Physics 243A--Surface and Interface Physics of Materials: Basic Concepts and Spectroscopy—CRN 46760

Fall Quarter, 2016

Surface and interface physics has had a dramatic growth in importance in recent years due to the increased interest in nanometer-scale structures and materials, which may have a majority of their atoms at the surface or at buried interfaces between two phases. Such surface and interface structures are crucial in a wide variety of technological applications, including very large scale integrated circuits, magnetic storage media, photovoltaic cells, batteries and fuel cells, chemical catalysis, corrosion inhibition, tribology (friction and lubrication), environmental science, and biological science. Such surface/interface systems often exhibit markedly different properties from those of the constituent bulk materials, as for example surface composition alterations, surface relaxations or distortions of atomic positions relative to the underlying lattice, and unusual surface electronic or magnetic properties (e.g., superconductivity or ferromagnetism). Buried surfaces or interfaces are ubiquitous in technology and are similarly varied in properties. Beyond this, the component bulk materials are often complex mixtures of several elements, which also can exhibit surprising "emergent" properties that require detailed characterization.

A number of experimental techniques, theoretical models, and computational methods have thus been developed in order to better understand and control such surfaces, interfaces, and complex materials. Synchrotron radiation has also become an indispensible tool for such systems, with about 50 such facilities worldwide, and the number growing steadily.

Physics 243A will introduce these subjects as the first of a two-quarter A/B sequence that will be offered in 2016-2017. 243A will first consider some basic properties of surfaces, including their thermodynamics, their electronic structure, and the theoretical approaches that are used to model them, and then turn to the principal spectroscopic probes of surfaces, interfaces, and complex multi-element materials. Special emphasis will be on photoelectron spectroscopy (photoemission) and the complementary Auger electron spectroscopy, using both laboratory excitation sources and synchrotron radiation, and the various other spectroscopies and techniques provided by synchrotron radiation: x-ray absorption and x-ray emission spectroscopies, as enhanced by standing-wave excitation. This course is designed to be complementary in subject matter to the subsequent quarters of Physics 243. 243B will probably be taught in 2016-17 by Prof. Chiang, and will stress surface atomic structure and microscopy.

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Consultant and substitute lecturer: Shh-Chieh Lin, Physics 221, E-mail: shclin@ucdavis.edu

Some recommended prior course experience:

- **Introduction to quantum mechanics (Physics 115A and/or 215A) and/or quantum chemistry (Chemistry 210A)**
- **Introduction to solid state physics or materials science (Physics 140A and/or Physics 240A)**
- **Introduction to surface analytical chemistry (Chemistry 241A)**
- **Introduction to structure and properties of materials (Chem. Eng. And Mat. Sci. 162 and/or 272)**

Course website: http://243a.physics.ucdavis.edu/ , to be updated regularly from the current 2014 version

Time and place: Tuesdays, Thursdays, 12:10-1:30, Physics 185, plus possible supplementary lectures to be arranged to compensate for some instructor absence during the quarter.

Textbooks:

Required:

- ***"Modern Techniques of Surface Science",* D.P. Woodruff and T.A. Delchar, 2nd Edition (Cambridge University Press, 1994)—a readable text on experimental methods in surface science**
- ***"Physics at Surfaces*", A. Zangwill (Cambridge University Press, 1988)--a thorough treatment of the various aspects of surface physics, including concise theoretical discussions of many topics, free download from course website**
- ***"Physics of Surfaces and Interfaces*", H. Ibach (Springer, 2006)--a thorough treatment of the various aspects of surface physics, and available for free download from course website**
- **Copies of current review articles on photoelectron spectroscopy and diffraction, synchrotron radiation, and other topics, to be handed out in class**

Recommended for additional theoretical background:

- ***"Concepts in Surface Physics"*, M.C. Desjonqueres and D. Spanjaard, 2nd Edition (Springer Verlag, 1996, corrected printing 1998)-- contains much more detail concerning the theoretical methods of surface physics, and a useful general reference, e.g. to augment the two textbooks. Derivations are done in detail. Excerpts from this book will be handed out in class.**

--*Course assessment*: *Grading in the course will be based on the following:*

Graded problem sets	40%
Midterm exam-Tuesday, 1 Nov.	20% (Open books and notes, calculators allowed, but not computers/phones)
Comprehensive final	40% (Open books and notes, calculators allowed, but not computers/phones)
	100%

--*Final examination:* Tuesday, December 6th, 10:30-12:30 PM, Physics 185, or, if desirable, another timeslot by unanimous agreement.

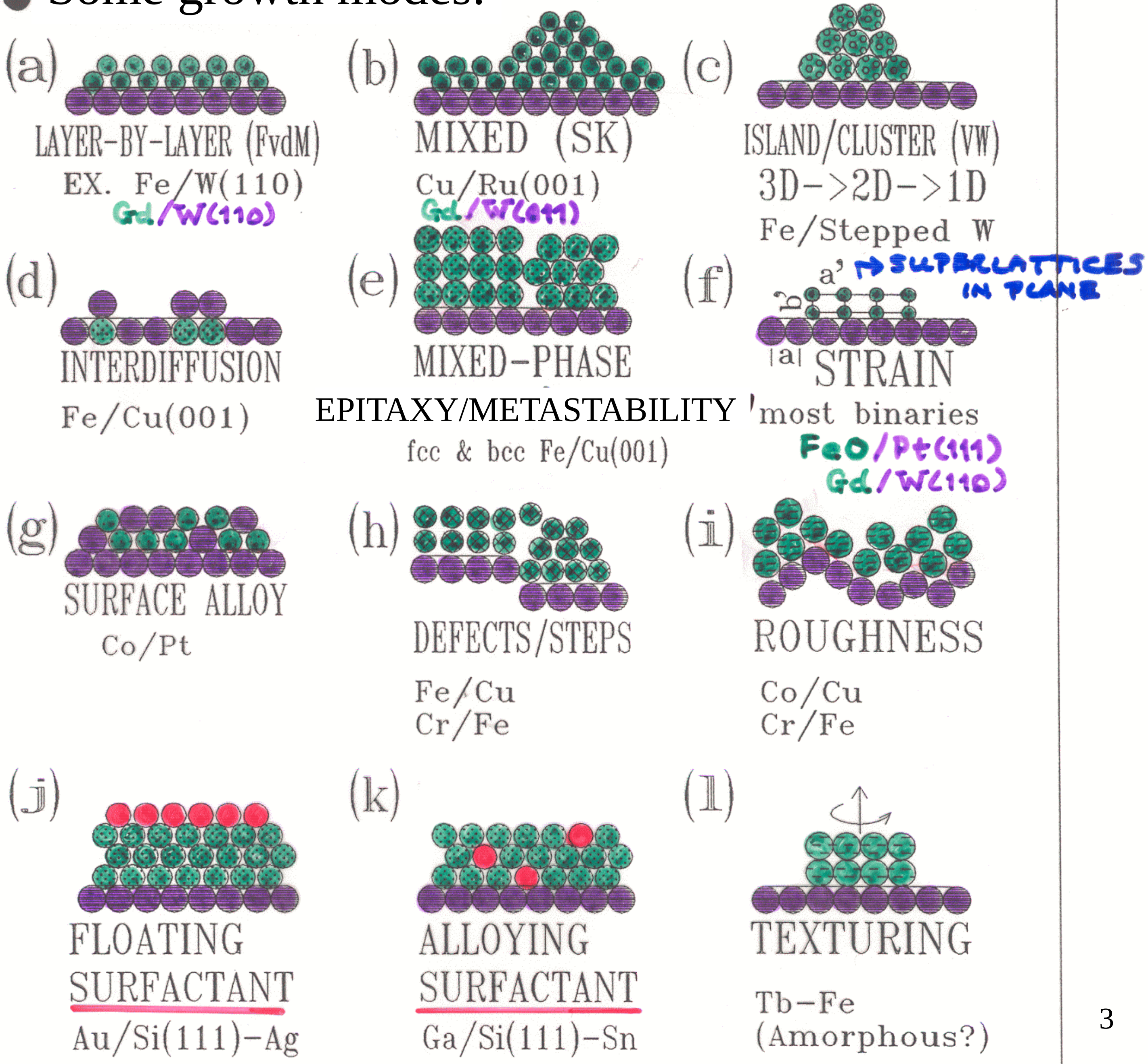
Texts, lecture slides and other reading material will be available as pdf e-files at the course website: http://www.physics.ucdavis.edu/Classes/Physics243A/

God made the bulk; surfaces were invented by the devil.

Wolfgang Pauli

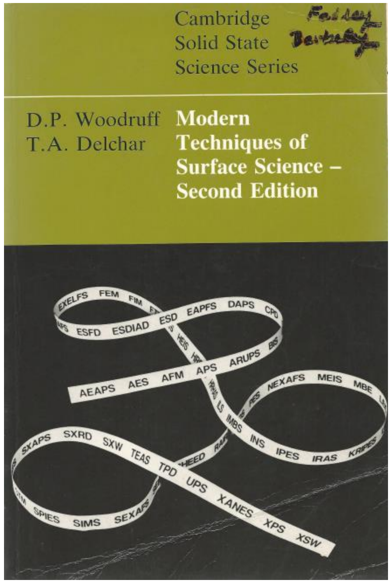
- **Frank-van der Merwe (FvdM) = layer-by-layer growth (2D).**
- **Stranski-Krastanow (SK) = layer-by-layer + island ...**
- **Volmer-Weber (VW) = island growth (3D).**

- Some growth modes:

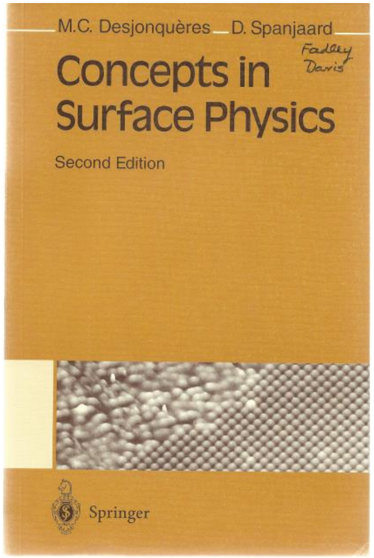


EPITAXY/METASTABILITY

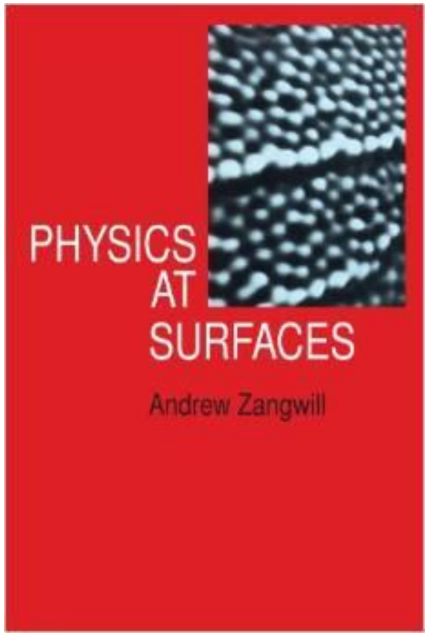
Text for surface techniques

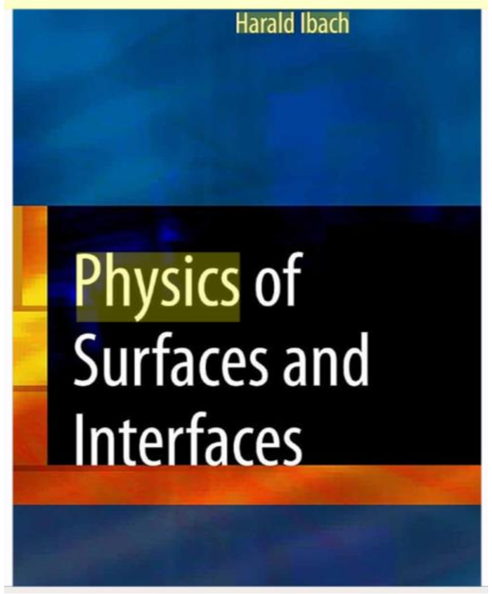


Excellent for deeper theoretical discussions of electronic structure, techniques, etc.-Excerpts at website



Downloadable Springer textbooks from course website-with a few assignments in them





Reading and Problem Assignments for Physics 243A
Surface Physics of Materials: Spectroscopy, Fall, 2014
(In order of coverage in lecture)

Reading:

- **Woodruff and Delchar, "Modern Techniques of Surface Science", 2nd Edition--**
  - **Chapter 1**
  - **Chapter 2: Sections 2.1, pp.22 (bottom)-23(top) on Wood notation for surface structures, 2.4, and 2.5 (pp. 31-37)**
  - **Chapter 6: 6.1, 6.9, 6.10, 6.11**
  - **Chapter 3: Sections 3.1, 3.2, 3.3, 3.5**

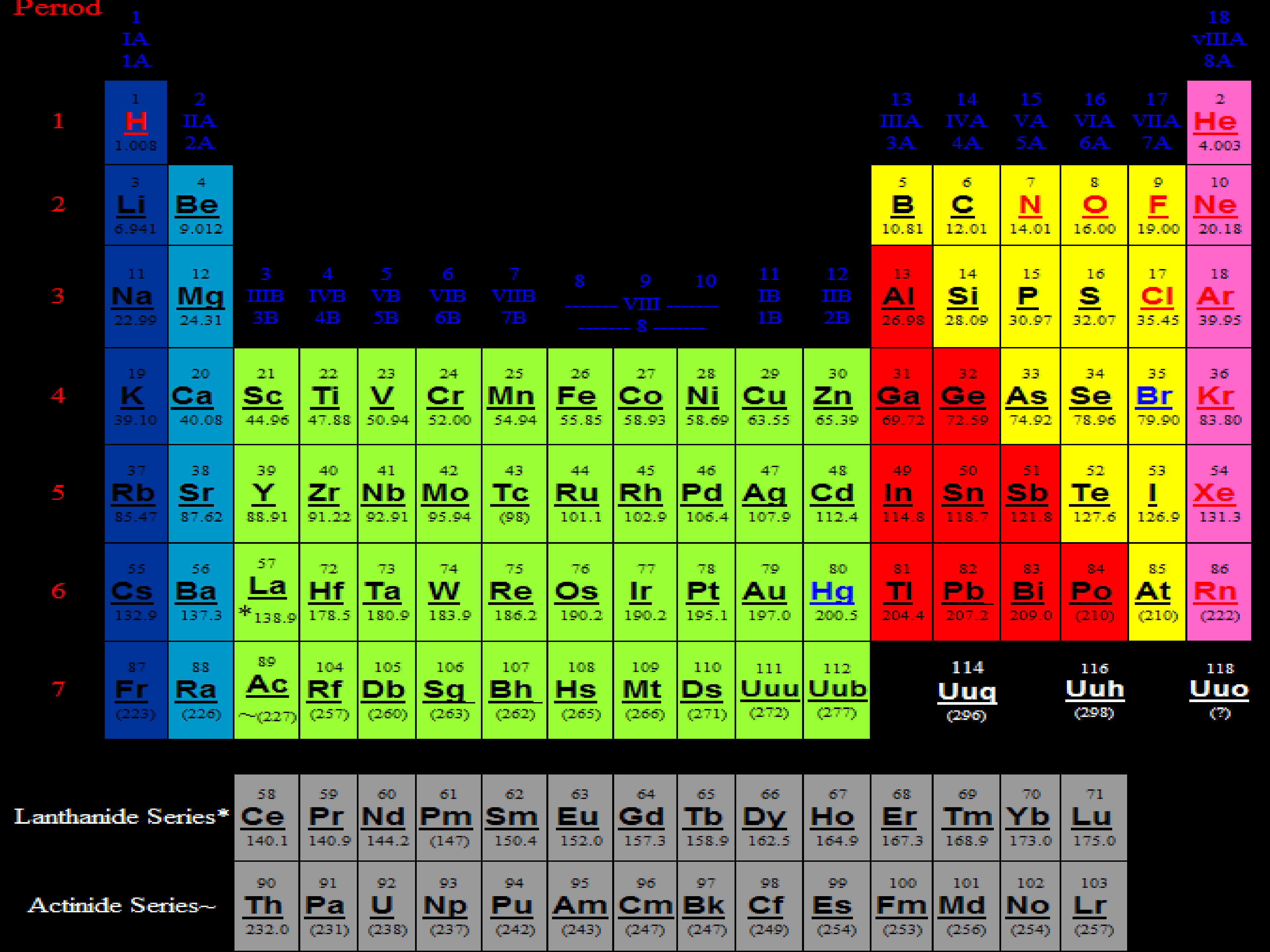
- **Zangwill, "Physics at Surfaces", downloadable Chapters 1-5 (see course website)--**
  - **Chapter 1: Everything except "The roughening transition"**
  - **Chapter 3: pp. 28-34, pp. 49-52 on STM**
  - **Pages 85-86, 192-196, 204-212**
  - **Chapter 2: All**
  - **Chapter 4: Introduction, with lighter reading of *The jellium model*, *One-dimensional band theory, and Three-dimensional band theory*, and detailed reading of *Photoelectron spectroscopy, Metals, and Alloys***

- **Ibach, "Physics of Surfaces and Interfaces", downloadable book (see course website)—**
  - **Chapter 2: 2.1, 2.2**

- **Attwood, Downloadeable excerpt on synchrotron radiation from the book "Soft X-Rays and Extreme Ultraviolet Radiation" (see course website)**

