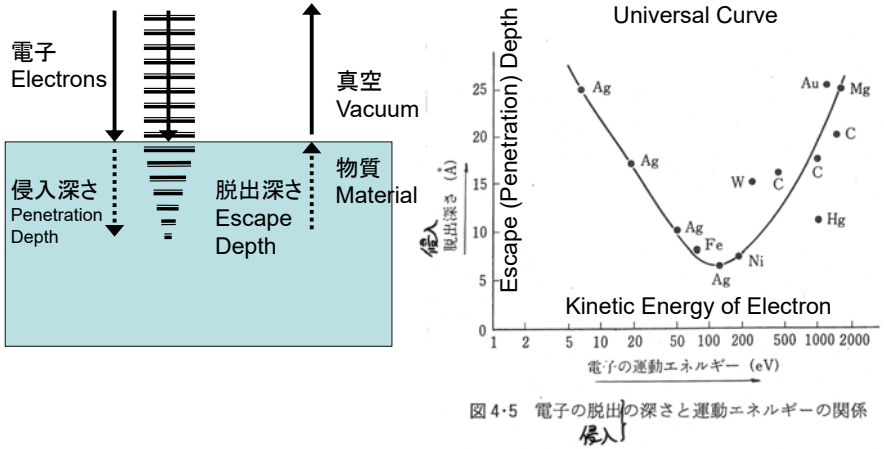
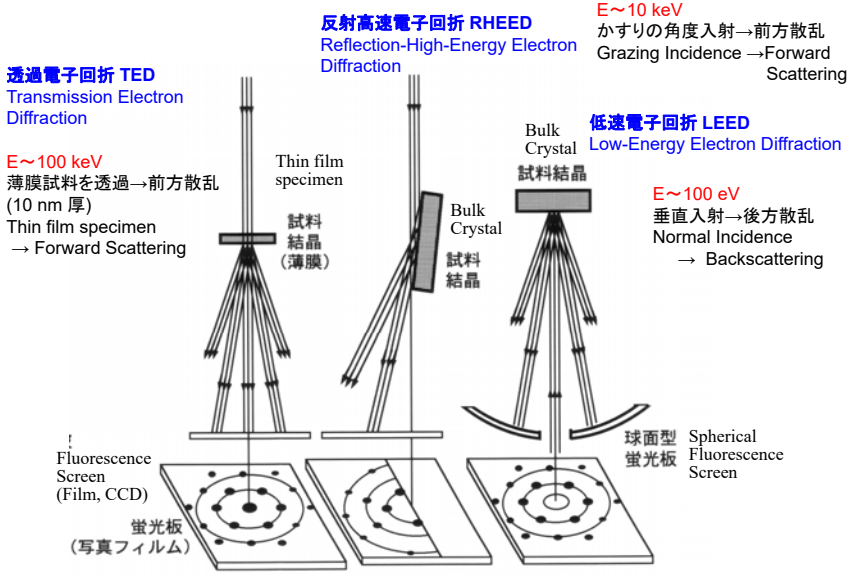


図4·5　電子の脱出の深さと運動エネルギーの関係

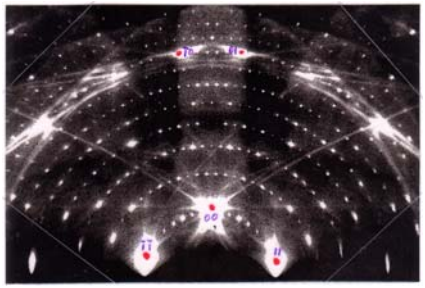
電子回折いろいろ Various Types of Electron Diffraction



Electron Diffraction Pattern from Si(111)-7×7 Clean Surface

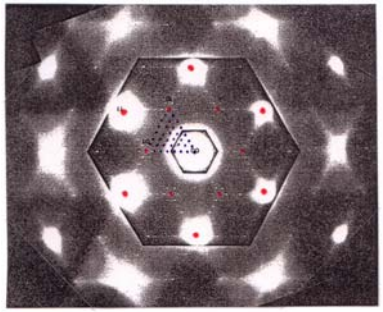
- 基本格子反射点
  Fundamental Spots
  (Diffraction spots from bulk crystal)

他の細かいスポット
超格子反射点
Superlattice Spots
(Diffraction spots from surface superstructure)

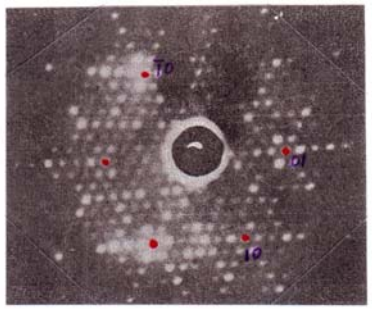


RHEED

TED（Takayanagi）

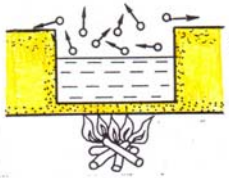


LEED（Ino）

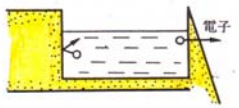


電子線源　― 熱電子銃と電界放射電子銃 ―
Electron Beam Source –Thermal Electron Gun & Field-Emission Electron Gun-

熱電子銃 Thermal EG
（1901 Richardson）



電界放射電子銃 Field-Emission EG
（1968 Crewe）

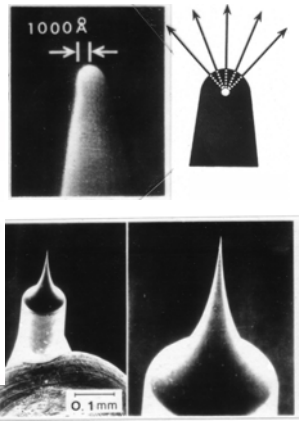


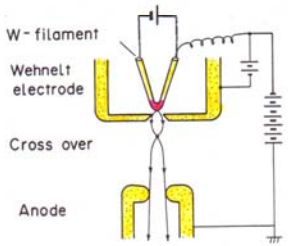
Tunneling

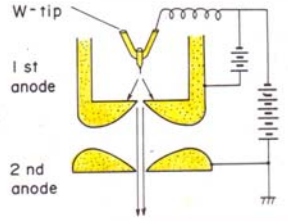
壁が10Å以下になると，電子はトンネル効果で外に飛び出す．

Field Emission Tip（W）

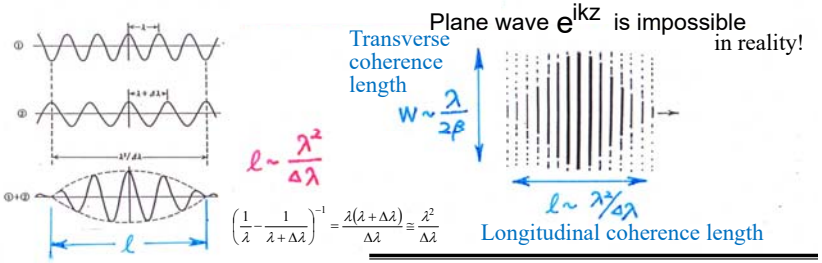
仮想光源
Virtual Source
～ 100 Å



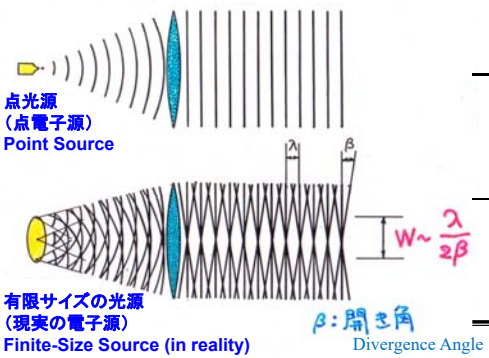




電子波束の大きさ Size of Electron Wave Packet



	熱電子銃（ヘアピン型）	電界放射電子銃（冷陰極型）
光源サイズ (μm)	～20	～0.01
エネルギー幅 (eV)	～ 2	～ 0.3
輝度 at 100 keV (A/cm²/st)	～5×10⁵	～5 ×10⁸
波束		
長さ l (μm)	～ 0.2	～ 1.3
幅 W (μm)	～ 0.02	～ 0.6
（レンズで拡大）	2	60



点光源
（点電子源）
Point Source

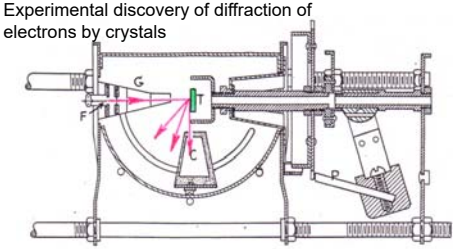
有限サイズの光源
（現実の電子源）
Finite-Size Source (in reality)

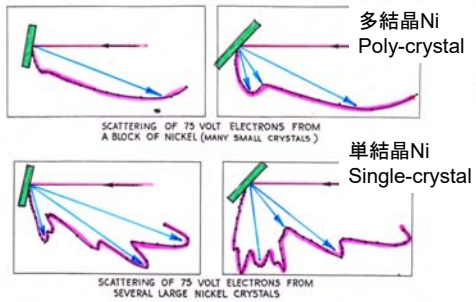
Divergence Angle

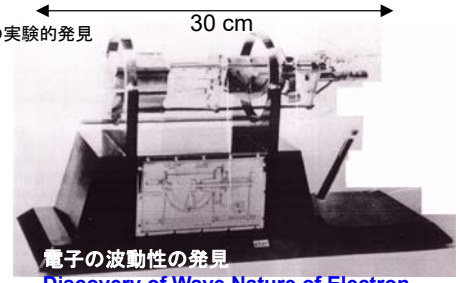
First Electron Diffraction – Davisson & Germer ―（LEED 75 eV）

C. Davisson and L. H. Germer, Phys. Rev. 30, 705-740 (1927)

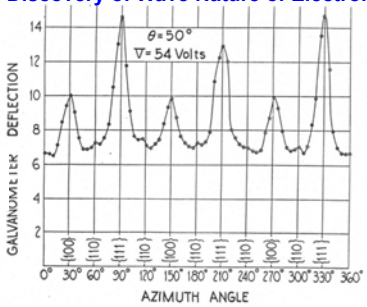
1937 Nobel Prize in Physics 結晶による電子の干渉現象の実験的発見
Experimental discovery of diffraction of electrons by crystals







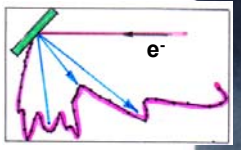
Discovery of Wave Nature of Electron



The Nobel Prize in Physics 1937

"for their experimental discovery of the diffraction of electrons by crystals"

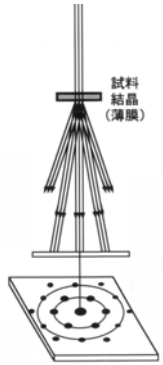
結晶による電子の回折の実験的発見

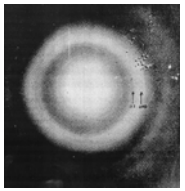


Ni Crystal : LEED

Clinton Joseph Davisson
USA
Bell Telephone Laboratories

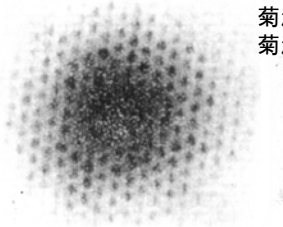
George Paget Thomson
Great Britain
London University



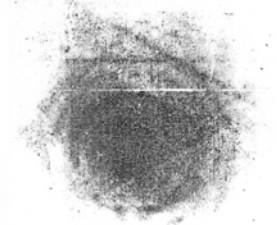


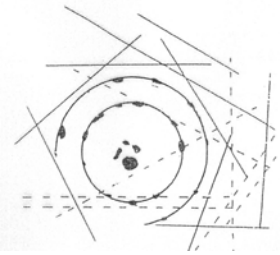
Au Thin Film :TED

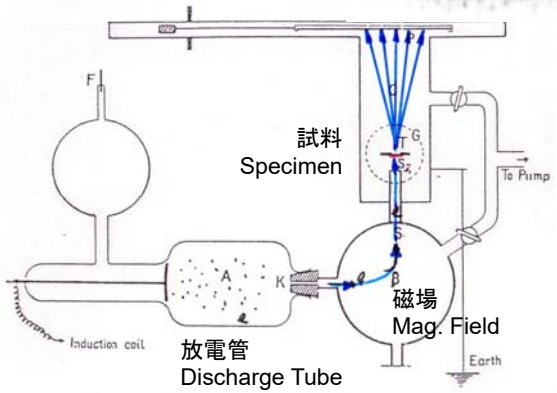
菊池正士 の電子回折　ー雲母薄膜のTED ー
Electron Diffraction by Seishi Kikuchi ー TED of Mica Thin Film



菊池線 Kikuchi Lines
菊池パターン Kikuchi Patterns

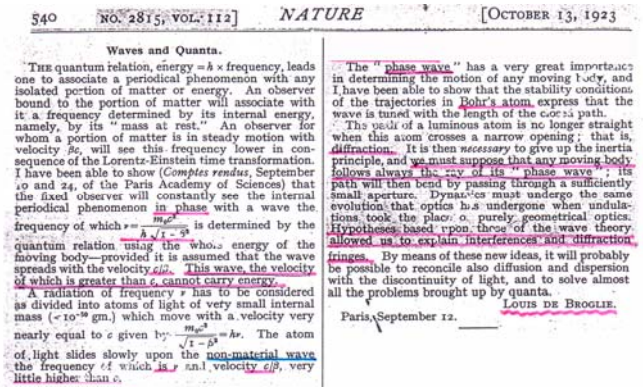






The Nobel Prize in Physics 1929

"for his discovery of the wave nature of electrons" 電子の波動性に発見に対して



540 NO. 2815, VOL. 112] NATURE [OCTOBER 13, 1923

Waves and Quanta.

THE quantum relation, energy = h × frequency, leads one to associate a periodical phenomenon with any isolated portion of matter or energy. An observer bound to the portion of matter will associate with it a frequency determined by its internal energy, namely, by its "mass at rest." An observer for whom a portion of matter is in steady motion with velocity βc, will see this frequency lower in consequence of the Lorentz-Einstein time transformation. I have been able to show (*Comptes rendus*, September 10 and 24, of the Paris Academy of Sciences) that the fixed observer will constantly see the internal periodical phenomenon in phase with a wave the frequency of which $\nu = \frac{m_0 c^2}{h\sqrt{1-\beta^2}}$ is determined by the quantum relation using the whole energy of the moving body—provided it is assumed that the wave spreads with the velocity c/β. This wave, the velocity of which is greater than c, cannot carry energy.