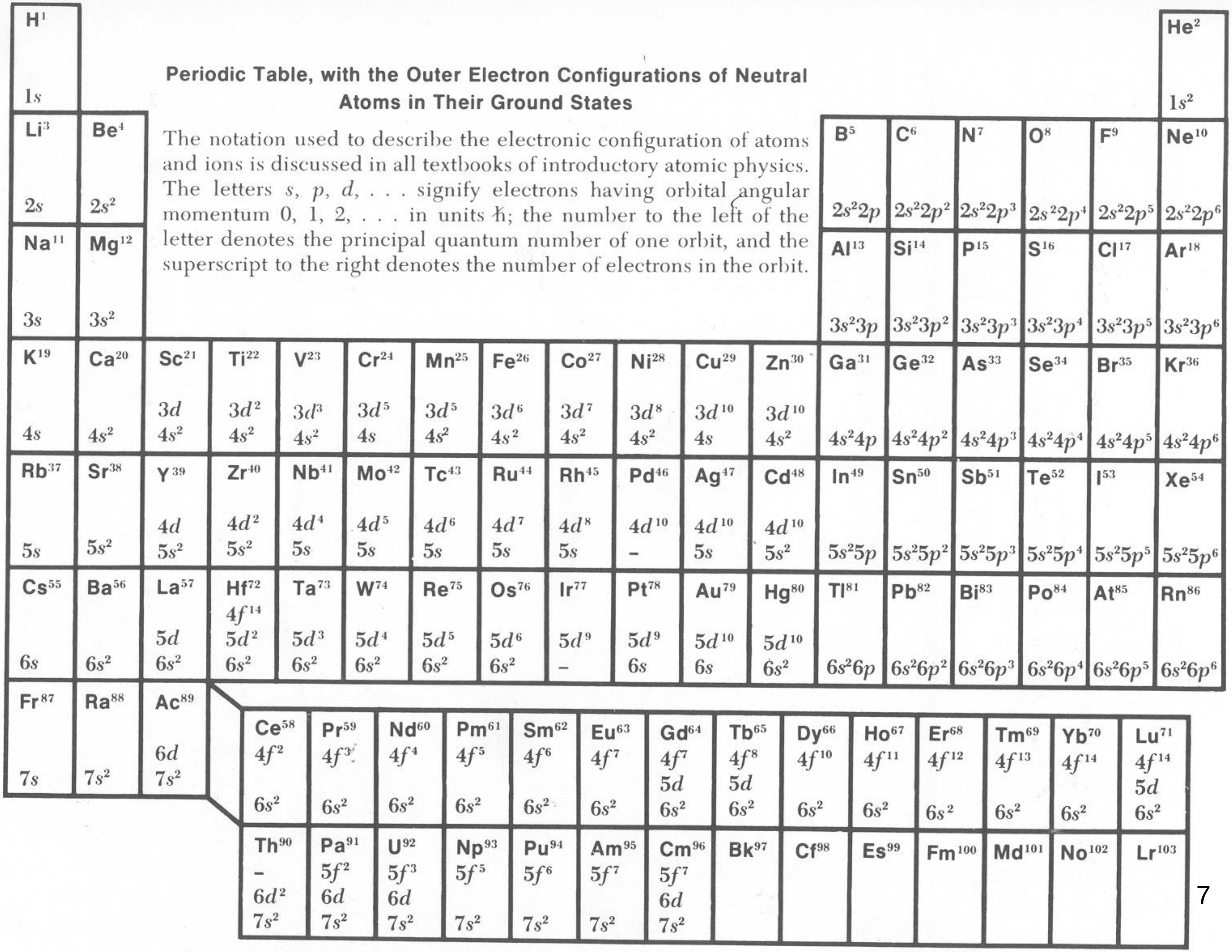
Problem assignments:

Problem set 1-all. Due Thursday, October 13th



Period	1 IA 1A																	18 VIIIA 8A
1	1 H 1.008	2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57 La *138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 190.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	89 Ac ~(227)	104 Rf (257)	105 Db (260)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Ds (271)	111 Uuu (272)	112 Uub (277)		114 Uuq (296)		116 Uuh (298)		118 Uuo (?)

Lanthanide Series*	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
Actinide Series~	90 Th 232.0	91 Pa (231)	92 U (238)	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)



Periodic Table, with the Outer Electron Configurations of Neutral Atoms in Their Ground States

The notation used to describe the electronic configuration of atoms and ions is discussed in all textbooks of introductory atomic physics. The letters *s*, *p*, *d*, . . . signify electrons having orbital angular momentum 0, 1, 2, . . . in units ħ; the number to the left of the letter denotes the principal quantum number of one orbit, and the superscript to the right denotes the number of electrons in the orbit.

H^{1} $1s$																	**He**^{2} $1s^2$
Li^{3} $2s$	**Be**^{4} $2s^2$											**B**^{5} $2s^22p$	**C**^{6} $2s^22p^2$	**N**^{7} $2s^22p^3$	**O**^{8} $2s^22p^4$	**F**^{9} $2s^22p^5$	**Ne**^{10} $2s^22p^6$
Na^{11} $3s$	**Mg**^{12} $3s^2$											**Al**^{13} $3s^23p$	**Si**^{14} $3s^23p^2$	**P**^{15} $3s^23p^3$	**S**^{16} $3s^23p^4$	**Cl**^{17} $3s^23p^5$	**Ar**^{18} $3s^23p^6$
K^{19} $4s$	**Ca**^{20} $4s^2$	**Sc**^{21} $3d$ $4s^2$	**Ti**^{22} $3d^2$ $4s^2$	**V**^{23} $3d^3$ $4s^2$	**Cr**^{24} $3d^5$ $4s$	**Mn**^{25} $3d^5$ $4s^2$	**Fe**^{26} $3d^6$ $4s^2$	**Co**^{27} $3d^7$ $4s^2$	**Ni**^{28} $3d^8$ $4s^2$	**Cu**^{29} $3d^{10}$ $4s$	**Zn**^{30} $3d^{10}$ $4s^2$	**Ga**^{31} $4s^24p$	**Ge**^{32} $4s^24p^2$	**As**^{33} $4s^24p^3$	**Se**^{34} $4s^24p^4$	**Br**^{35} $4s^24p^5$	**Kr**^{36} $4s^24p^6$
Rb^{37} $5s$	**Sr**^{38} $5s^2$	**Y**^{39} $4d$ $5s^2$	**Zr**^{40} $4d^2$ $5s^2$	**Nb**^{41} $4d^4$ $5s$	**Mo**^{42} $4d^5$ $5s$	**Tc**^{43} $4d^6$ $5s$	**Ru**^{44} $4d^7$ $5s$	**Rh**^{45} $4d^8$ $5s$	**Pd**^{46} $4d^{10}$ –	**Ag**^{47} $4d^{10}$ $5s$	**Cd**^{48} $4d^{10}$ $5s^2$	**In**^{49} $5s^25p$	**Sn**^{50} $5s^25p^2$	**Sb**^{51} $5s^25p^3$	**Te**^{52} $5s^25p^4$	**I**^{53} $5s^25p^5$	**Xe**^{54} $5s^25p^6$
Cs^{55} $6s$	**Ba**^{56} $6s^2$	**La**^{57} $5d$ $6s^2$	**Hf**^{72} $4f^{14}$ $5d^2$ $6s^2$	**Ta**^{73} $5d^3$ $6s^2$	**W**^{74} $5d^4$ $6s^2$	**Re**^{75} $5d^5$ $6s^2$	**Os**^{76} $5d^6$ $6s^2$	**Ir**^{77} $5d^9$ –	**Pt**^{78} $5d^9$ $6s$	**Au**^{79} $5d^{10}$ $6s$	**Hg**^{80} $5d^{10}$ $6s^2$	**Tl**^{81} $6s^26p$	**Pb**^{82} $6s^26p^2$	**Bi**^{83} $6s^26p^3$	**Po**^{84} $6s^26p^4$	**At**^{85} $6s^26p^5$	**Rn**^{86} $6s^26p^6$
Fr^{87} $7s$	**Ra**^{88} $7s^2$	**Ac**^{89} $6d$ $7s^2$															

Ce^{58} $4f^2$ $6s^2$	**Pr**^{59} $4f^3$ $6s^2$	**Nd**^{60} $4f^4$ $6s^2$	**Pm**^{61} $4f^5$ $6s^2$	**Sm**^{62} $4f^6$ $6s^2$	**Eu**^{63} $4f^7$ $6s^2$	**Gd**^{64} $4f^7$ $5d$ $6s^2$	**Tb**^{65} $4f^8$ $5d$ $6s^2$	**Dy**^{66} $4f^{10}$ $6s^2$	**Ho**^{67} $4f^{11}$ $6s^2$	**Er**^{68} $4f^{12}$ $6s^2$	**Tm**^{69} $4f^{13}$ $6s^2$	**Yb**^{70} $4f^{14}$ $6s^2$	**Lu**^{71} $4f^{14}$ $5d$ $6s^2$
Th^{90} – $6d^2$ $7s^2$	**Pa**^{91} $5f^2$ $6d$ $7s^2$	**U**^{92} $5f^3$ $6d$ $7s^2$	**Np**^{93} $5f^5$ $7s^2$	**Pu**^{94} $5f^6$ $7s^2$	**Am**^{95} $5f^7$ $7s^2$	**Cm**^{96} $5f^7$ $6d$ $7s^2$	**Bk**^{97}	**Cf**^{98}	**Es**^{99}	**Fm**^{100}	**Md**^{101}	**No**^{102}	**Lr**^{103}

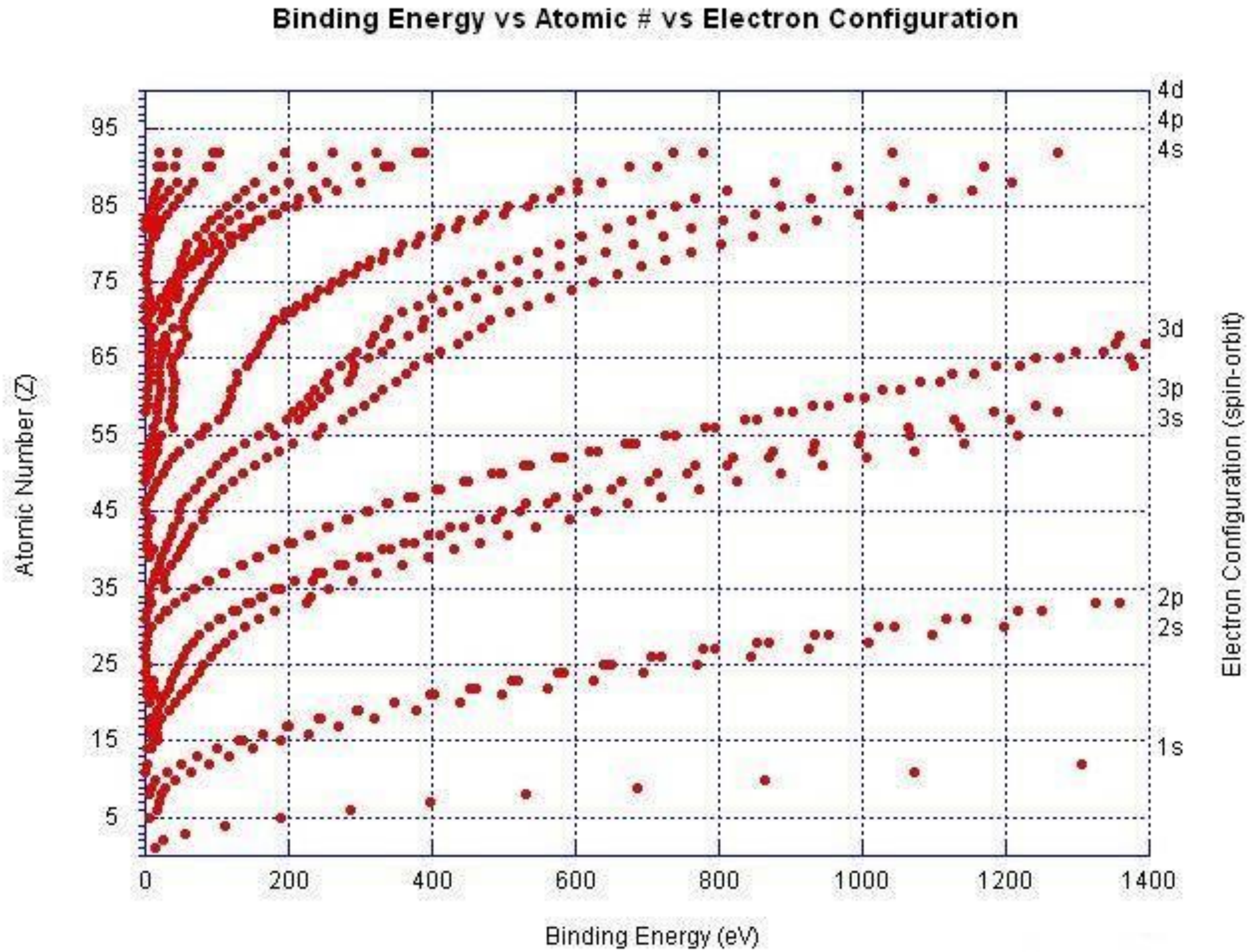

Binding Energy vs Atomic # vs Electron Configuration
Atomic Number (Z)
95
85
75
65
55
45
35
25
15
5
0
200
400
600
800
1000
1200
1400
Binding Energy (eV)
4d
4p
4s
3d
3p
3s
2p
2s
1s
Electron Configuration (spin-orbit)

Table 3 Crystal structures of the elements

The data given are at room temperature for the most common form, or at the stated temperature in deg K. For further descriptions of the elements see Wyckoff, Vol. 1, Chap. 2. Structures labeled complex are described there.

← Crystal structure →
← *a* lattice parameter, in Å →
← *c* lattice parameter, in Å →

H^1 4K hcp 3.75 6.12																	**He**^{4} 2K hcp 3.57 5.83
Li 78K bcc 3.491	**Be** hcp 2.27 3.59											**B** rhomb.	**C** diamond 3.567	**N** 20K cubic 5.66 (N$_2$)	**O** complex (O$_2$)	**F**	**Ne** 4K fcc 4.46
Na 5K bcc 4.225	**Mg** hcp 3.21 5.21											**Al** fcc 4.05	**Si** diamond 5.430	**P** complex	**S** complex	**Cl** complex (Cl$_2$)	**Ar** 4K fcc 5.31
K 5K bcc 5.225	**Ca** fcc 5.58	**Sc** hcp 3.31 5.27	**Ti** hcp 2.95 4.68	**V** bcc 3.03	**Cr** bcc 2.88	**Mn** cubic complex	**Fe** bcc 2.87	**Co** hcp 2.51 4.07	**Ni** fcc 3.52	**Cu** fcc 3.61	**Zn** hcp 2.66 4.95	**Ga** complex	**Ge** diamond 5.658	**As** rhomb.	**Se** hex. chains	**Br** complex (Br$_2$)	**Kr** 4K fcc 5.64
Rb 5K bcc 5.585	**Sr** fcc 6.08	**Y** hcp 3.65 5.73	**Zr** hcp 3.23 5.15	**Nb** bcc 3.30	**Mo** bcc 3.15	**Tc** hcp 2.74 4.40	**Ru** hcp 2.71 4.28	**Rh** fcc 3.80	**Pd** fcc 3.89	**Ag** fcc 4.09	**Cd** hcp 2.98 5.62	**In** tetr. 3.25 4.95	**Sn** (α) diamond 6.49	**Sb** rhomb.	**Te** hex. chains	**I** complex (I$_2$)	**Xe** 4K fcc 6.13
Cs 5K bcc 6.045	**Ba** bcc 5.02	**La** hex. 3.77 *ABAC*	**Hf** hcp 3.19 5.05	**Ta** bcc 3.30	**W** bcc 3.16	**Re** hcp 2.76 4.46	**Os** hcp 2.74 4.32	**Ir** fcc 3.84	**Pt** fcc 3.92	**Au** fcc 4.08	**Hg** rhomb.	**Tl** hcp 3.46 5.52	**Pb** fcc 4.95	**Bi** rhomb.	**Po** sc 3.34	**At** —	**Rn** —
Fr —	**Ra** —	**Ac** fcc 5.31															

Ce fcc 5.16	**Pr** hex. 3.67 *ABAC*	**Nd** hex. 3.66	**Pm** —	**Sm** complex	**Eu** bcc 4.58	**Gd** hcp 3.63 5.78	**Tb** hcp 3.60 5.70	**Dy** hcp 3.59 5.65	**Ho** hcp 3.58 5.62	**Er** hcp 3.56 5.59	**Tm** hcp 3.54 5.56	**Yb** fcc 5.48	**Lu** hcp 3.50 5.55
Th fcc 5.08	**Pa** tetr. 3.92 3.24	**U** complex	**Np** complex	**Pu** complex	**Am** hex. 3.64 *ABAC*	**Cm** —	**Bk** —	**Cf** —	**Es** —	**Fm** —	**Md** —	**No** —	**Lr** —

CPK Atomic-Ionic Radii

This image was generated using CrystalMaker®

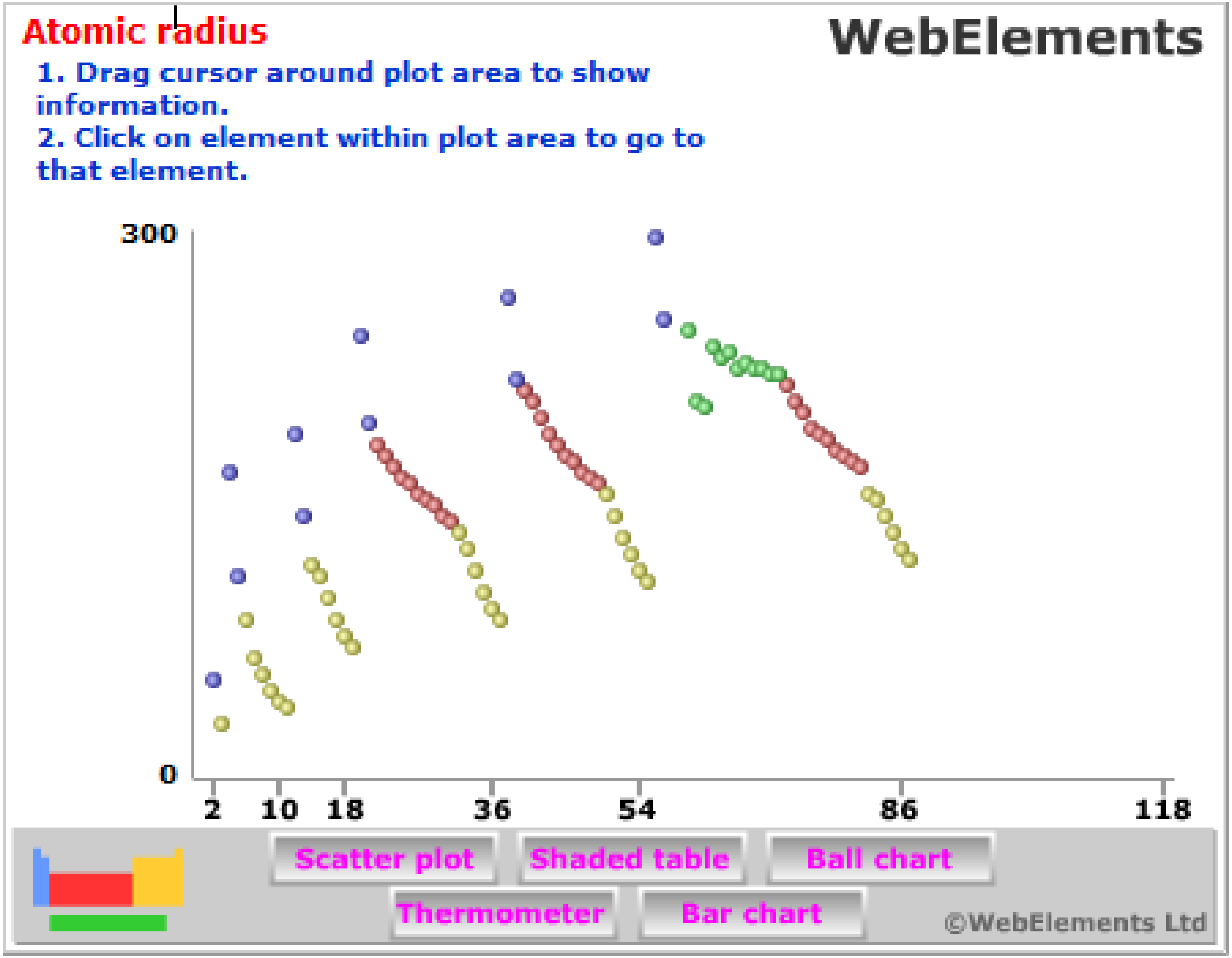
This dataset uses colours derived from those of the plastic spacefilling models developed by Corey, Pauling and Kultun ("CPK"). The atomic radii data are taken from an empirical system of unified atomic-ionic radii, which is suitable for describing anion-cation contacts in ionic structures. Calculated data (Clementi et al., 1963) have been used for: He, Ne, Ar, Kr, Xe, At and Rn.