A radiation of frequency ν has to be considered as divided into atoms of light of very small internal mass ($< 10^{-50}$ gm.) which move with a velocity very nearly equal to c given by $\frac{m_0 c^2}{\sqrt{1-\beta^2}} = h\nu$. The atom of light slides slowly upon the non-material wave the frequency of which is, and velocity c/β, very little higher than c.

The "phase wave" has a very great importance in determining the motion of any moving body, and I have been able to show that the stability conditions of the trajectories in Bohr's atom express that the wave is tuned with the length of the circular path.

This result of a luminous atom is no longer straight when this atom crosses a narrow opening; that is, diffraction. It is then *necessary* to give up the inertia principle, and we must suppose that any moving body follows always the ray of its "phase wave"; its path will then bend by passing through a sufficiently small aperture. Dynamics must undergo the same evolution that optics has undergone when undulations took the place of purely geometrical optics. Hypotheses based upon those of the wave theory allowed us to explain interferences and diffraction fringes. By means of these new ideas, it will probably be possible to reconcile also diffusion and dispersion with the discontinuity of light, and to solve almost all the problems brought up by quanta.

LOUIS DE BROGLIE.

Paris, September 12.

Prince Louis-Victor Pierre Raymond de Broglie

France

Sorbonne University, Institut Henri Poincaré, Paris, France

b. 1892 d. 1987

運動する物体($V = c\beta$)には**位相波**を伴っている！ $mc^2 = h\nu$

non-material wave （⇒ material wave (物質波)）

光速より速く走る、エネルギーを運ばない $V_\phi = c/\beta$

$$\lambda = \frac{V_\phi}{\nu} = \frac{ch}{\beta mc^2} = \frac{h}{\beta mc} = \frac{h}{mV} = \frac{h}{p}$$

→ 干渉・回折縞を説明できる！

電子の波長 Wavelength of Electron

- では電子の波長は？ How long is the wavelength of electron?

de Broglie's formula

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} = \sqrt{\frac{150.412}{V[\text{ボルト}]}} \quad \text{(非相対論)}$$

$$eV = \frac{p^2}{2m}$$

$$= \sqrt{\frac{150.412}{V[\text{ボルト}]}} \times \left(1 - 4.89 \times 10^{-7} \times V\right) \quad \text{(相対論)}$$

加速電圧 Acc. Voltage	λ(非相対論)	λ(相対論)
100 V	1.23 Å	1.23 Å
500 V	0.548 Å	0.548 Å
1 kV	0.388 Å	0.388 Å
5 kV	0.173 Å	0.173 Å
10 kV	0.123 Å	0.122 Å
50 kV	0.0548 Å	0.0535 Å
100 kV	0.0388 Å	0.0369 Å
500 kV	0.0173 Å	0.0131 Å

Atomic-Scale

電子の速度は光速に近い
The speed approaches c.

Huygens の原理と回折　Huygens' Principle & Diffraction

電子線が物質に照射されると、物質内の静電ポテンシャル $V(\vec{r})$ によって散乱される；

$$\Delta\psi(\vec{r}) + \frac{8\pi^2 me}{h^2}[E + V(\vec{r})]\psi(\vec{r}) = 0 \qquad (1)$$

(E; 加速電圧)。入射電子波として平面波 $exp(2\pi i\vec{K}_0\cdot\vec{r})$ をとると $(K = |\vec{K}_0| = \frac{\sqrt{2meE}}{h} = \frac{1}{\lambda})$

この解は、形式的に

$$\psi(\vec{r}) = exp(2\pi i\vec{K}_0\cdot\vec{r}) + \frac{2\pi me}{h^2}\int \frac{exp(2\pi iK\cdot|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}V(\vec{r}')\psi(\vec{r}')d\vec{r}' \qquad (2)$$

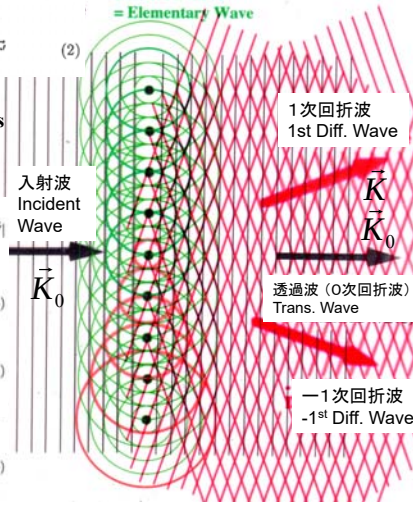
第１項：入射波 **Plane wave**

第２項：散乱波＝球面波の合成（ホイヘンスの原理） **Spherical waves**

その振幅は、その場所でのポテンシャルと波の振幅に比例する

散乱波（球面波）＝素元波

Scattered Wave
= Elementary Wave



1.1. Born 近似　Born approximation

(2) 式の第２項の $\psi(\vec{r})$ を入射波そのものの $exp(2\pi i\vec{K}_0\cdot\vec{r})$ で置き換える近似。$|\vec{r}| >> |\vec{r}'|$ とすると、

透過波（平面波）　散乱波（球面波）

$$\psi(\vec{r}) = exp(2\pi i\vec{K}_0\cdot\vec{r}) + \frac{exp(2\pi iKr)}{r}\Psi(\vec{K}-\vec{K}_0) \qquad (3)$$

ここで、$\vec{K}$ で決まる方向の微分散乱断面積は $|\Psi|^2$ で書け、 Differential Scattering Cross Section

$$\Psi(\vec{K}-\vec{K}_0) = \frac{2\pi me}{h^2}\int V(r')exp[-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r}']d\vec{r}' \qquad (4)$$

であり、$V(\vec{r})$ のフーリエ変換。

散乱波の強度 I は、入射波の強度を I_0 とすると

Intensity of Scattered Wave　$I = I_0\frac{1}{r^2}|\Psi|^2$ (5)

1.2. 結晶による回折

静電ポテンシャル $V(\vec{r})$ ＝各原子による静電ポテンシャルの和 $V_j(\vec{r}-\vec{r}_j)$

$(\vec{r}_K$：k 番目の原子の位置)；

Superposition of atomic potentials of all atoms

$$V(\vec{r}) = \sum_j V_j(\vec{r}-\vec{r}_j). \qquad (6)$$

$\vec{r}_j$: **position of the *j*–th atom**

そうすると、散乱振幅 Ψ は　f_j Scattering Amplitude

$$\Psi = \frac{2\pi me}{h^2}\sum_j\{\int V_j(\vec{r})exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r})d\vec{r}\}exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r}_j) \qquad (7)$$

$$= \sum_j f_j exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r}_j) \qquad (8)$$

ここで、f_j は j 番目の原子散乱因子。$\sum_{j(全原子)} = \sum_{全単位胞}\sum_{単位胞内の原子}$ と和をとる；　Atomic Scattering Factor of the j-th Atom