References: J C Slater (1964) Journal of Chemical Physics 41:3199-

J C Slater (1965) Quantum Theory of Molecules and Solids. Symmetry and Bonds in Crystals Vol 2. McGraw-Hill, NY.

Clementi E, Raimondi DL, Reinhardt WP (1963) Journal of Chemical Physics 38:2686-

http://www.webelements.com/titanium/atom_sizes.htm



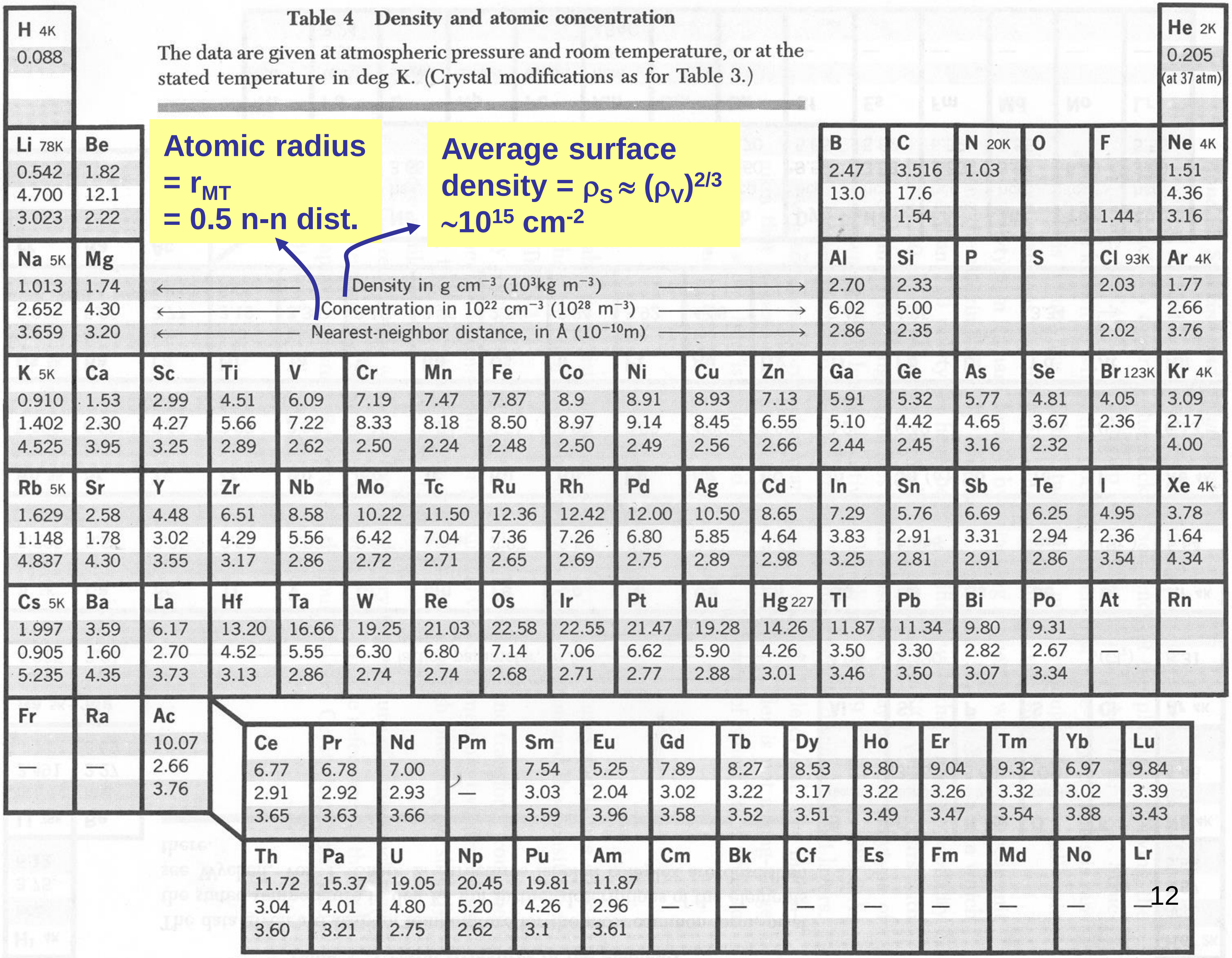


Table 4 Density and atomic concentration

The data are given at atmospheric pressure and room temperature, or at the stated temperature in deg K. (Crystal modifications as for Table 3.)

Atomic radius = r_{MT} = 0.5 n-n dist.

Average surface density = $\rho_S \approx (\rho_V)^{2/3}$ ~10^{15} cm^{-2}

Density in g cm^{-3} ($10^3 kg\ m^{-3}$)

Concentration in 10^{22} cm^{-3} (10^{28} m^{-3})

Nearest-neighbor distance, in Å (10^{-10}m)

H 4K 0.088																	He 2K 0.205 (at 37 atm)
Li 78K 0.542 4.700 3.023	Be 1.82 12.1 2.22											B 2.47 13.0	C 3.516 17.6 1.54	N 20K 1.03	O	F 1.44	Ne 4K 1.51 4.36 3.16
Na 5K 1.013 2.652 3.659	Mg 1.74 4.30 3.20											Al 2.70 6.02 2.86	Si 2.33 5.00 2.35	P	S	Cl 93K 2.03 2.02	Ar 4K 1.77 2.66 3.76
K 5K 0.910 1.402 4.525	Ca 1.53 2.30 3.95	Sc 2.99 4.27 3.25	Ti 4.51 5.66 2.89	V 6.09 7.22 2.62	Cr 7.19 8.33 2.50	Mn 7.47 8.18 2.24	Fe 7.87 8.50 2.48	Co 8.9 8.97 2.50	Ni 8.91 9.14 2.49	Cu 8.93 8.45 2.56	Zn 7.13 6.55 2.66	Ga 5.91 5.10 2.44	Ge 5.32 4.42 2.45	As 5.77 4.65 3.16	Se 4.81 3.67 2.32	Br 123K 4.05 2.36	Kr 4K 3.09 2.17 4.00
Rb 5K 1.629 1.148 4.837	Sr 2.58 1.78 4.30	Y 4.48 3.02 3.55	Zr 6.51 4.29 3.17	Nb 8.58 5.56 2.86	Mo 10.22 6.42 2.72	Tc 11.50 7.04 2.71	Ru 12.36 7.36 2.65	Rh 12.42 7.26 2.69	Pd 12.00 6.80 2.75	Ag 10.50 5.85 2.89	Cd 8.65 4.64 2.98	In 7.29 3.83 3.25	Sn 5.76 2.91 2.81	Sb 6.69 3.31 2.91	Te 6.25 2.94 2.86	I 4.95 2.36 3.54	Xe 4K 3.78 1.64 4.34
Cs 5K 1.997 0.905 5.235	Ba 3.59 1.60 4.35	La 6.17 2.70 3.73	Hf 13.20 4.52 3.13	Ta 16.66 5.55 2.86	W 19.25 6.30 2.74	Re 21.03 6.80 2.74	Os 22.58 7.14 2.68	Ir 22.55 7.06 2.71	Pt 21.47 6.62 2.77	Au 19.28 5.90 2.88	Hg 227 14.26 4.26 3.01	Tl 11.87 3.50 3.46	Pb 11.34 3.30 3.50	Bi 9.80 2.82 3.07	Po 9.31 2.67 3.34	At —	Rn —
Fr —	Ra —	Ac 10.07 2.66 3.76															

Ce 6.77 2.91 3.65	Pr 6.78 2.92 3.63	Nd 7.00 2.93 3.66	Pm —	Sm 7.54 3.03 3.59	Eu 5.25 2.04 3.96	Gd 7.89 3.02 3.58	Tb 8.27 3.22 3.52	Dy 8.53 3.17 3.51	Ho 8.80 3.22 3.49	Er 9.04 3.26 3.47	Tm 9.32 3.32 3.54	Yb 6.97 3.02 3.88	Lu 9.84 3.39 3.43
Th 11.72 3.04 3.60	Pa 15.37 4.01 3.21	U 19.05 4.80 2.75	Np 20.45 5.20 2.62	Pu 19.81 4.26 3.1	Am 11.87 2.96 3.61	Cm —	Bk —	Cf —	Es —	Fm —	Md —	No —	Lr —

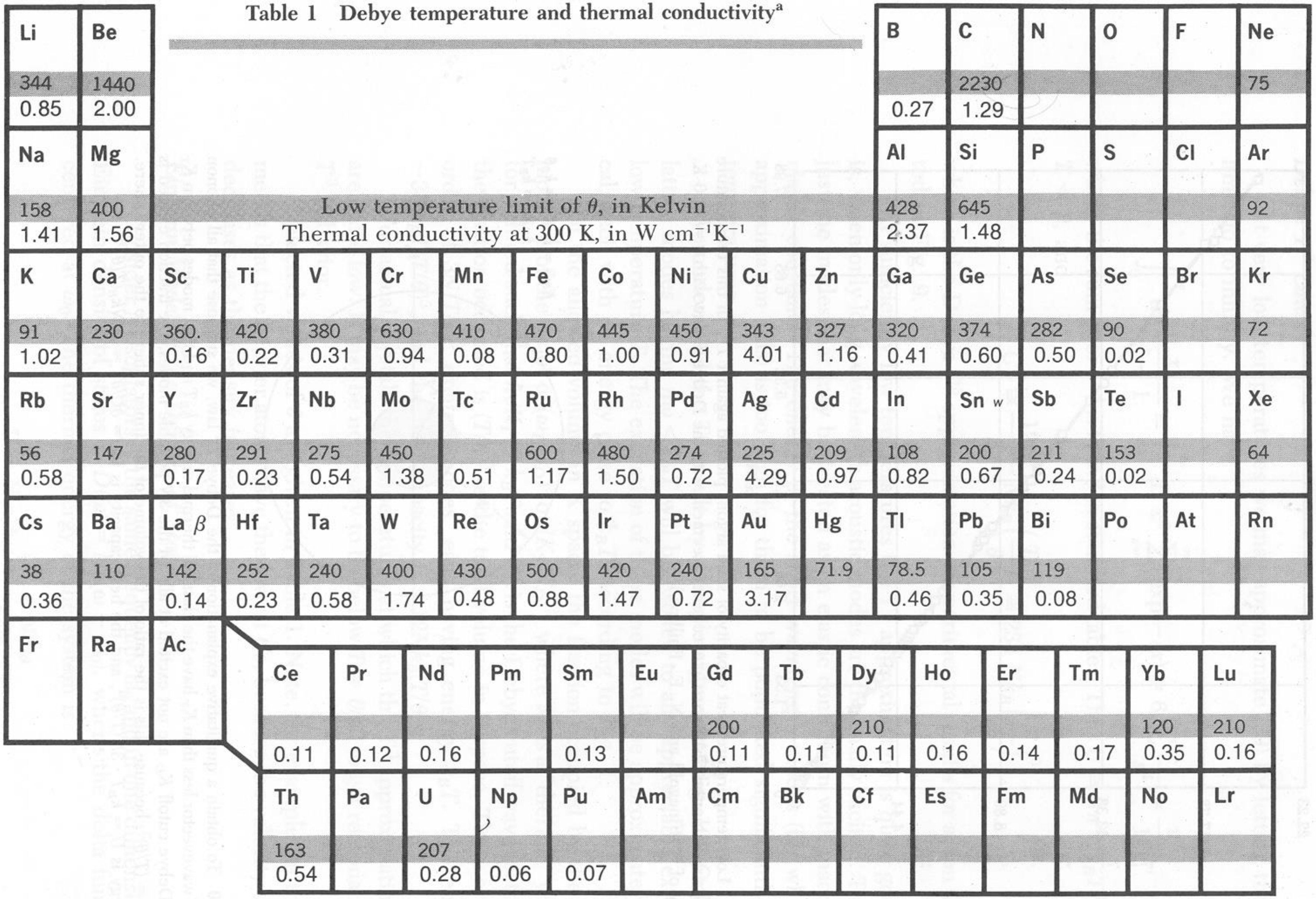


Table 1 Debye temperature and thermal conductivity[a]

Low temperature limit of θ, in Kelvin
Thermal conductivity at 300 K, in W $cm^{-1}K^{-1}$

Li 344 0.85	**Be** 1440 2.00											**B** 0.27	**C** 2230 1.29	**N**	**O**	**F**	**Ne** 75
Na 158 1.41	**Mg** 400 1.56											**Al** 428 2.37	**Si** 645 1.48	**P**	**S**	**Cl**	**Ar** 92
K 91 1.02	**Ca** 230	**Sc** 360. 0.16	**Ti** 420 0.22	**V** 380 0.31	**Cr** 630 0.94	**Mn** 410 0.08	**Fe** 470 0.80	**Co** 445 1.00	**Ni** 450 0.91	**Cu** 343 4.01	**Zn** 327 1.16	**Ga** 320 0.41	**Ge** 374 0.60	**As** 282 0.50	**Se** 90 0.02	**Br**	**Kr** 72
Rb 56 0.58	**Sr** 147	**Y** 280 0.17	**Zr** 291 0.23	**Nb** 275 0.54	**Mo** 450 1.38	**Tc** 0.51	**Ru** 600 1.17	**Rh** 480 1.50	**Pd** 274 0.72	**Ag** 225 4.29	**Cd** 209 0.97	**In** 108 0.82	**Sn** *w* 200 0.67	**Sb** 211 0.24	**Te** 153 0.02	**I**	**Xe** 64
Cs 38 0.36	**Ba** 110	**La** β 142 0.14	**Hf** 252 0.23	**Ta** 240 0.58	**W** 400 1.74	**Re** 430 0.48	**Os** 500 0.88	**Ir** 420 1.47	**Pt** 240 0.72	**Au** 165 3.17	**Hg** 71.9	**Tl** 78.5 0.46	**Pb** 105 0.35	**Bi** 119 0.08	**Po**	**At**	**Rn**
Fr	**Ra**	**Ac**															

Ce 0.11	**Pr** 0.12	**Nd** 0.16	**Pm**	**Sm** 0.13	**Eu**	**Gd** 200 0.11	**Tb** 0.11	**Dy** 210 0.11	**Ho** 0.16	**Er** 0.14	**Tm** 0.17	**Yb** 120 0.35	**Lu** 210 0.16
Th 163 0.54	**Pa**	**U** 207 0.28	**Np** 0.06	**Pu** 0.07	**Am**	**Cm**	**Bk**	**Cf**	**Es**	**Fm**	**Md**	**No**	**Lr**

---

[a] Most of the θ values were supplied by N. Pearlman; references are given the *A.I.P. Handbook*, 3rd ed; the thermal conductivity values are from R. W. Powell and Y. S. Touloukian, Science **181**, 999 (1973).

Table 1 Cohesive Energies* of the elements

Energy required to form separated neutral atoms from the solid at 0°K; the values in parentheses are at 298.15°K or at the melting point, whichever temperature is lower. To obtain the energy in J mol^{-1}, multiply the energy in kcal mol^{-1} by 4.184 = 10^3. To obtain the energy in ergs per atom, multiply the energy in eV per atom by 1.60219 × 10^{-12}.

← eV per atom →

← kcal per mole →

H 4.48 103																	He
Li 1.65 38.0	Be 3.33 76.9											B 5.81 134.	C 7.36 170.	N (114)	O (60)	F (20)	Ne 0.02 0.45
Na 1.13 26.0	Mg 1.53 35.3											Al 3.34 76.9	Si 4.64 107	P (79.2)	S 2.86 66.1	Cl (32.2)	Ar 0.080 1.85
K 0.941 21.7	Ca 1.825 42.1	Sc 3.93 90.6	Ti 4.855 112.0	V 5.30 122.	Cr 4.10 94.5	Mn 2.98 68.7	Fe 4.29 98.9	Co 4.387 101.2	Ni 4.435 102.3	Cu 3.50 80.8	Zn 1.35 31.1	Ga 2.78 64.2	Ge 3.87 89.3	As 3.0 69.	Se 2.13 49.2	Br 1.22 (28.2)	Kr 0.116 2.67
Rb 0.858 19.8	Sr (39.1)	Y 4.387 101.2	Zr 6.316 145.7	Nb 7.47 172.	Mo 6.810 157.1	Tc	Ru 6.615 152.6	Rh 5.752 132.7	Pd 3.936 90.8	Ag 2.96 68.3	Cd 1.160 26.76	In 2.6 59	Sn 3.12 71.9	Sb 2.7 62.	Te 2.0 46	I (25.6)	Xe (3.57)
Cs 0.827 19.1	Ba 1.86 (42.8)	La 4.491 103.6	Hf 6.35 146.	Ta 8.089 186.6	W 8.66 200.	Re 8.10 187.	Os (187)	Ir 6.93 160.	Pt 5.852 135.0	Au 3.78 87.3	Hg (0.694) (16.0)	Tl 1.87 43.2	Pb 2.04 47.0	Bi 2.15 49.6	Po (34.5)	At	Rn
Fr	Ra	Ac															

Ce 4.77 110	Pr 3.9 89	Nd 3.35 77.2	Pm	Sm 2.11 48.6	Eu 1.80 41.5	Gd 4.14 95.4	Tb 4.1 94	Dy 3.1 71	Ho 3.0 70	Er 3.3 77	Tm 2.6 59	Yb 1.6 36	Lu (4.4) (102)
Th 5.926 136.7	Pa 5.46 126	U 5.405 124.7	Np 4.55 105	Pu 4.0 92	Am 2.6 60	Cm	Bk	Cf	Es	Fm	Md	No	Lw

Work functions of the Elements
[eV]

After L. Ley and M. Cardona,
"Photoemission in Solids", Springer 1979

Low

1 **H** -																	2 **He** -
3 **Li** 2.4	4 **Be** 1.5											5 **B** 4.5	6 **C** 4.7	7 **N** -	8 **O** -	9 **F** -	10 **Ne** -
11 **Na** 2.35	12 **Mg** 3.6											13 **Al** 4.25	14 **Si** 4.8	15 **P** -	16 **S** -	17 **Cl** -	18 **Ar** -
19 **K** 2.2	20 **Ca** 2.8	21 **Sc** 3.3	22 **Ti** 3.95	23 **V** 4.1	24 **Cr** 4.6	25 **Mn** 3.8	26 **Fe** 4.3	27 **Co** 4.4	28 **Ni** 4.5	29 **Cu** 4.4	30 **Zn** 4.2	31 **Ga** 4.0	32 **Ge** 4.8	33 **As** 5.1	34 **Se** 4.7	35 **Br** -	36 **Kr** -
37 **Rb** 2.2	38 **Sr** 2.35	39 **Y** 3.3	40 **Zr** 3.9	41 **Nb** 4.0	42 **Mo** 4.3	43 **Tc** -	44 **Ru** 4.6	45 **Rh** 4.75	46 **Pd** 4.8	47 **Ag** 4.3	48 **Cd** 4.1	49 **In** 3.8	50 **Sn** 4.4	51 **Sb** 4.1	52 **Te** 4.7	53 **I** -	54 **Xe** -
55 **Cs** 1.8	56 **Ba** 2.5	57 **La** 3.3	72 **Hf** 3.5	73 **Ta** 4.1	74 **W** 4.5	75 **Re** 5.0	76 **Os** 4.7	77 **Ir** 5.3	78 **Pt** 5.3	79 **Au** 4.3	80 **Hg** 4.5	81 **Tl** 3.7	82 **Pb** 4.0	83 **Bi** 4.4	84 **Po** -	85 **At** -	86 **Rn** -
87 **Fr** -	88 **Ra** -	89 **Ac** -															

High

58 **Ce** 2.7	59 **Pr** -	60 **Nd** -	61 **Pm** -	62 **Sm** -	63 **Eu** -	64 **Gd** -	65 **Tb** -	66 **Dy** -	67 **Ho** -	68 **Er** -	69 **Tm** -	70 **Yb** -	71 **Lu** -
90 **Th** 3.3	91 **Pa** -	92 **U** 3.3	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

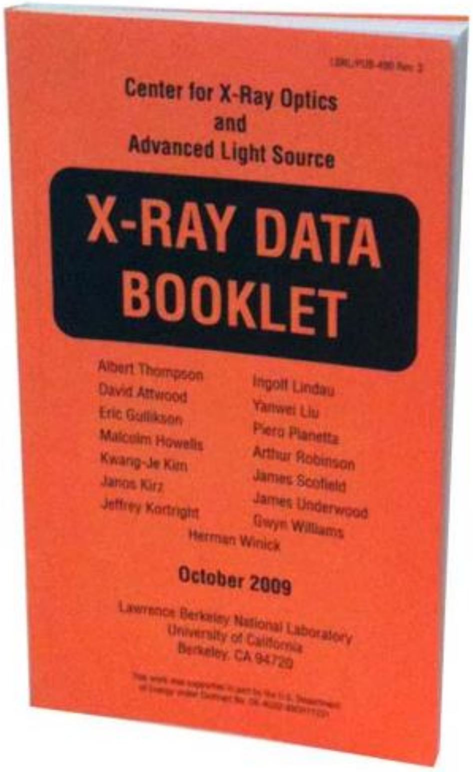
X-RAY DATA BOOKLET
Center for X-ray Optics and Advanced Light Source
Lawrence Berkeley National Laboratory

- Introduction
- X-Ray Properties of Elements
- Electron Binding Energies
- X-Ray Energy Emission Energies
- Fluorescence Yields for K and L Shells
- Principal Auger Electron Energies
- Subshell Photoionization Cross-Sections
- Mass Absorption Coefficients
- Atomic Scattering Factors
- Energy Levels of Few Electron Ions
- Periodic Table of X-Ray Properties
- Synchrotron Radiation
- Characteristics of Synchrotron Radiation
- History of X-rays and Synchrotron Radiation
- Synchrotron Facilities
- Scattering Processes
- Scattering of X-rays from Electrons and Atoms
- Low-Energy Electron Ranges in Matter
- Optics and Detectors
- Crystal and Multilayer Elements
- Specular Reflectivities for Grazing-Incidence Mirrors
- Gratings and Monochromators
- Zone Plates
- X-Ray Detectors
- Miscellaneous
- Physical Constants
- Physical Properties of the Elements
- Electromagnetic Relations
- Radioactivity and Radiation Protection
- Useful Formulas

X-ray data booklet

Download the PDF [8 Mb]

http://cxro.lbl.gov/x-ray-data-booklet



Center for X-Ray Optics
and
Advanced Light Source

X-RAY DATA
BOOKLET

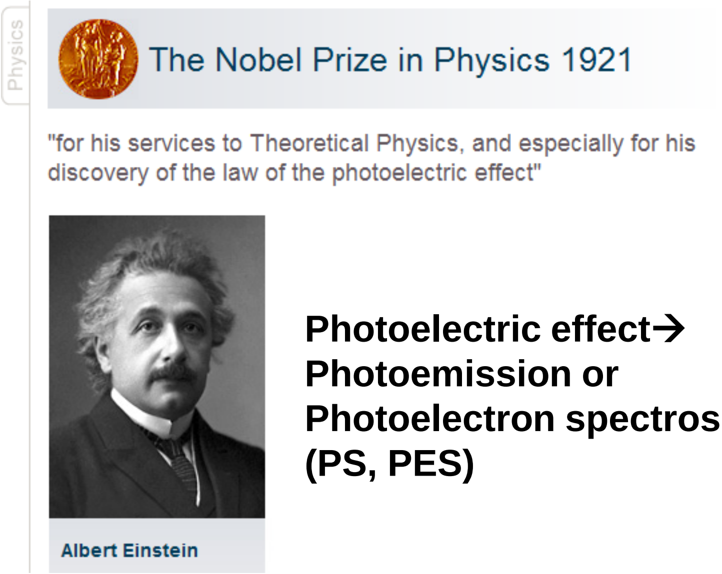
Albert Thompson
David Attwood
Eric Gullikson
Malcolm Howells
Kwang-Je Kim
Janos Kirz
Jeffrey Kortright
Ingolf Lindau
Yanwei Liu
Piero Pianetta
Arthur Robinson
James Scofield
James Underwood
Gwyn Williams
Herman Winick

October 2009

Lawrence Berkeley National Laboratory
University of California
Berkeley, CA 94720

- *Why surfaces, interfaces, structures at the nanometer scale?*
  1 nm = 10 Å = 0.001 micron
  Cube of 1 nm sides has 75% of its atoms on the surface
  ➡ *Many areas of science/technology*

→*Driven by advances in experimental techniques for characterizing them, many important applications areas and Nobel Prizes along the way*



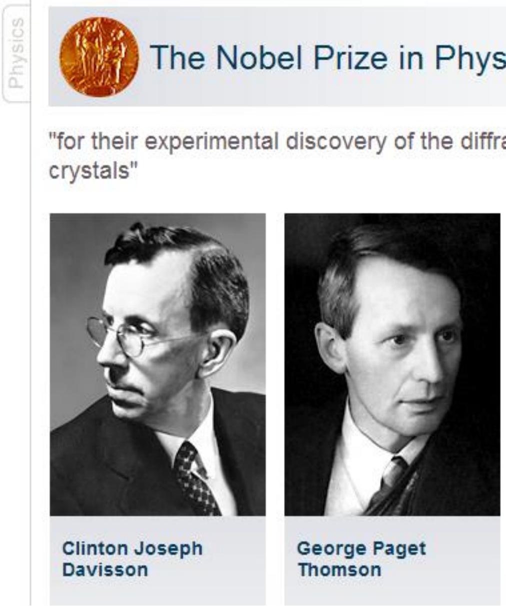
Physics

The Nobel Prize in Physics 1921

"for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect"

Albert Einstein

Photoelectric effect→ Photoemission or Photoelectron spectroscopy (PS, PES)



Physics

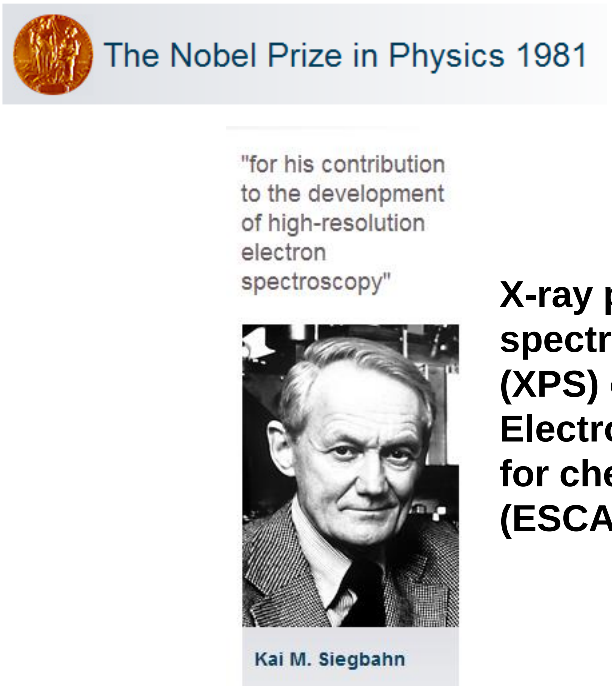
The Nobel Prize in Physics 1937

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

Clinton Joseph Davisson

George Paget Thomson

Low energy electron diffraction (LEED)

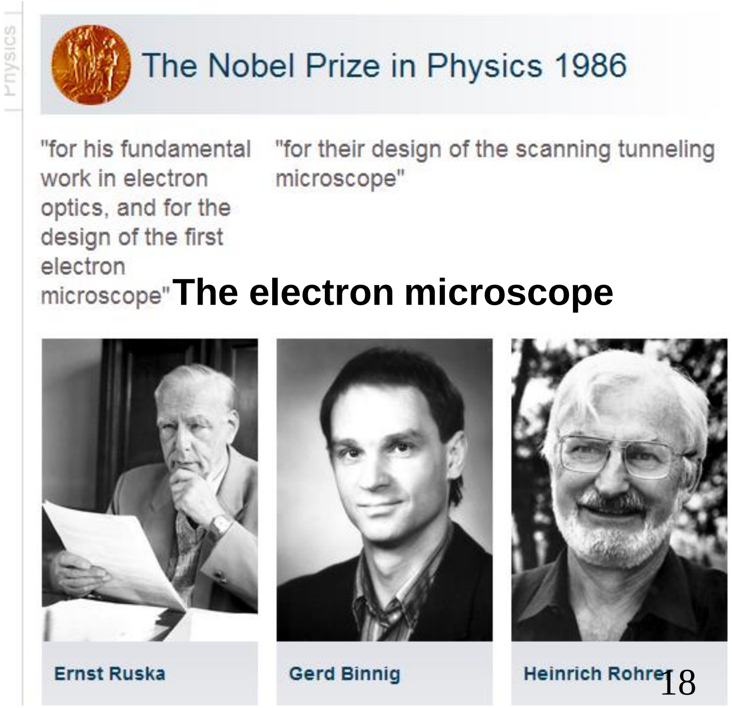


The Nobel Prize in Physics 1981

"for his contribution to the development of high-resolution electron spectroscopy"

Kai M. Siegbahn

X-ray photoelectron spectroscopy (XPS) or Electron spectroscopy for chemical analysis (ESCA)



Physics

The Nobel Prize in Physics 1986

"for his fundamental work in electron optics, and for the design of the first electron microscope"

"for their design of the scanning tunneling microscope"

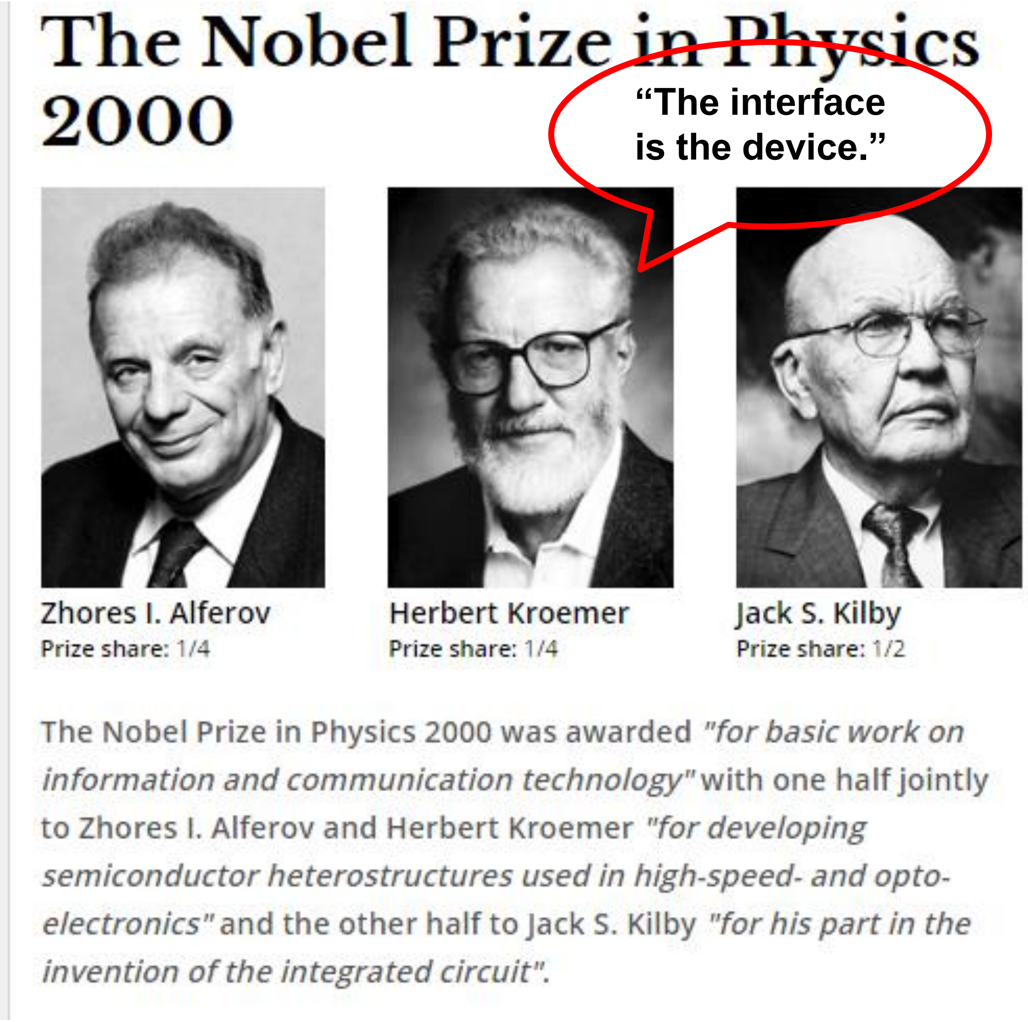
The electron microscope

Ernst Ruska

Gerd Binnig

Heinrich Rohrer

Scanning tunneling microscopy (STM)



The Nobel Prize in Physics 2000

“The interface is the device.”