$(\vec{r}_j \leftarrow \vec{R}_n + \vec{r}_l)$、($\vec{R}_n$；単位胞の位置ベクトル、$\vec{r}_l$；単位胞内の原子の位置ベクトル)

Sum in Unit Cell => F

$$\Psi = \sum_{全単位胞\ n}\{\sum_{単位胞内の原子\ l} f_l exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r}_l)\}exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{R}_n) \qquad (9)$$

Crystal Structure Factor

ここで単位胞の和、$F(\vec{K}-\vec{K}_0) = \sum_l f_l exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{r}_l)$ を結晶構造因子という。

$G(\vec{K}=\vec{K}_0)\sum_{全単位胞\ n} exp(-2\pi i(\vec{K}-\vec{K}_0)\cdot\vec{R}_n)$ と置くと、

G: Laue Function

$$\Psi = F(\vec{K}-\vec{K}_0)\cdot G(\vec{K}-\vec{K}_0) \qquad (10)$$

$$\vec{r}_j = \vec{R} + \vec{r}_\ell$$

$\vec{R}_n$: **position of the n–th unit cell**

$\vec{r}_\ell$: **position of the ℓ–th atom in the unit cell**

となり、散乱波の強度 I は、

Intensity of Scattered Wave　$I = |\Psi|^2 = I_0|F(\vec{K}-\vec{K}_0)|^2|G(\vec{K}-\vec{K}_0)|^2$ (11)

結晶が $N_1\vec{a}_1$, $N_2\vec{a}_2$, $N_3\vec{a}_3$ を稜とする平行六面体であるとすると、単位胞の位置ベクトルは $\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$,(ここで、$n_1 = 1,2,---,N_1, n_2 = 1,2,---,N_2, n_3 = 1,2,---,N_3$) だから、

$$|G(\vec{K}-\vec{K}_0)|^2 = \frac{sin^2\{\frac{1}{2}N_1(\vec{K}-\vec{K}_0)\cdot\vec{a}_1\}}{sin^2\{\frac{1}{2}(\vec{K}-\vec{K}_0)\cdot\vec{a}_1\}}\cdot\frac{sin^2\{\frac{1}{2}N_2(\vec{K}-\vec{K}_0)\cdot\vec{a}_2\}}{sin^2\{\frac{1}{2}(\vec{K}-\vec{K}_0)\cdot\vec{a}_2\}}\cdot\frac{sin^2\{\frac{1}{2}N_3(\vec{K}-\vec{K}_0)\cdot\vec{a}_3\}}{sin^2\{\frac{1}{2}(\vec{K}-\vec{K}_0)\cdot\vec{a}_3\}} \qquad (12)$$

となり、Laue 関数と呼ばれ、$(\vec{K}-\vec{K}_0)\cdot\vec{a}_i = 2\pi h_i$,(ここで、$i = 1,2,3$, h_iは整数) のとき（Laue 条件）、極大値 $N_1^2N_2^2N_3^2$ をとる次ページのような関数。(h_1,h_2,h_3) を逆格子点（回折スポット）の指数。

Laue Function

Indexes of Reciprocal Lattice Points (Diffraction Spots)

Procedure of Structure Analysis: Trial and Error

(1) Measure the intensity $I(\vec{k})$ of each diffraction spot

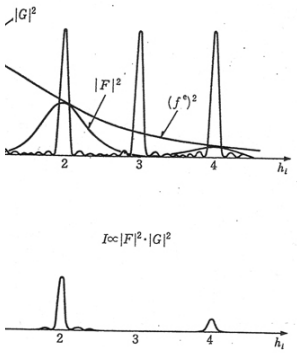
(2) Assume a model of the atomic arrangement in the unit cell.

(3) Calculate $V(\vec{r})$ from the model.

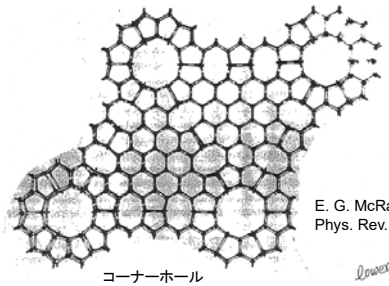
(4) Fourier transform the $V(\vec{r})$ to obtain the crystal structure factor $F(\vec{k})$.

(5) Compare the calculated $|F(\vec{k})|^2$ with the measured spot intensity $I(\vec{k})$.

(6) If they do not agree with each other, modify the model, and repeat the process (2)-(5).

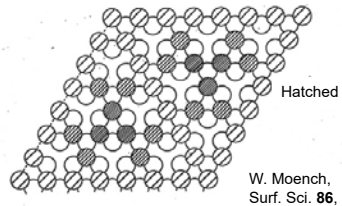


Proposed Models for Si(111)-7x7 Surface Superstructure



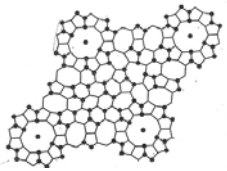
コーナーホール
ダイマー

E. G. McRae,
Phys. Rev. B **28**, 2305 (1983).



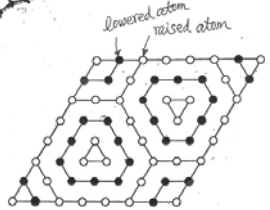
Hatched atoms; raised atoms

W. Moench,
Surf. Sci. **86**, 672 (1979).

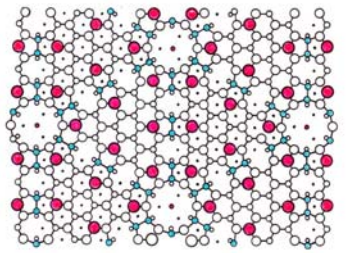


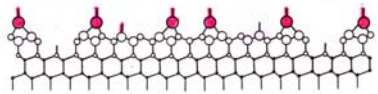
コーナーホール
ダイマー、非対称な半単位胞

F. J. Himpsel,
Phys. Rev. B **27**, 7782 (1983).



D. J. Chadi,
Surf. Sci. **99**, 1 (1980).



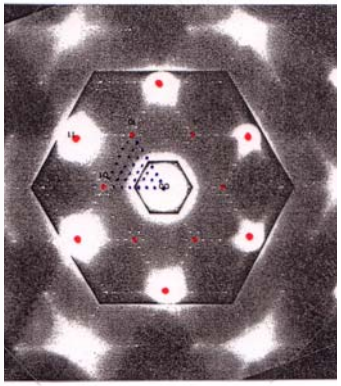


K. Takayanagi, et al., Surf. Sci. **164**, 367 (1985).

TED Analysis of Si(111)-7x7 Surface Superstructure by Takayanagi etal.
—Proposal of DAS Structure —