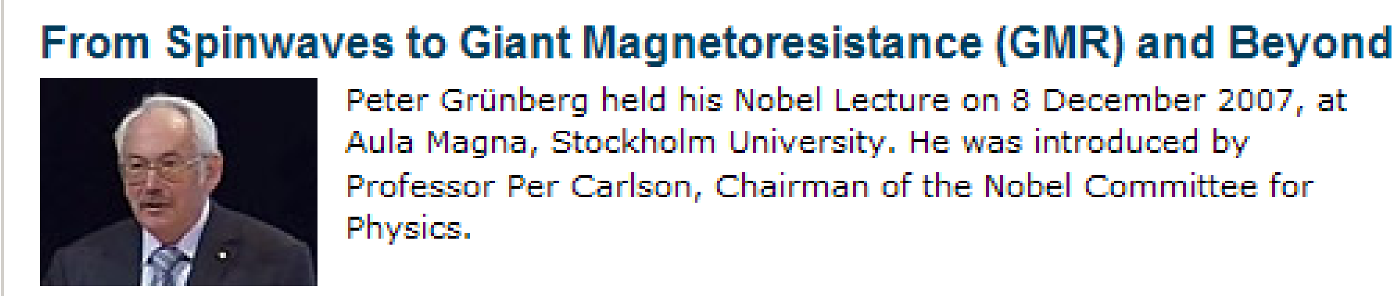
Zhores I. Alferov
Prize share: 1/4

Herbert Kroemer
Prize share: 1/4

Jack S. Kilby
Prize share: 1/2

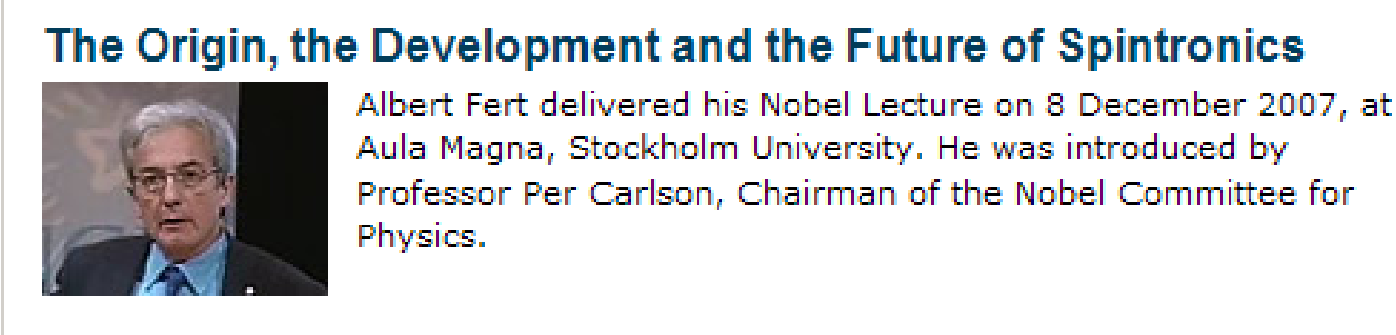
The Nobel Prize in Physics 2000 was awarded *"for basic work on information and communication technology"* with one half jointly to Zhores I. Alferov and Herbert Kroemer *"for developing semiconductor heterostructures used in high-speed- and opto-electronics"* and the other half to Jack S. Kilby *"for his part in the invention of the integrated circuit"*.

Nobel Prizes in Physics and Chemistry--2007



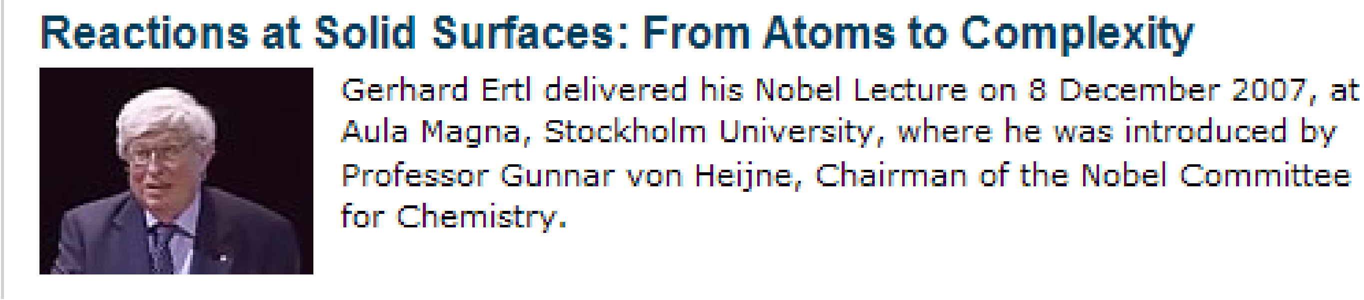
From Spinwaves to Giant Magnetoresistance (GMR) and Beyond

Peter Grünberg held his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University. He was introduced by Professor Per Carlson, Chairman of the Nobel Committee for Physics.



The Origin, the Development and the Future of Spintronics

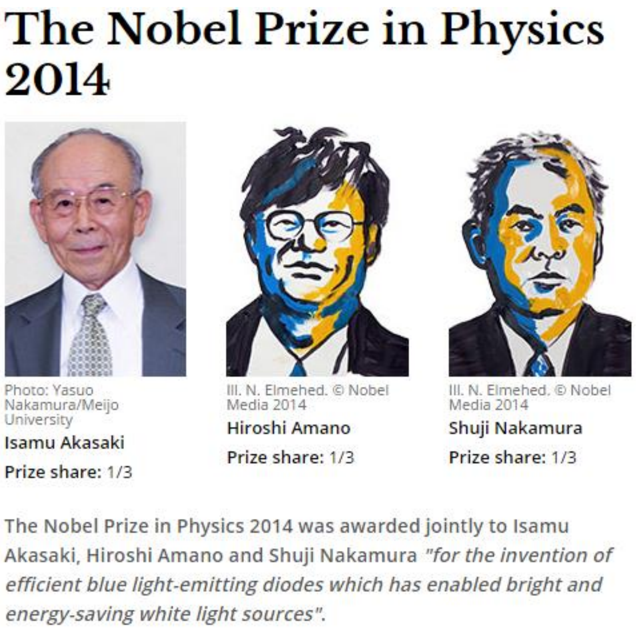
Albert Fert delivered his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University. He was introduced by Professor Per Carlson, Chairman of the Nobel Committee for Physics.



Reactions at Solid Surfaces: From Atoms to Complexity

Gerhard Ertl delivered his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University, where he was introduced by Professor Gunnar von Heijne, Chairman of the Nobel Committee for Chemistry.

Nobel Prize in Physics--2014



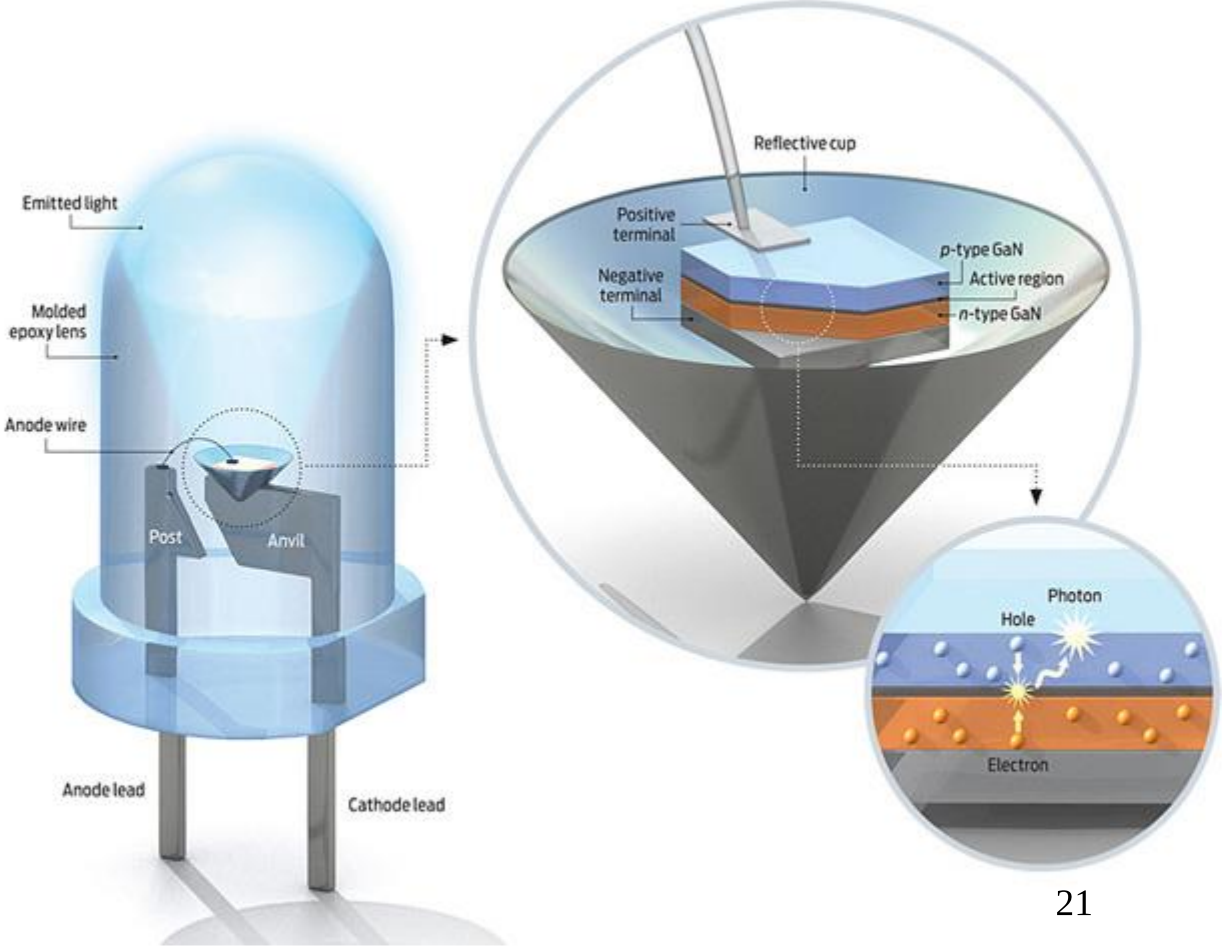
The Nobel Prize in Physics 2014

Photo: Yasuo Nakamura/Meijo University
Isamu Akasaki
Prize share: 1/3

Ill. N. Elmehed. © Nobel Media 2014
Hiroshi Amano
Prize share: 1/3

Ill. N. Elmehed. © Nobel Media 2014
Shuji Nakamura
Prize share: 1/3

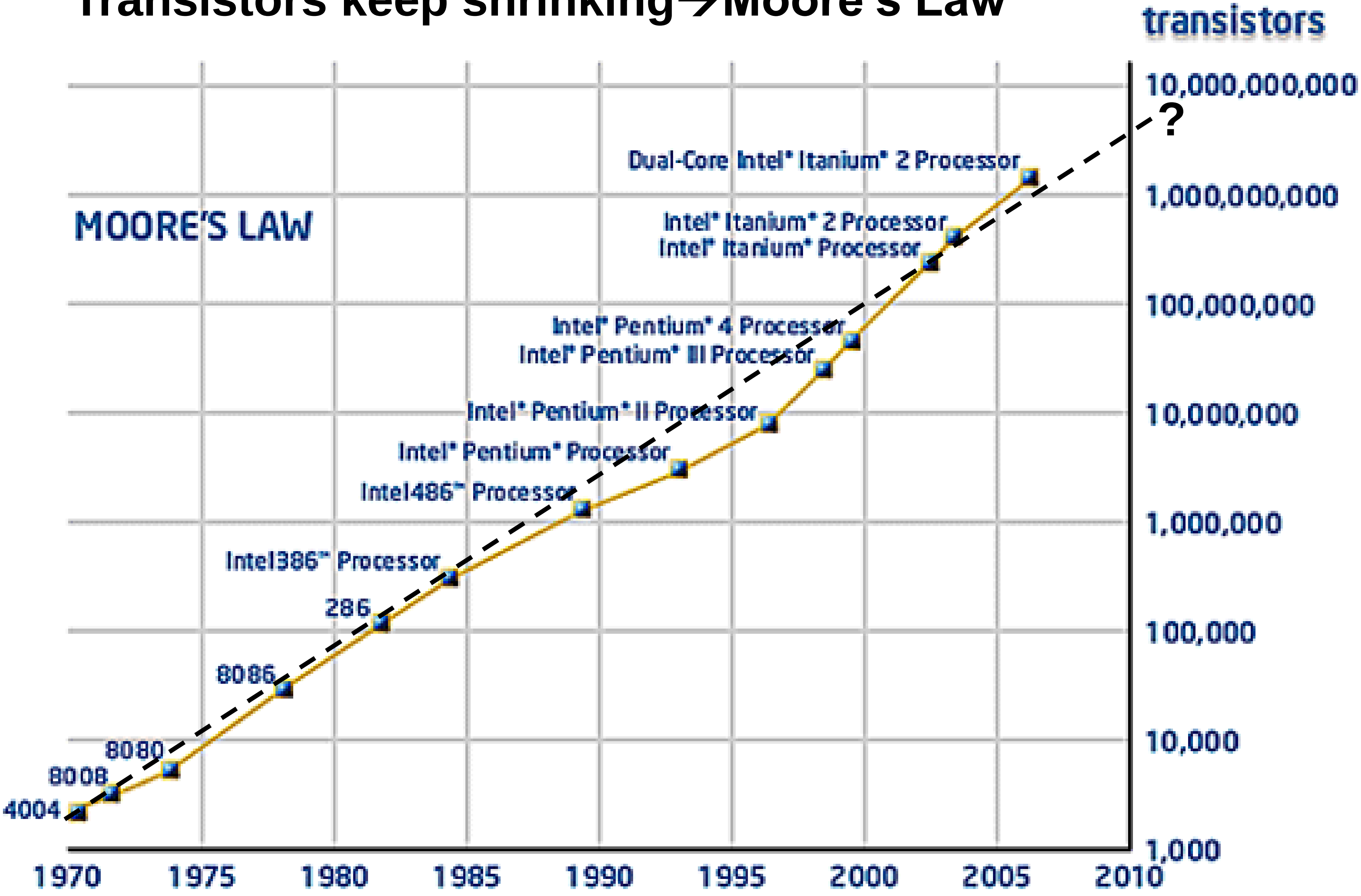
The Nobel Prize in Physics 2014 was awarded jointly to Isamu Akasaki, Hiroshi Amano and Shuji Nakamura *"for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources".*



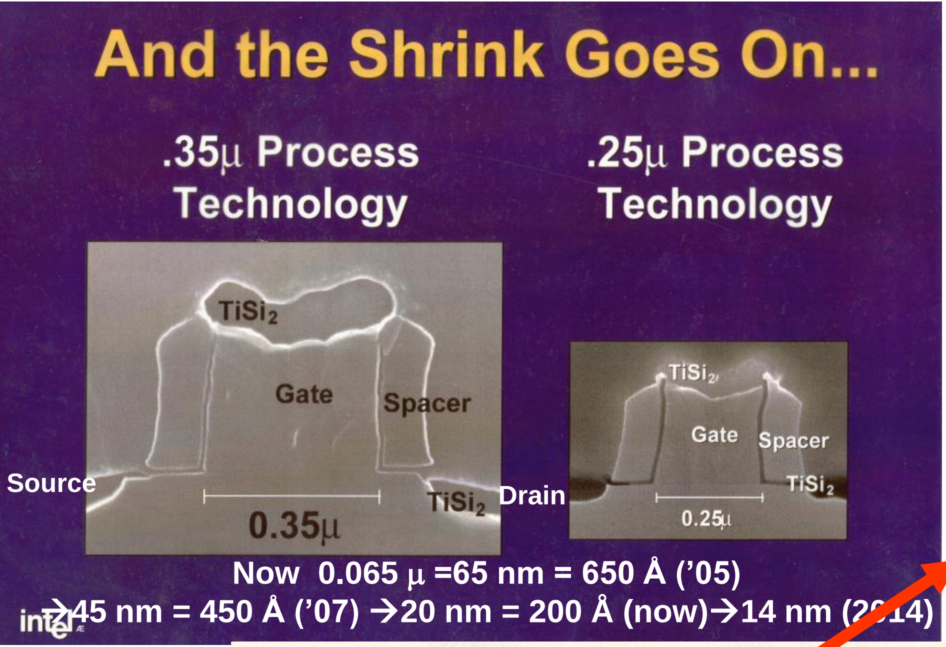
Scientific and technological areas involving surface/interface/nano science:

- **Integrated circuits—higher speed, higher density**

Transistors keep shrinking→Moore's Law



http://www.intel.com/technology/mooreslaw/index.htm



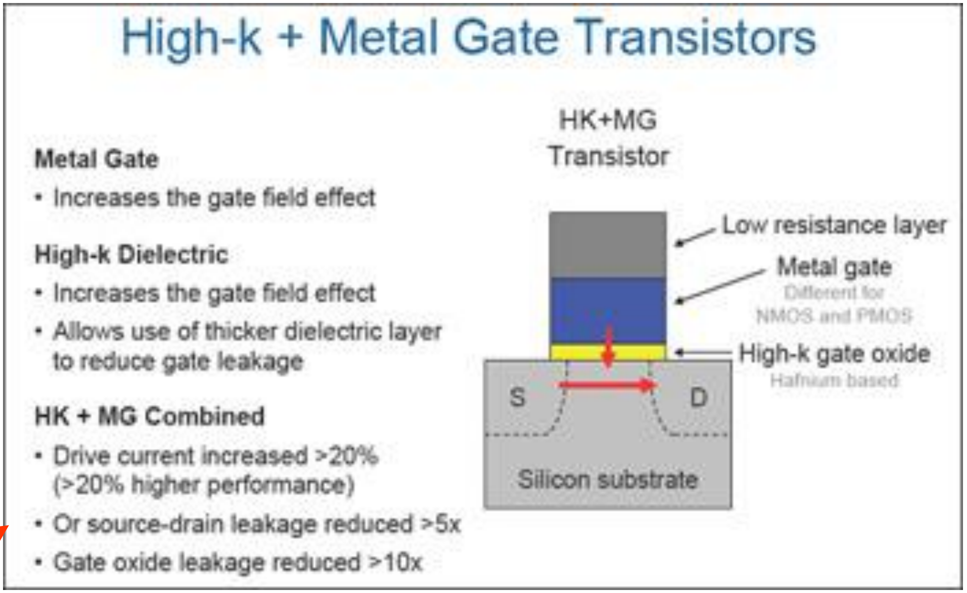
And the Shrink Goes On...