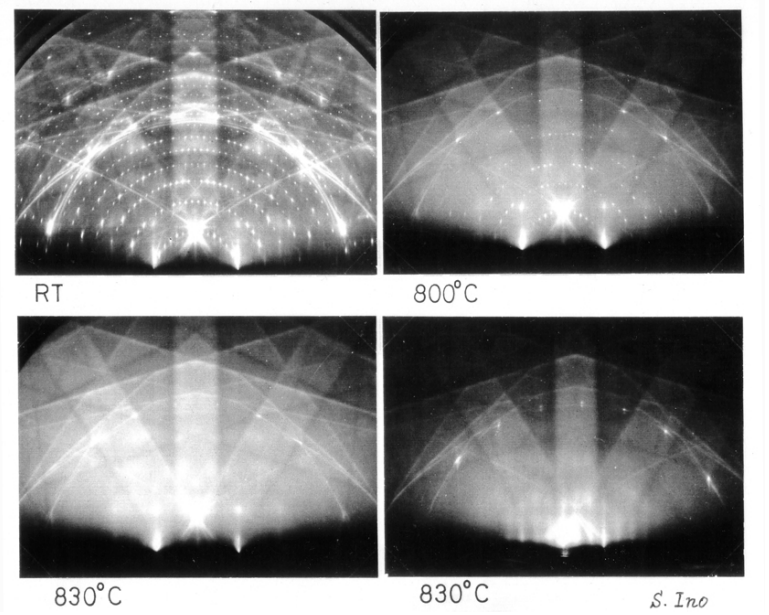
Relative intensities of $(h/7\ k/7, 0)$ reflections for the observation and for calculations of DAS, DAS-Refined, McRae [30], Bennett et al. [12], Himpsel and Batra [21] models; intensities of (1 1/7) reflection, which were calculated to be 146×10^{-7}, 147×10^{-7}, 562×10^{-7}, 103×10^{-7}, 57×10^{-7} for the unit incidence of electrons, respectively, are normalized to 100; on account of the limited space, the intensities of only 80 of the observed 460×6 reflections are listed

Reflections $(h/7\ k/7)$	TED intensity					
	Obs.	DAS	DAS-RFN	McRae	Bennett	Himpsel
3/7 0	160	150	159	57	285	236
3/7 1/7	37	24	25	0	25	39
4/7 0	9	18	13	0	25	21
3/7 3/7	10	2	1	9	10	24
4/7 3/7	10	1	1	8	1	3
4/7 4/7	64	42	45	9	80	0
6/7 0	96	79	83	78	69	327
6/7 1/7	80	58	59	64	128	101
1 1/7	100	100	100	100	100	100
8/7 0	77	60	46	68	128	47
5/7 0	15	19	13	16	13	31
5/7 2/7	15	11	9	15	36	28
1 2/7	62	40	43	37	42	65
9/7 0	37	10	15	12	26	62
1 3/7	123	86	100	47	122	54
8/7 3/7	37	14	12	2	17	1
1 4/7	10	4	5	0	11	41
6/7 4/7	0	6	4	0	5	54
5/7 3/7	0	5	3	1	2	1
5/7 4/7	25	9	10	2	16	2
6/7 3/7	19	7	7	2	6	20
8/7 2/7	23	10	10	5	11	12
9/7 1/7	25	11	8	6	8	8
9/7 2/7	25	8	9	3	13	7
5/7 5/7	0	0	0	1	0	14
6/7 5/7	17	4	5	9	1	136
8/7 4/7	0	1	1	3	0	5
9/7 4/7	12	0	1	1	1	17
9/7 3/7	0	1	1	0	0	5
10/7 0	0	6	5	0	4	50
10/7 1/7	25	7	6	0	16	3

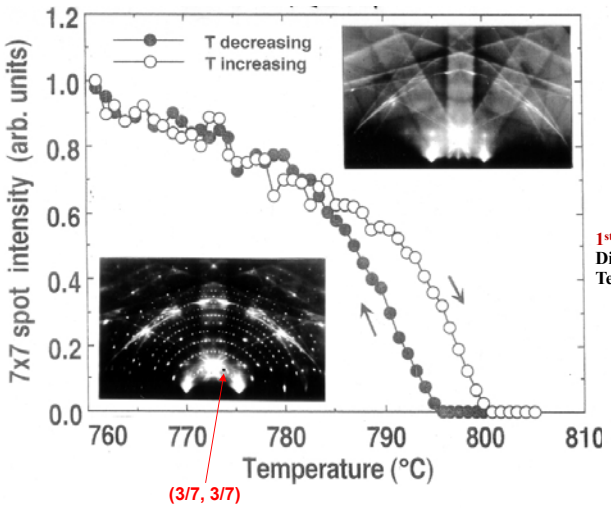


K. Takayanagi, et al.,
Surf. Sci. **164**, 367 (1985).

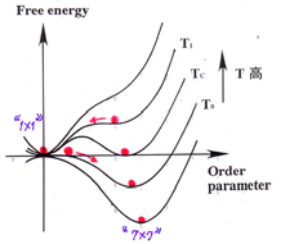
Phase Transition: Si(111)-7x7 ⇔ 1x1 at ～830℃



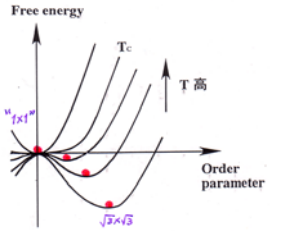
Phase Transition Si(111)-7x7 ⇔ 1x1; 1st Order



S. Hasegawa, et al., Phys. Rev. B **47**, 9903 (1993).
Phase Transitions **53**, 87 (1995).

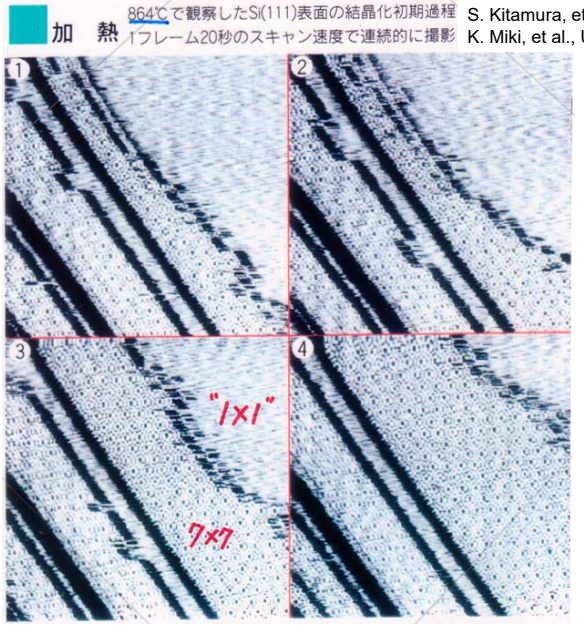


1st-order Phase Transition
Discontinuous change in order parameter
Temperature hysteresis



2nd-order Phase Transition
Continuous change in order parameter
No Temperature hysteresis

Phase Transition Si(111)-7x7 ⇔ 1x1; Real-Space Observation by STM



S. Kitamura, et al., Nature **351**, 215 (1991).
K. Miki, et al., Ultramicroscopy **42-44**, 851 (1992).

T_{sub}=864℃
20 sec per frame

Boundaries between 7x7 and 1x1 domains fluctuates from frame to frame.