.35µ Process Technology

.25µ Process Technology

Now 0.065 µ =65 nm = 650 Å ('05)

→45 nm = 450 Å ('07) →20 nm = 200 Å (now)→14 nm (2014)



High-k + Metal Gate Transistors

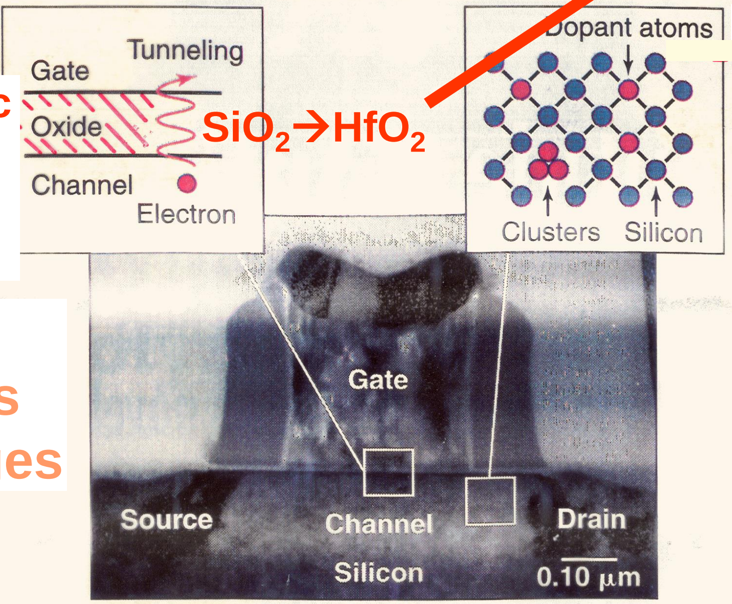
Metal Gate
- Increases the gate field effect

High-k Dielectric
- Increases the gate field effect
- Allows use of thicker dielectric layer to reduce gate leakage

HK + MG Combined
- Drive current increased >20% (>20% higher performance)
- Or source-drain leakage reduced >5x
- Gate oxide leakage reduced >10x

~few atomic layers— currently 15 Å SiO_2

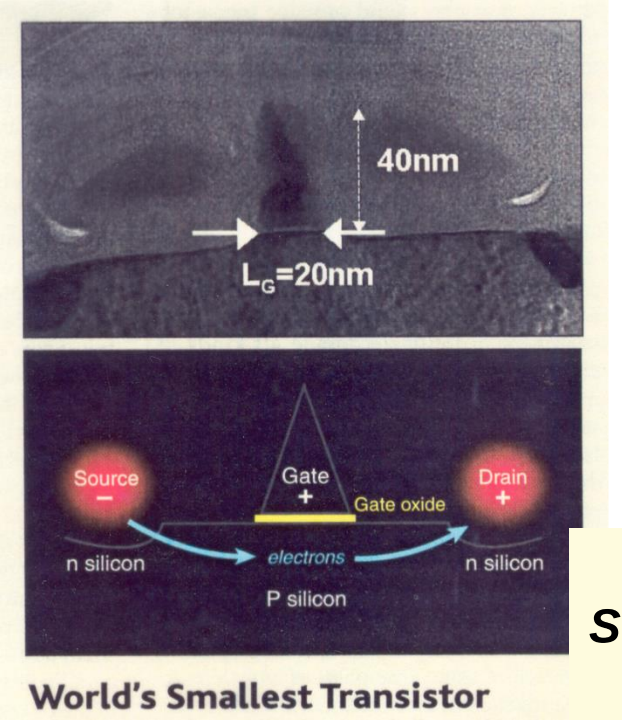
Some serious challenges



SiO_2→HfO_2

~1 %

Cross section of a MOS transistor. Electron tunneling through the gate oxide (**left inset**) and high-concentration dopant interactions (**right inset**) are posing fundamental limitations to continuing historical transistor scaling trends.

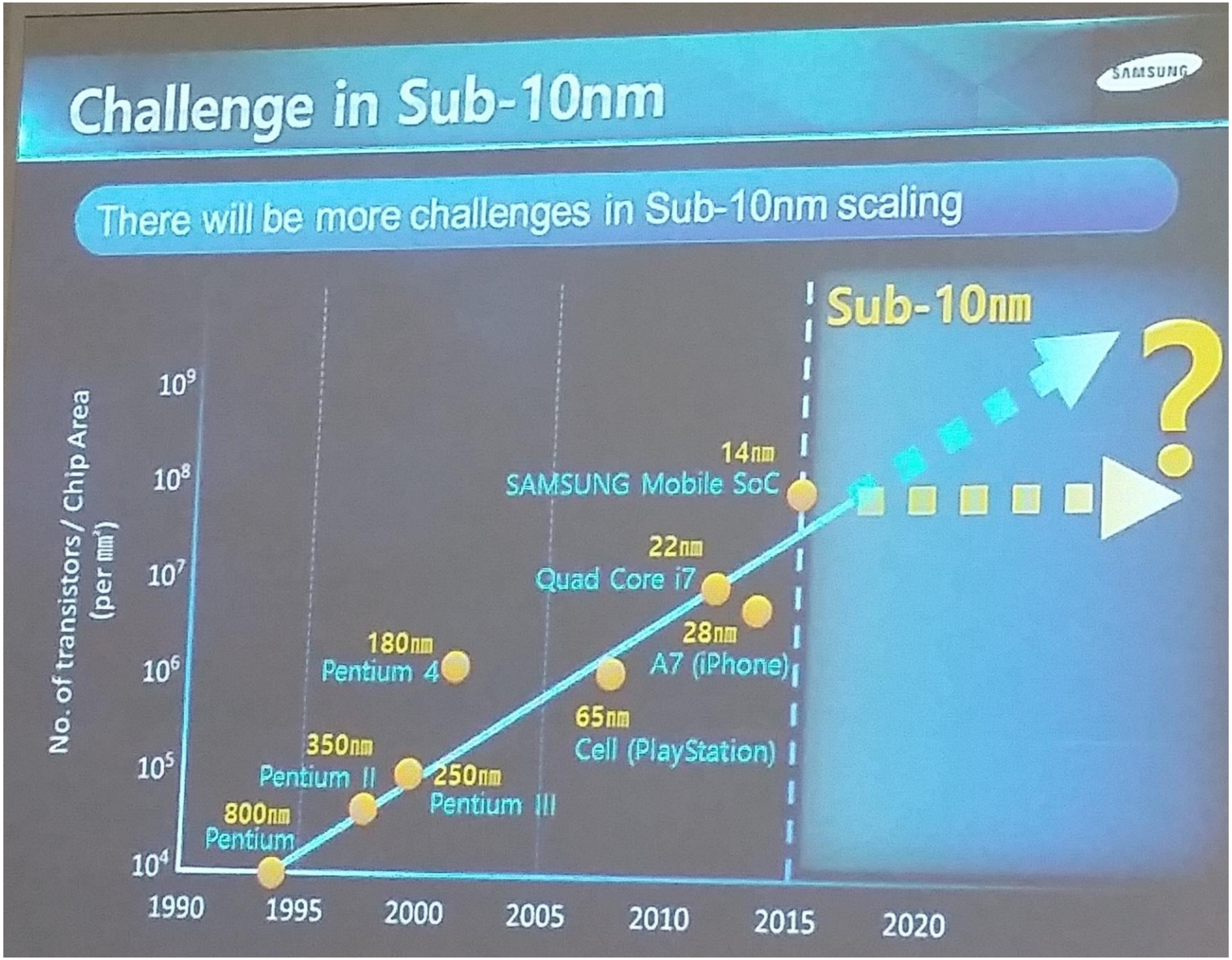


World's Smallest Transistor

IBM Science 2001

Some history

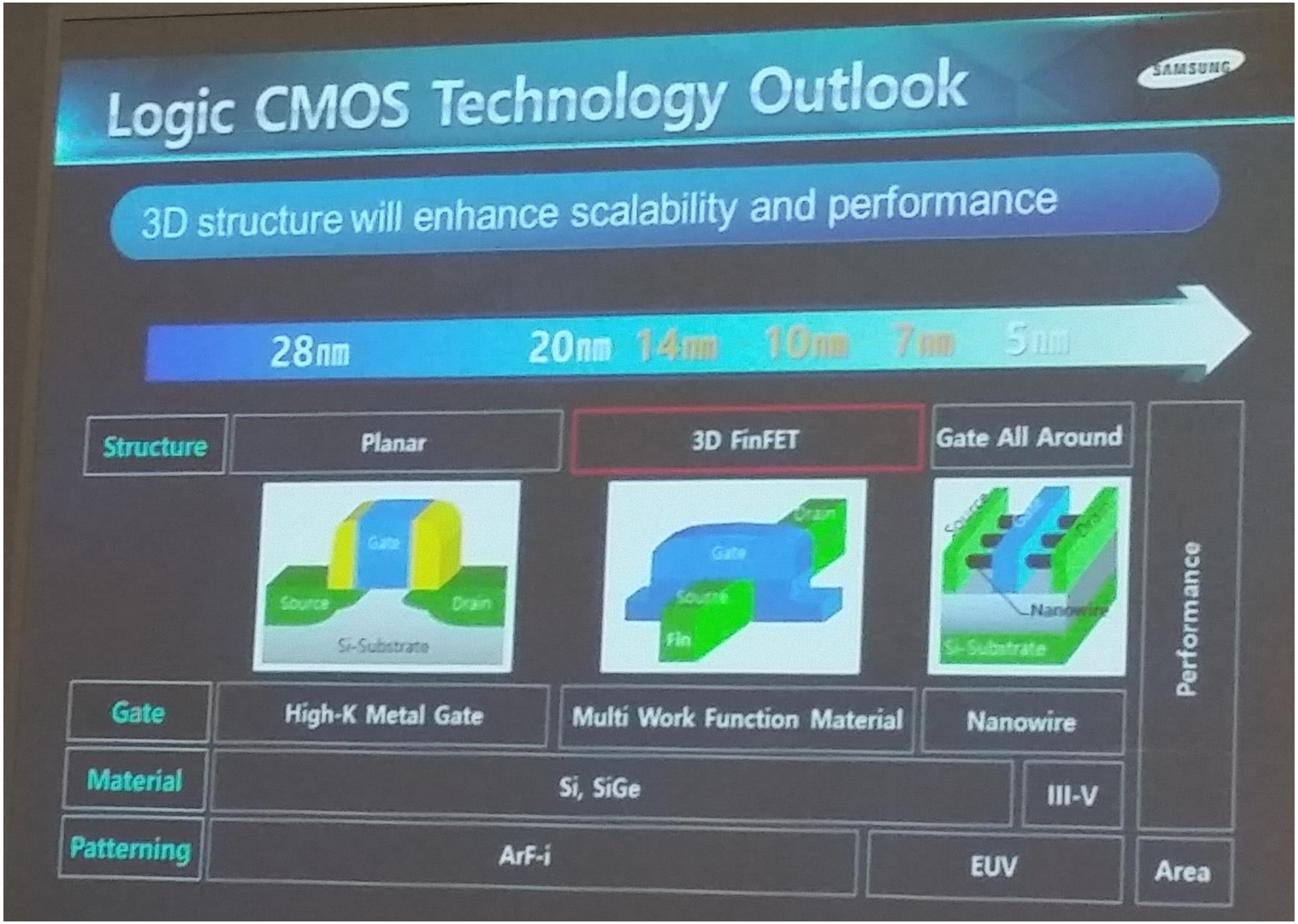
10 µm — 1971
3 µm — 1975
1.5 µm — 1982
1 µm — 1985
800 nm (.80 µm) — 1989
600 nm (.60 µm) — 1994
350 nm (.35 µm) — 1995
250 nm (.25 µm) — 1998
180 nm (.18 µm) — 1999
130 nm (.13 µm) — 2000
90 nm — 2002
65 nm — 2006
45 nm — 2008
32 nm — 2010
22 nm — 2012
14 nm — approx. 2014 (tunneling still a problem, heat density like sun)
10 nm — approx. 2016
7 nm — approx. 2018
5 nm — approx. 2020



Challenge in Sub-10nm

There will be more challenges in Sub-10nm scaling

Kinam Kim, Samsung
IVC Conference, Busan, Korea, August, 2016



Logic CMOS Technology Outlook

SAMSUNG

3D structure will enhance scalability and performance

28nm 20nm 14nm 10nm 7nm 5nm

Structure	Planar	3D FinFET	Gate All Around	Performance
Gate	High-K Metal Gate	Multi Work Function Material	Nanowire	
Material	Si, SiGe		III-V	
Patterning	ArF-i		EUV	Area

Kinam Kim, Samsung
IVC Conference, Busan, Korea, August, 2016

What do the interfaces look like? How thick are they?

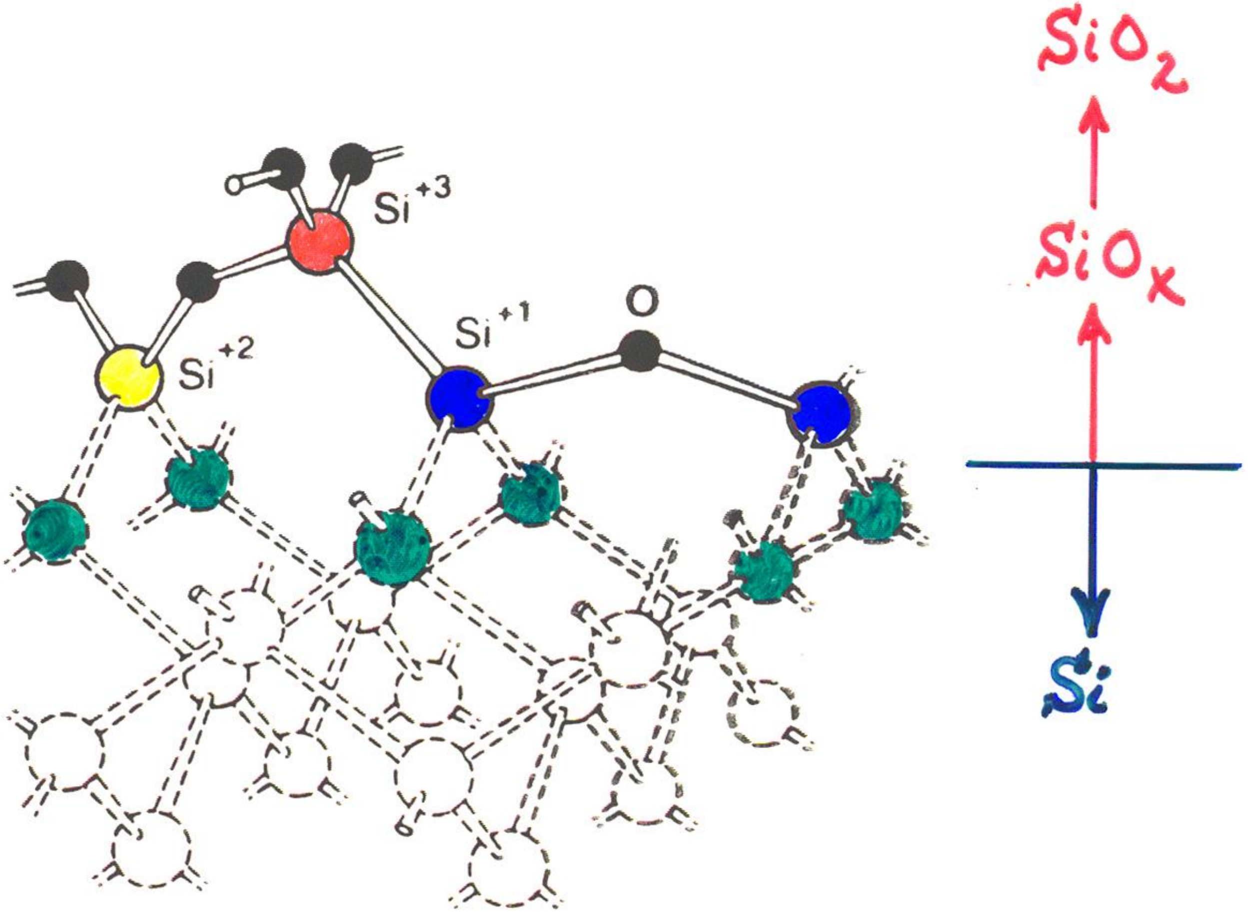
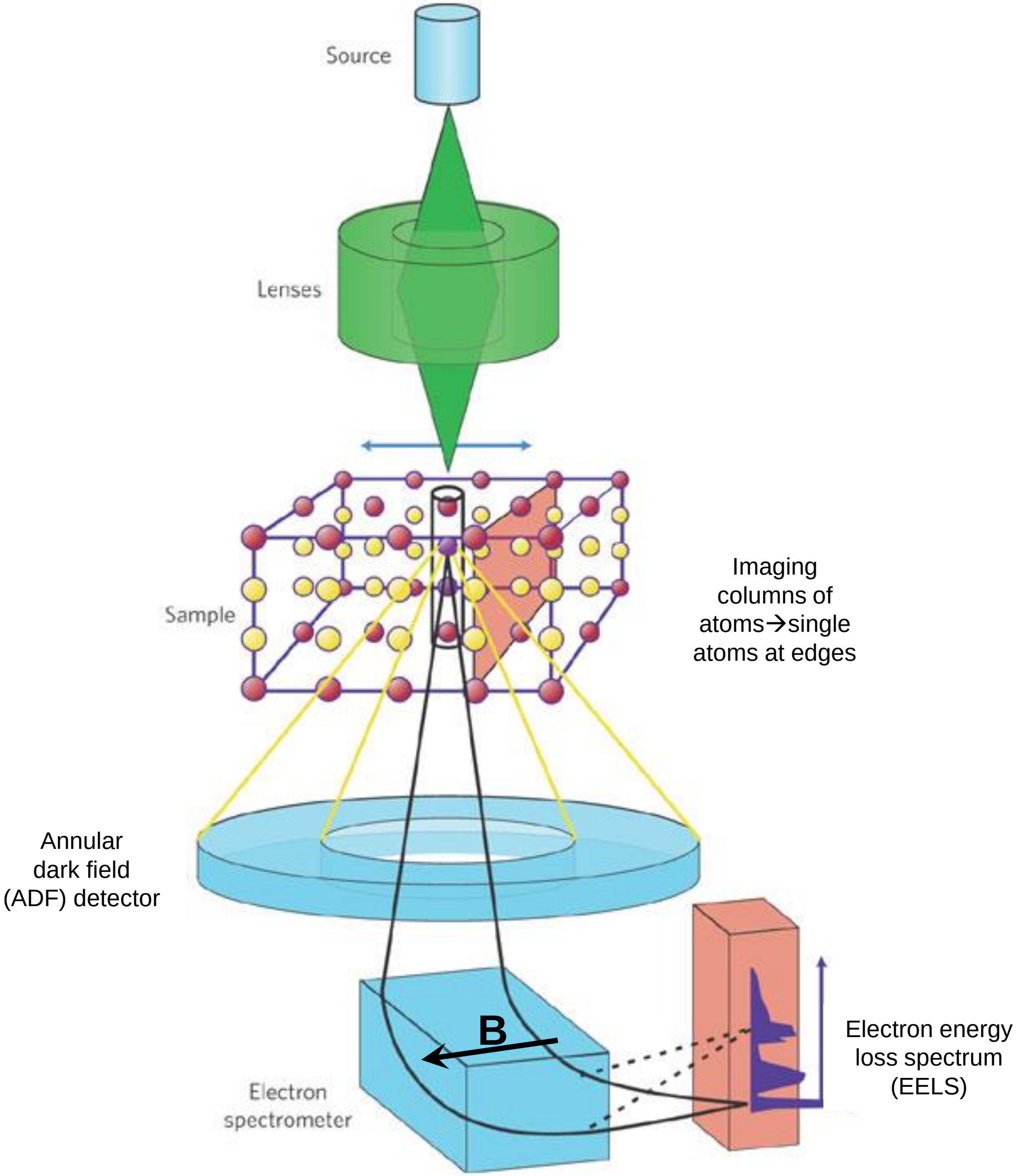