SPM
Scanning Probe Microscopy
走査プローブ顕微鏡

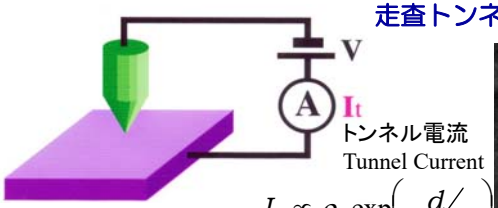
Scanning Tunneling Microscope (STM)
走査トンネル顕微鏡

Atomic Force Microscopy (AFM)
原子間力顕微鏡

磁気力･静電気力顕微鏡
摩擦力顕微鏡

Scanning Tunneling Microscope (STM) by Binnig and とRohrer

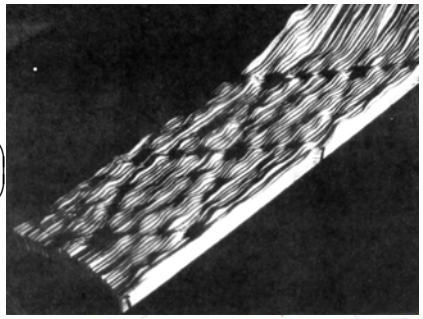
走査トンネル顕微鏡

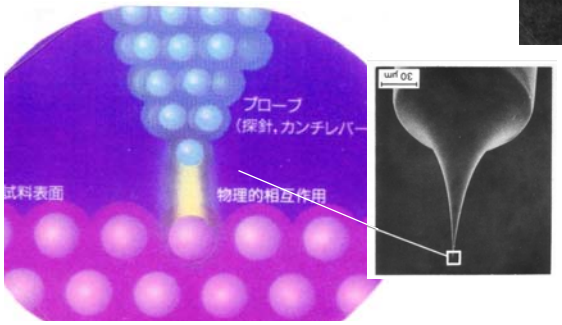


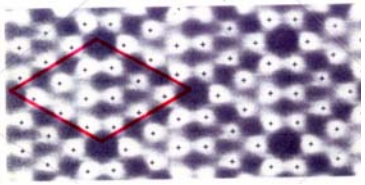
トンネル電流
Tunnel Current

$$I_t \propto \rho \cdot \exp\left(-d/d_0\right)$$

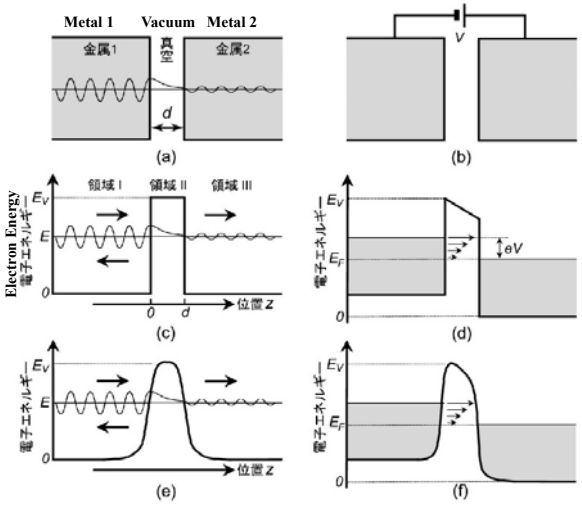
(トンネル電流) $\propto$ (電子密度)$\cdot e^{-a\cdot(\text{間隔})}$

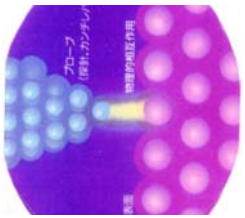






Si(111)-7×7 清浄表面のＳＴＭ像。
原子一個一個が輝点として分解されている。
STM image of Si(111)-7x7 surface in 1983
Individual atoms as bright spots





境界(z=0, d)での
波動関数とその
微係数が連続
WF and its derivative
should be continuous
at Boundaries (z=0, d)
⇒係数A_i, B_iを決定
Determine Coefficients
A_i, B_i

領域 I: $\psi_1 = A_1 \exp(ikz) + B_1 \exp(-ikz),$

領域 II: $\psi_2 = A_2 \exp(\kappa z) + B_2 \exp(-\kappa z),$

領域 III: $\psi_3 = A_3 \exp(ikz)$

$$k = \frac{\sqrt{2mE}}{h}$$

$$\kappa = \frac{\sqrt{2m(E_V - E)}}{h}$$

1個の電子のトンネル Tunneling of Single Electron

透過係数
Transmission Probability

$$T(E) = \left|\frac{A_3}{A_1}\right|^2 = \left[1 + \frac{E_V^2 \sinh^2 \kappa d}{4E(E_V - E)}\right]^{-1}$$

$$E_V - E \cong \text{仕事関数} \cong 4eV \Rightarrow \kappa = \frac{\sqrt{2m(E_V - E)}}{h} \approx 10nm^{-1}$$

$$\Rightarrow \sinh^2 \kappa d \cong \exp(2\kappa d)$$

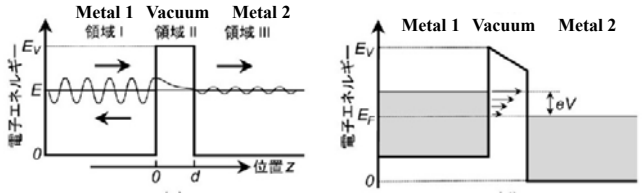
$$\Rightarrow T(E) \cong 16\left(1 - \frac{E}{E_V}\right)\left(\frac{E}{E_V}\right)\exp(-2\kappa d) \approx \exp(-2\kappa d) \approx 10^{-9} << 1$$

$when \quad d = 1nm$

$$T(E) \approx 10^{-8} \quad when \quad d = 0.9nm$$

トンネルギャップの距離 d が0.1 nm変化すると
トンネル電流は1桁変化する⇒原子レベルの凸凹を検出
When the distance d at tunneling gap changes by 0.1 nm,
the tunneling current changes by one order of magnitude.
⇒ Atomic-Level roughness is detectable.

トンネル電流と
状態密度
Tunneling Current &
DOS



$$I(V) = \int_{E_F}^{E_F+eV} \rho_1(E-eV) f(E-eV) \cdot \rho_2(E)[1-f(E)] \cdot T(E-eV) dE$$

Metal1 Metal 2

f: Fermi-Dirac Distr.

$$\cong \int_{E_F}^{E_F+eV} \rho_1(E-eV) \cdot \rho_2(E) \cdot T(E-eV) dE$$

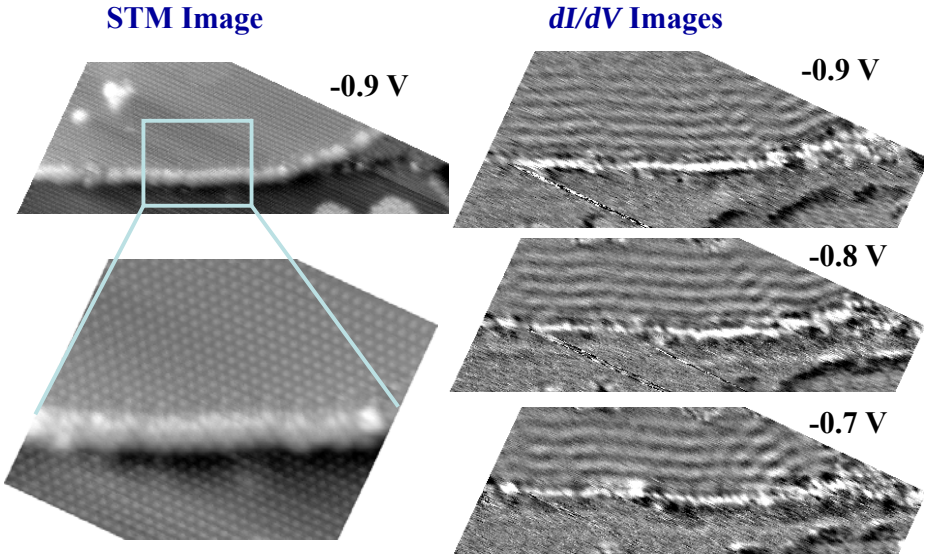
$$\cong \rho_1(E_F) \cdot \rho_2(E_F) \cdot \exp(-2\kappa d) \quad when \cdot V = small$$

$$\frac{dI(V)}{dV} = \rho_1(E_F) \cdot \rho_2(E_F+eV) \cdot T(E_F)$$ **Energy dependence of DOS**

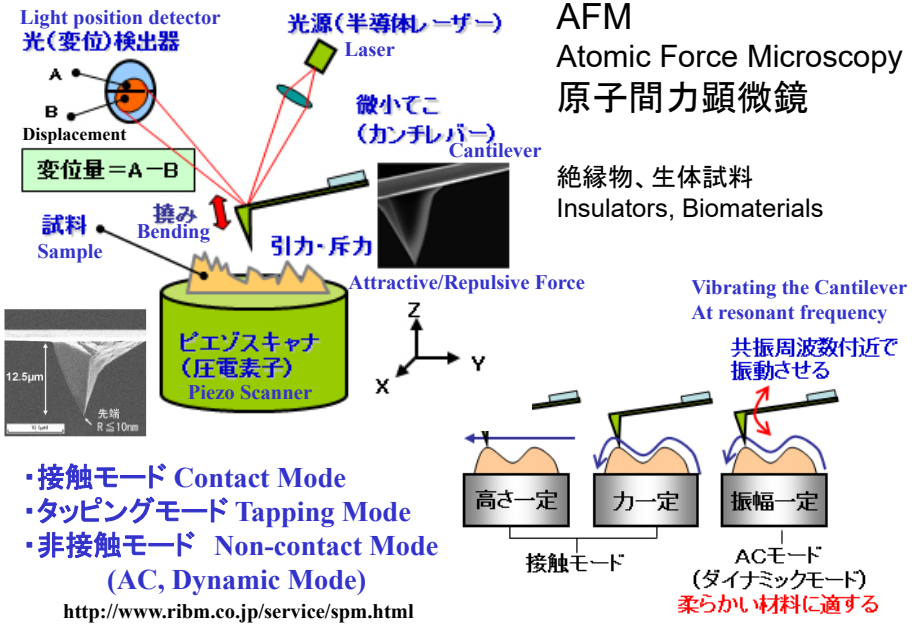
走査トンネルスペクトロスコピー Scanning Tunneling Spectroscopy

Electron Standing Wave on Si(111)-√3×√3-Ag at 65K

T. Hirahara, et al., Surface Science **563** (2004) 191–198



G. Binnig, C. F. Quate, & Ch. Gerber, "Atomic Force Microscope", Phys. Rev. Lett. 56, 930 (1986)

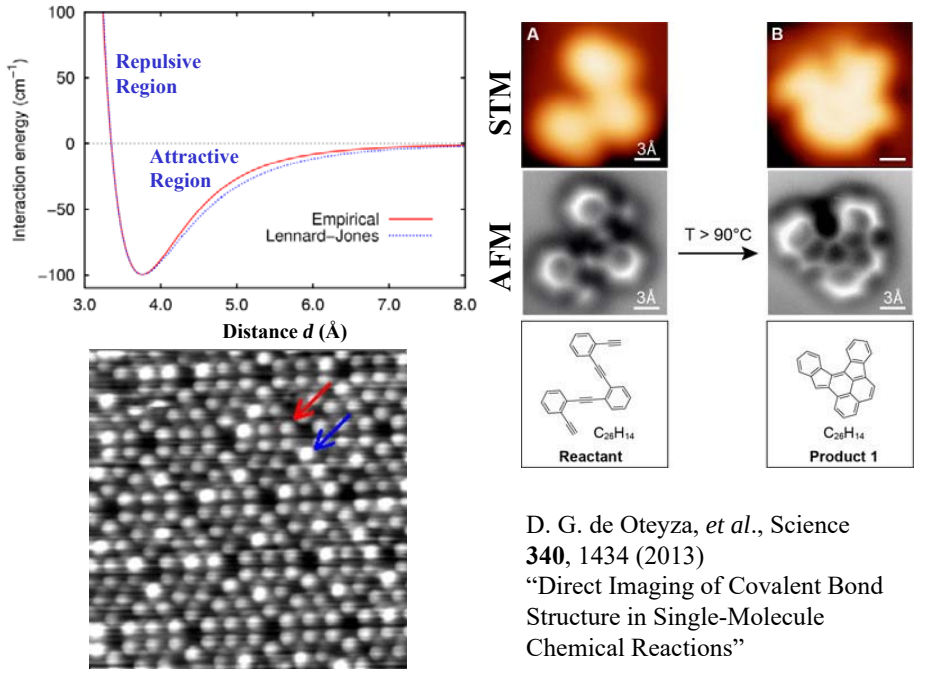


AFM
Atomic Force Microscopy
原子間力顕微鏡

絶縁物、生体試料
Insulators, Biomaterials

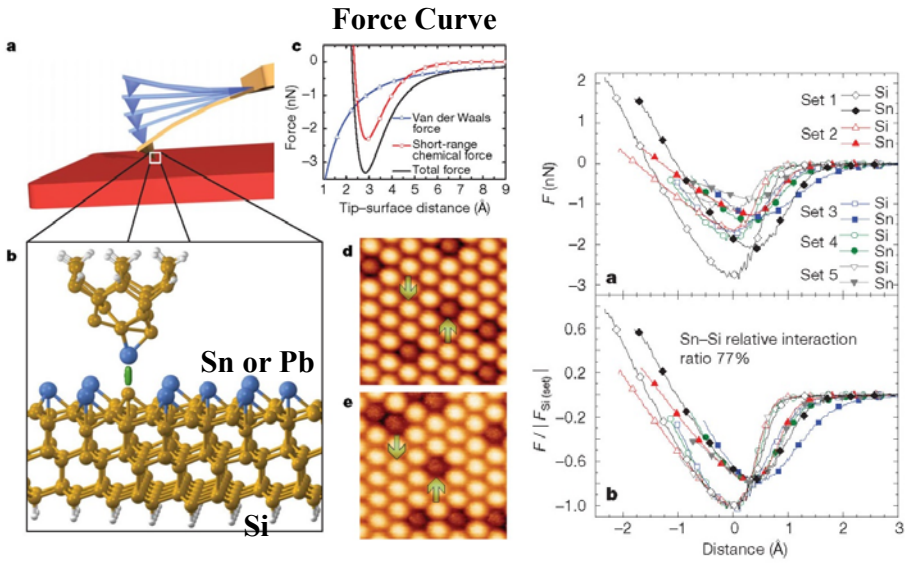
・接触モード Contact Mode
・タッピングモード Tapping Mode
・非接触モード Non-contact Mode
(AC, Dynamic Mode)