FIG. 2. Topological structure of various silicon suboxides at the SiO_2/Si (100) interface. The structure is based on the plastic ball and spoke model proposed by Ohdomari *et al.*[9]

SCANNING TRANSMISSION ELECTRON MICROSCOPY (STEM) WITH ELECTRON ENERGY LOSS SPECTROSCOPY (EELS)

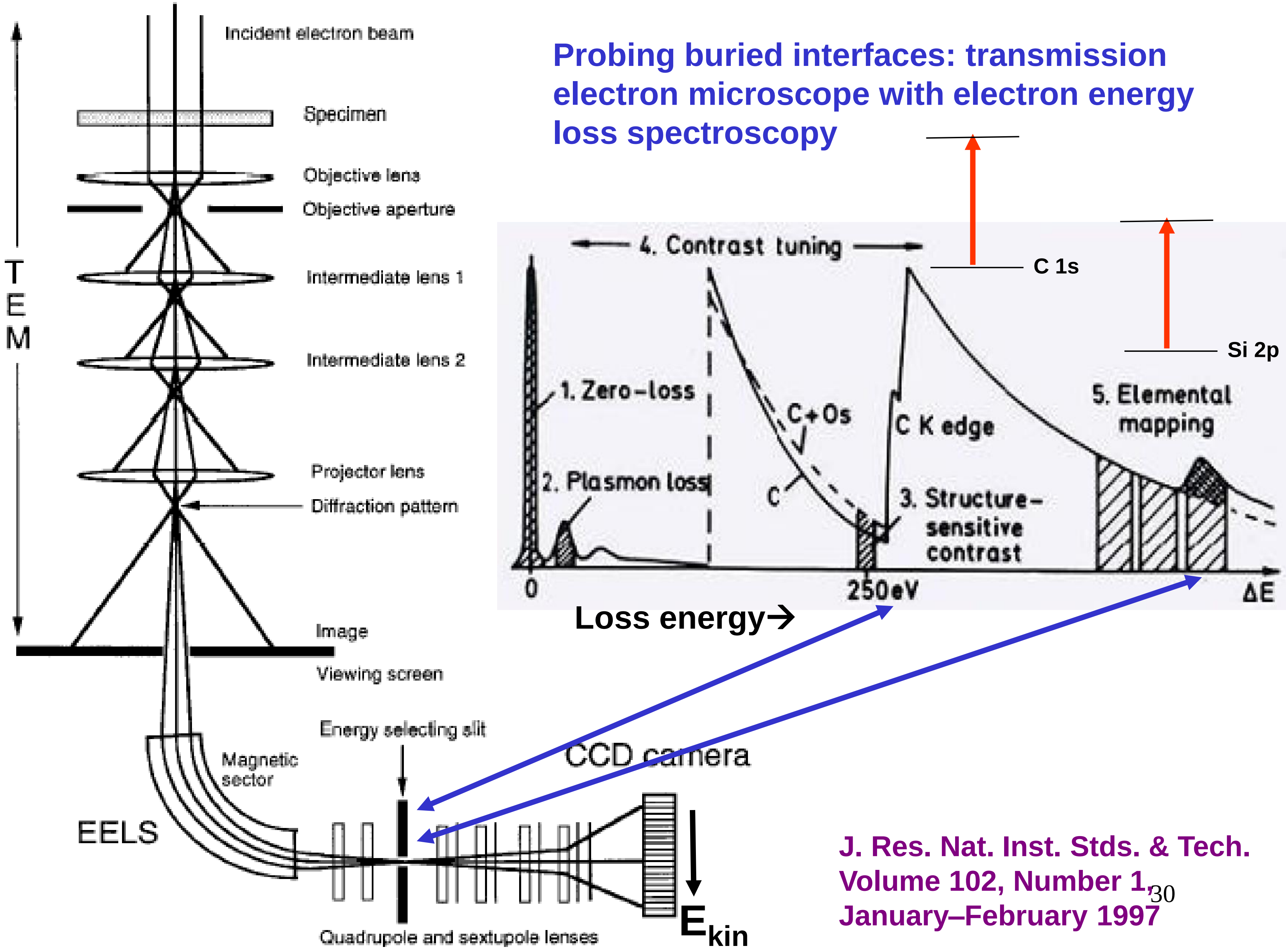


Imaging columns of atoms→single atoms at edges

Annular dark field (ADF) detector

Electron energy loss spectrum (EELS)

Probing buried interfaces: transmission electron microscope with electron energy loss spectroscopy



J. Res. Nat. Inst. Stds. & Tech.
Volume 102, Number 1,
January–February 1997

HIGH-RESOLUTION TRANSMISSION e^- MICROSCOPY OF SiO_2/Si INTERFACES

(GOODNICK ET AL., PHYS. REV. B <u>32</u>, 8171 ('85))

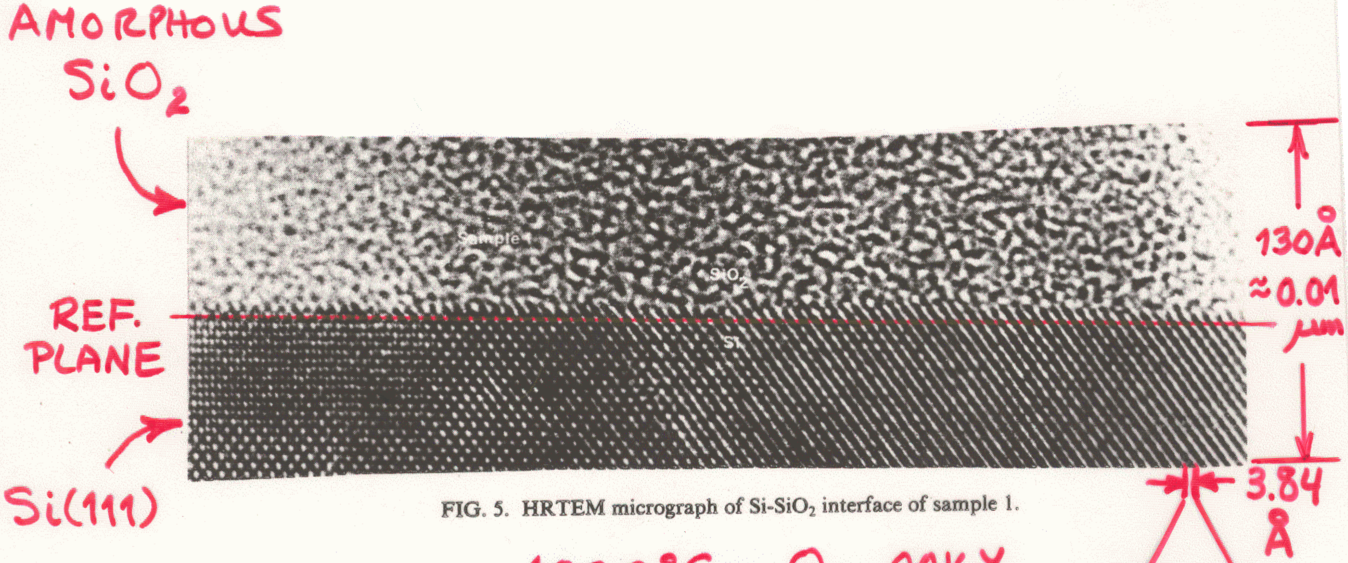
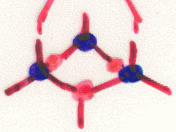


FIG. 5. HRTEM micrograph of Si-SiO$_2$ interface of sample 1.

1000°C, O_2 ONLY

SMOOTH INTERFACE



●,● = Si

IN TETRAHEDRAL "DIAMOND" STRUCTURE

⟹ 6-MEMBER RING

SCANNING TRANSMISSION e^- μSCOPY WITH EELS:

Si 2p excitations—like x-ray absorption spectra

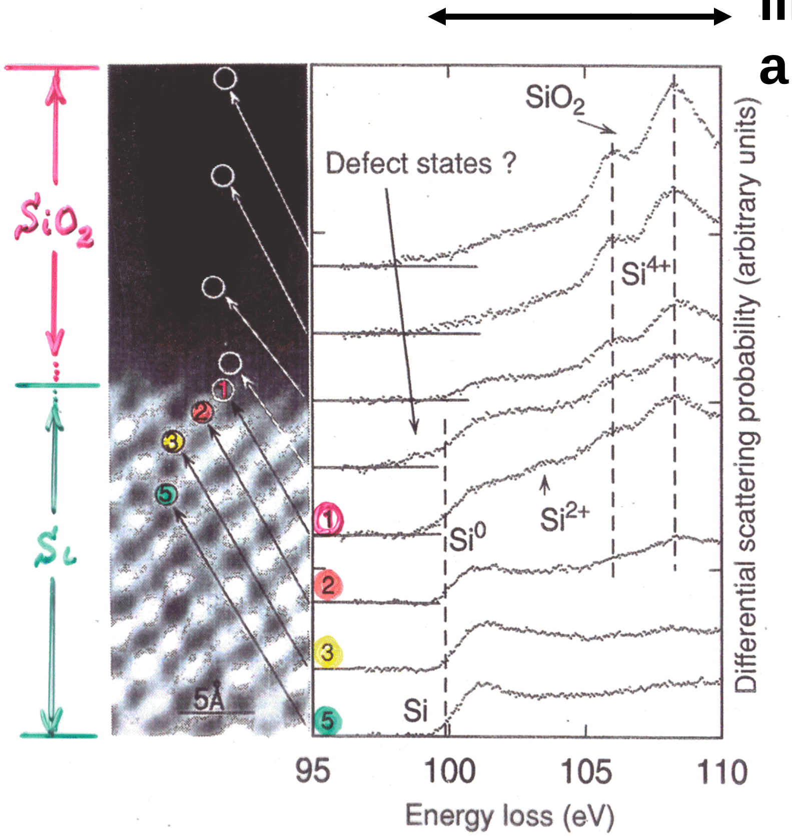
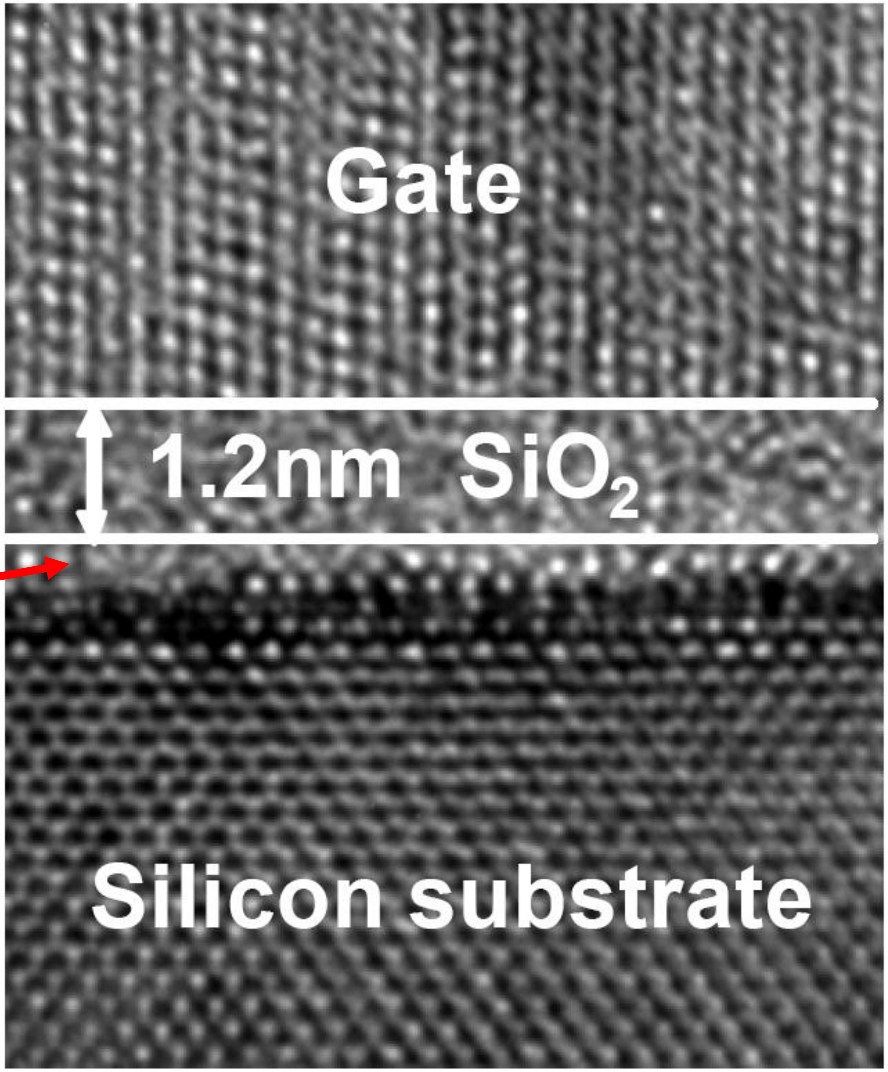


FIG. 1 Left, Incoherent dark-field image of the Si–SiO$_2$ interface for a steam-formed oxide. The elongated bright structures coincide with chains of Si atom pairs, oriented along the ⟨110⟩ directions. Right, EELS spectra obtained at eight locations indicated by the circles at the left. The bulk Si onset (Si^0) is near 100 eV. The SiO$_2$ (Si^{4+}) structure lies between 105 and 108 eV. At the interface, a fairly strong Si^{2+} signal is seen for the first time in the bulk. Some structure corresponding to electronic defect states in the silicon gap also appears to be present.

$\Delta E \approx 0.1$ eV
$\Delta x, \Delta y$
≈ 0.2 nm

P. E. BATSON,
NATURE, 366,
727 (1993)

Current SiO$_2$ gate oxide thicknesses in the 1 nm range → with high-k dielectrics, Si$_w$Hf$_x$N$_y$O$_z$,… a few nm or more



Mixed oxides:
Si^{+1}, Si^{+2}, Si^{+3}, and coord. sites

Chau et al., INTEL

Fig. 2 High resolution TEM cross section of 1.2nm physical SiO$_2$ gate oxide at the 90nm logic technology node.

→ 65 nm technology → 45 nm → 32 nm

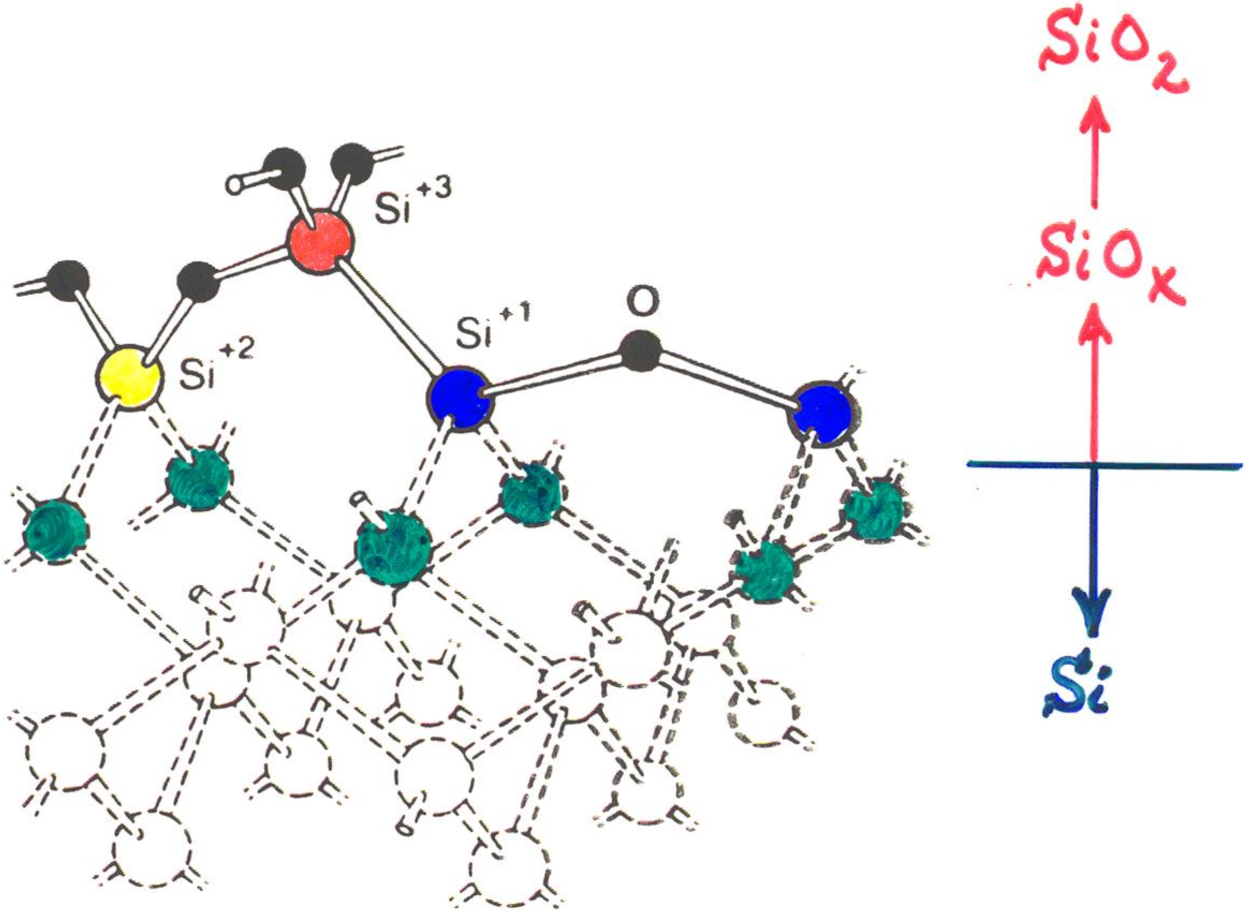
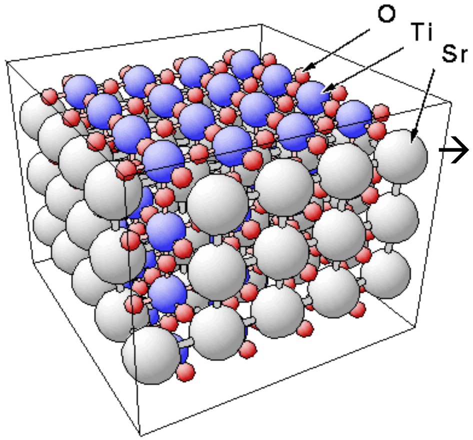