http://www.ribm.co.jp/service/spm.html

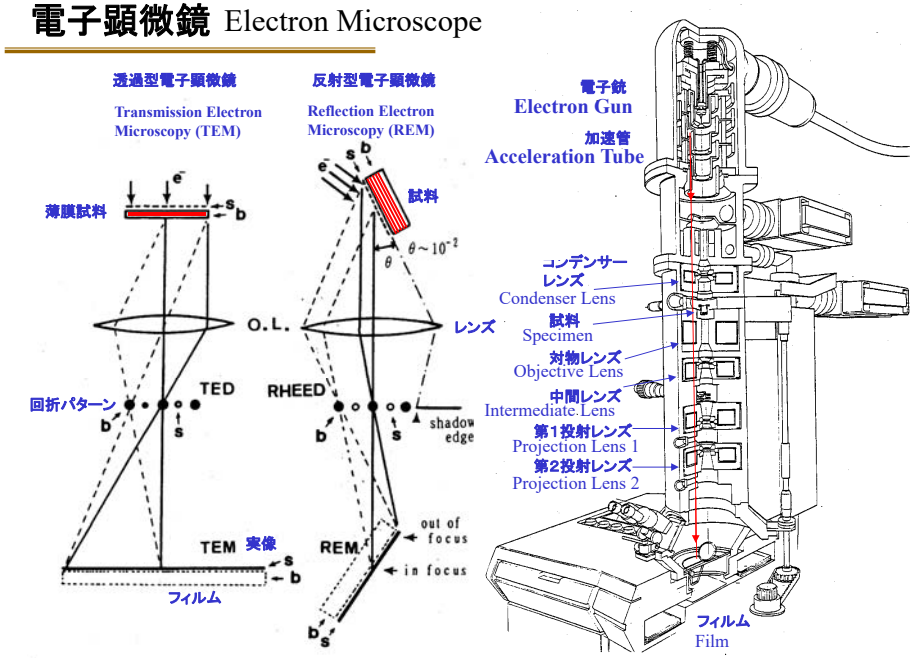


D. G. de Oteyza, *et al.*, Science **340**, 1434 (2013)
"Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions"

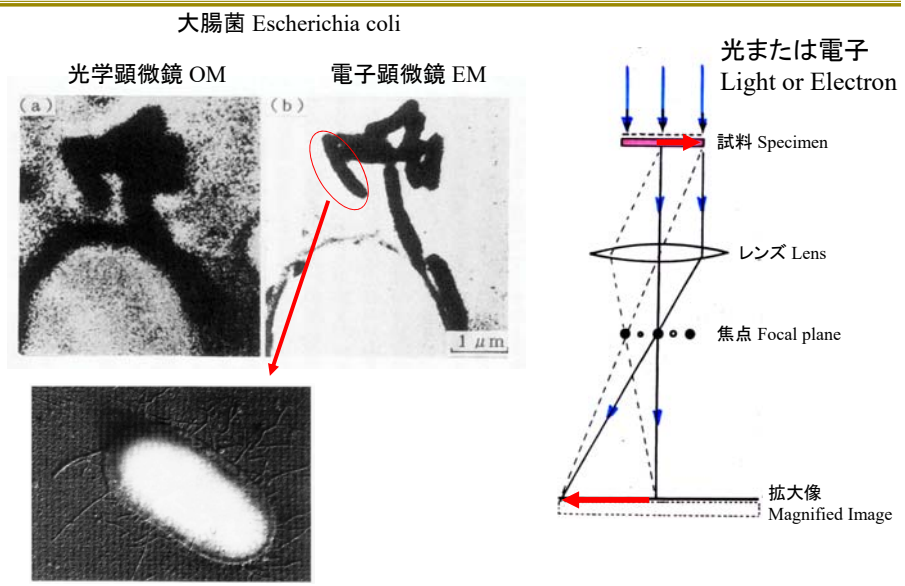
"Chemical identification of individual surface atoms by atomic force microscopy", Y. Sugimoto1, *et al*., Nature **446**, 64 (2007).



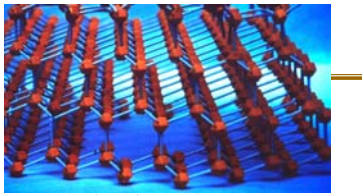
電子顕微鏡 Electron Microscope

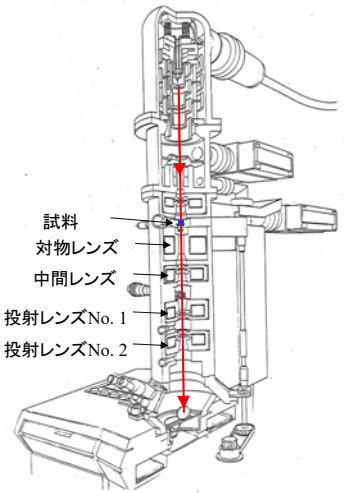


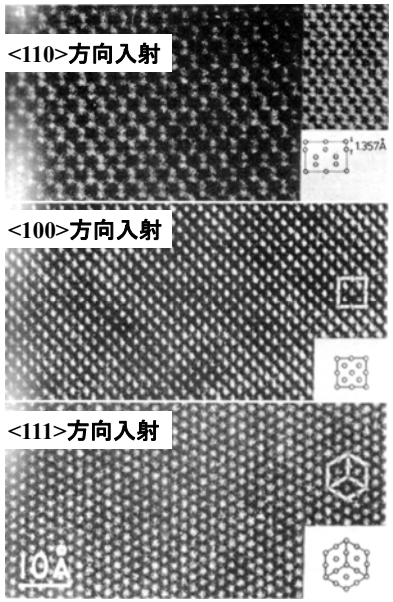
1934 E. Ruska Resolution of EM is superior to Optical Microscope.



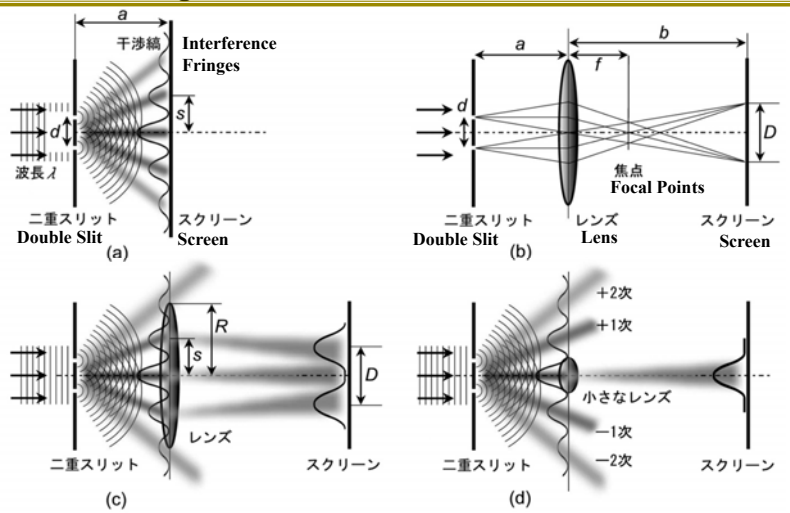
Si Crystal Observed by TEM







ヤングの二重スリットとレンズの分解能
Young's Double Slit & Resolution of Lens



$s = R \longrightarrow$ 分解能 Resolution $d_{\min} \cong \lambda \cdot \dfrac{f}{R}$