FIG. 2. Topological structure of various silicon suboxides at the SiO_2/Si (100) interface. The structure is based on the plastic ball and spoke model proposed by Ohdomari *et al.*[9]

Transmission electron microscopy images with energy loss spectroscopy

Perovskite lattice



→La,Sr

$La_{0.7}Sr_{0.3}MnO_3$

$SrTiO_3$

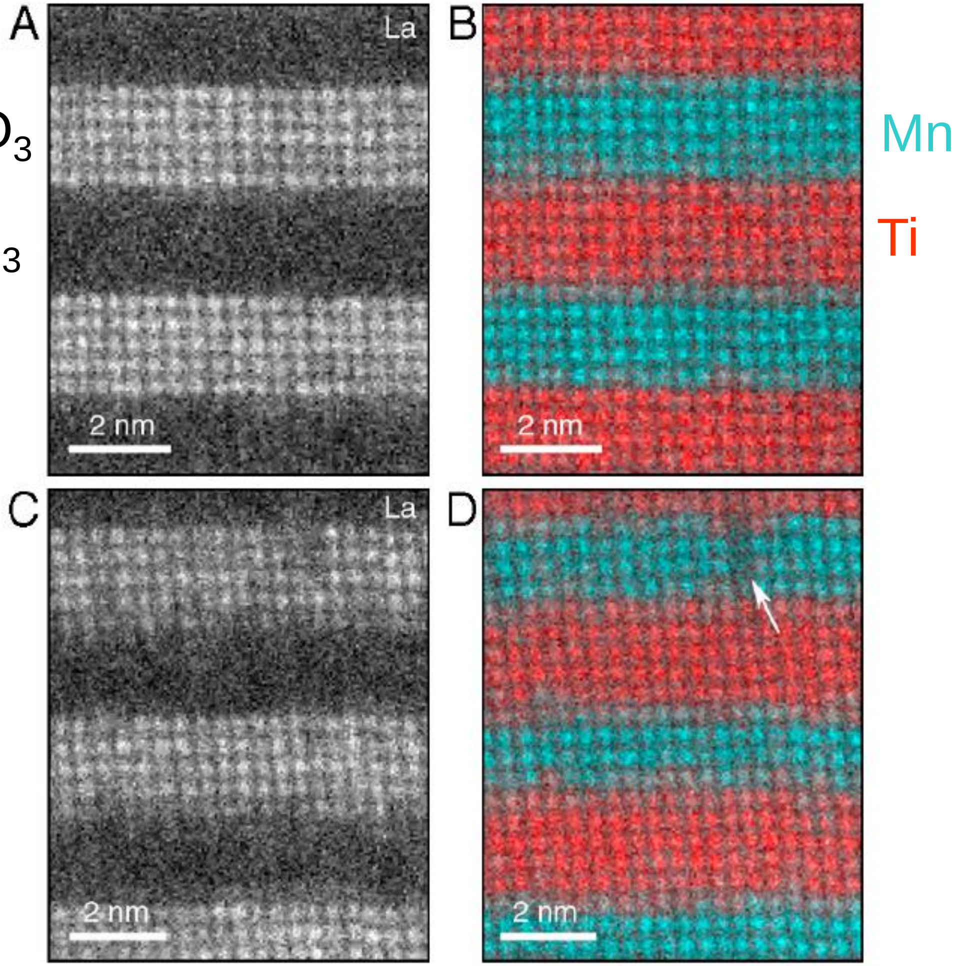
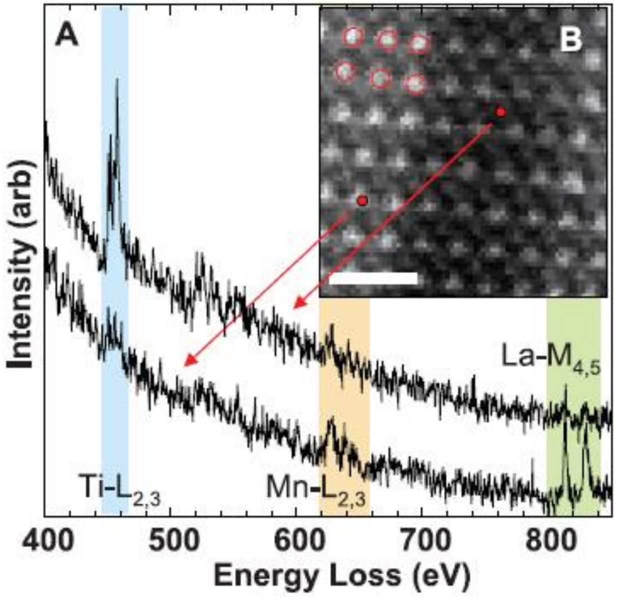


Fig. 2. Spectroscopic-imaging of $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ multilayers grown at $P_{O2} = 1$ m torr and at a laser spot size of (*A* and *B*) 7.5 and (*C* and *D*) 1.6×10^{-2} cm^2. (*A* and *C*) La elemental maps and (*B* and *D*) red-green-blue false color B-site maps, obtained by combining the Ti (red) and Mn (green and blue) maps extracted from the spectrum images. The multilayer grown with a smaller laser spot size shows less abrupt interfaces and an extended defect, marked by a white arrow in *D*. The growth direction is from bottom to top.



TEM+EELS:Nice intro.- Muller et al., Science 319, 1073 (2008)

Proc. Nat. Acad. Sci. 107, 11682 (2010)

PHOTOELECTRON SPECTROSCOPY

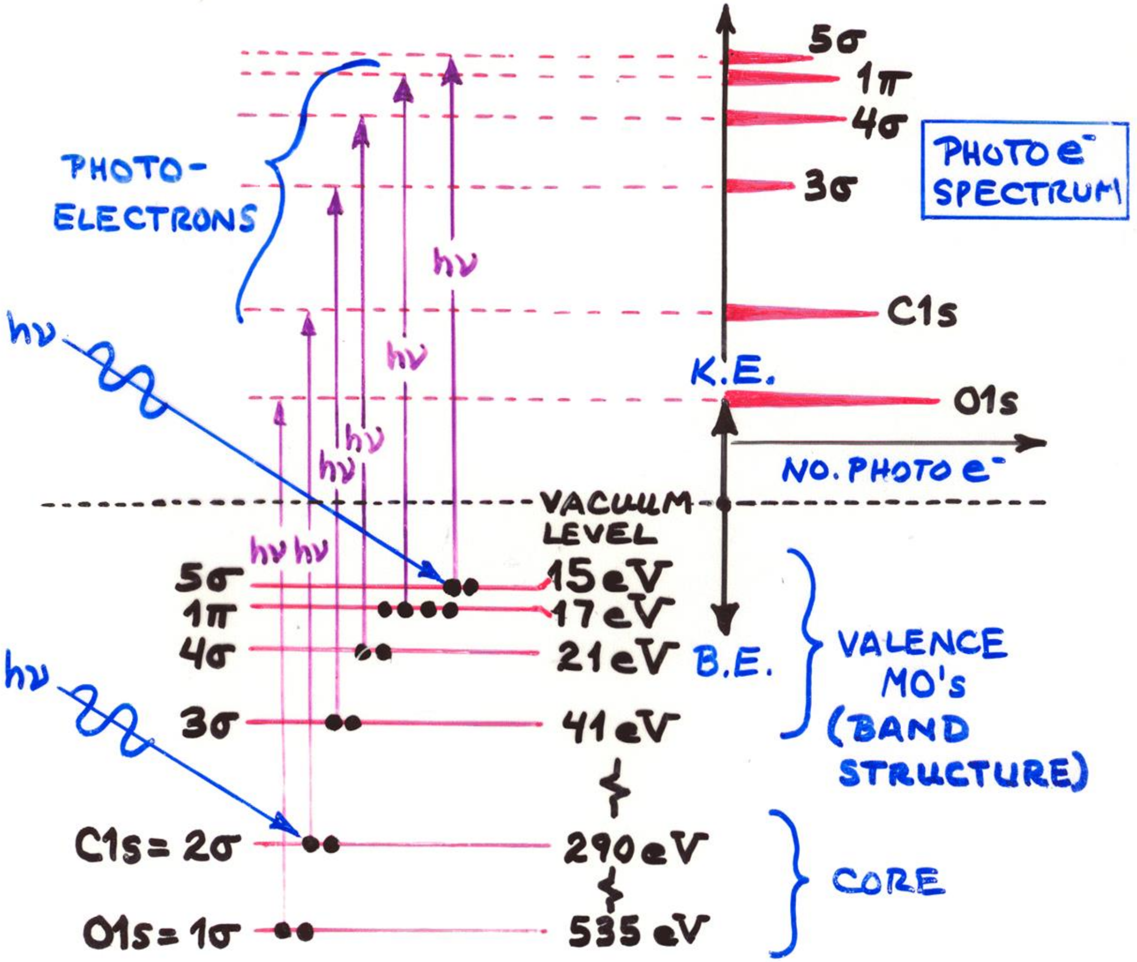
THE PHOTOELECTRIC EFFECT (EINSTEIN, 1905):

(PHOTON ENERGY) = (e⁻ BINDING ENERGY IN SYSTEM) + (PHOTOELECTRON KINETIC ENERGY)

(ABSORBED) (EMITTED)

= B.E. + K.E.

EXAMPLE – CO MOLECULE:

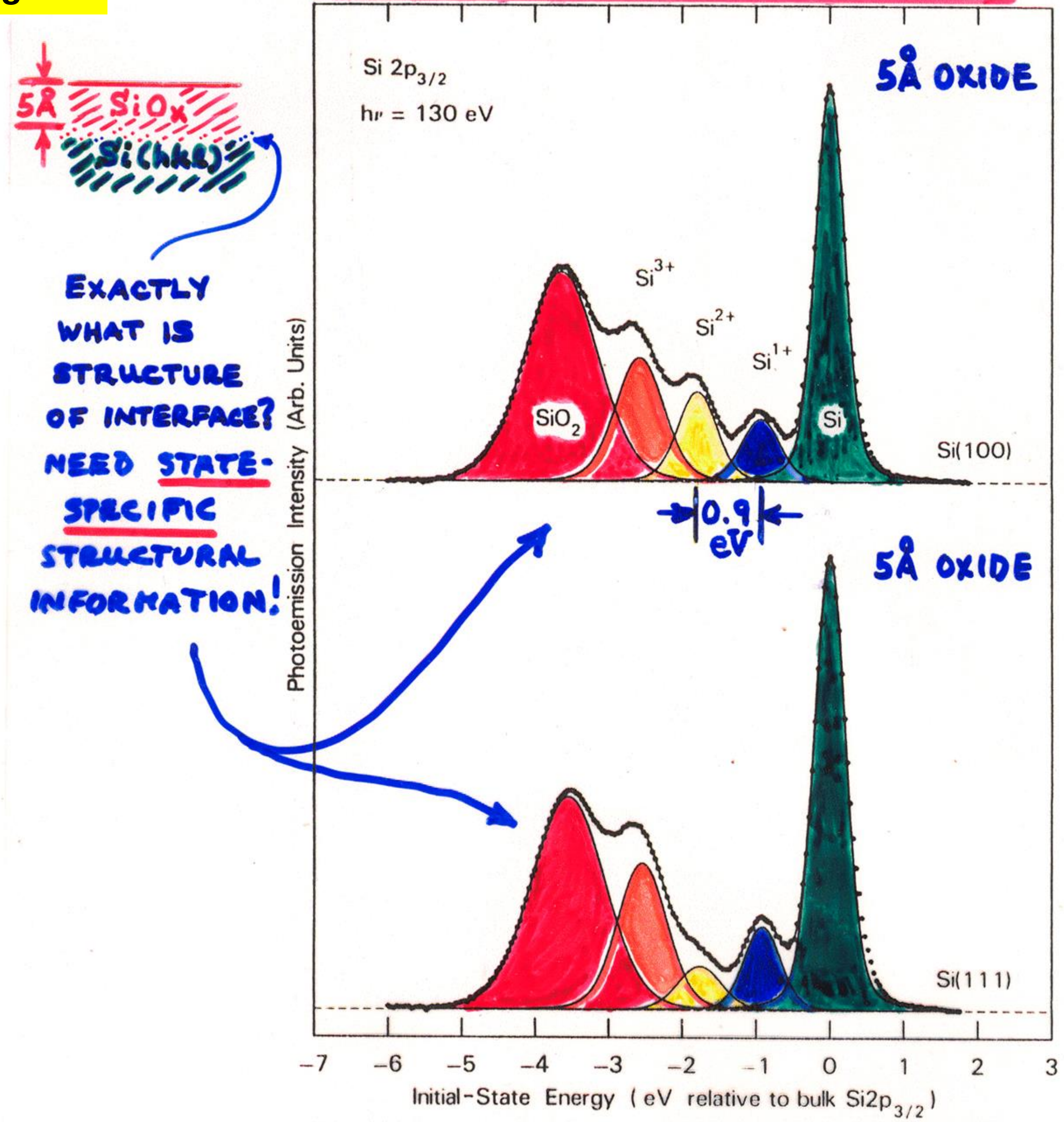


Chemical shifts
In core electron
binding energies

PHOTOELECTRON SPECTRA

OXIDIZED SILICON

CHEMICAL SHIFTS OF CORE LEVELS



EXACTLY WHAT IS STRUCTURE OF INTERFACE? NEED STATE-SPECIFIC STRUCTURAL INFORMATION!

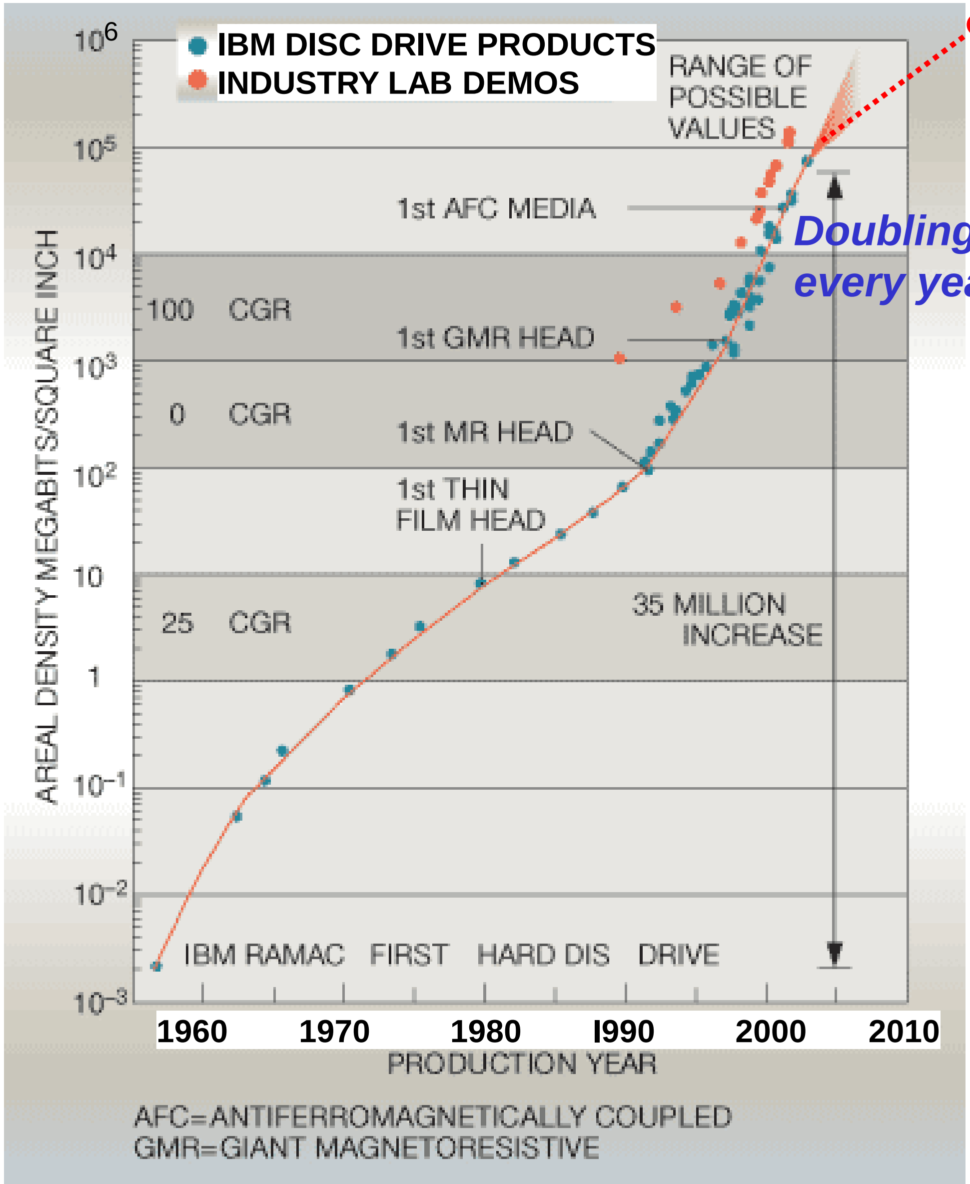
HIMPSEL ET AL., PHYS. REV. B, 38, 6084('90)

Scientific and technological areas related to surface/interface/nano science:

- **Integrated circuits—higher speed, higher density**
- **Magnetic storage and circuits—higher density, magnetic logic**

"Moore's Law" for magnetic storage

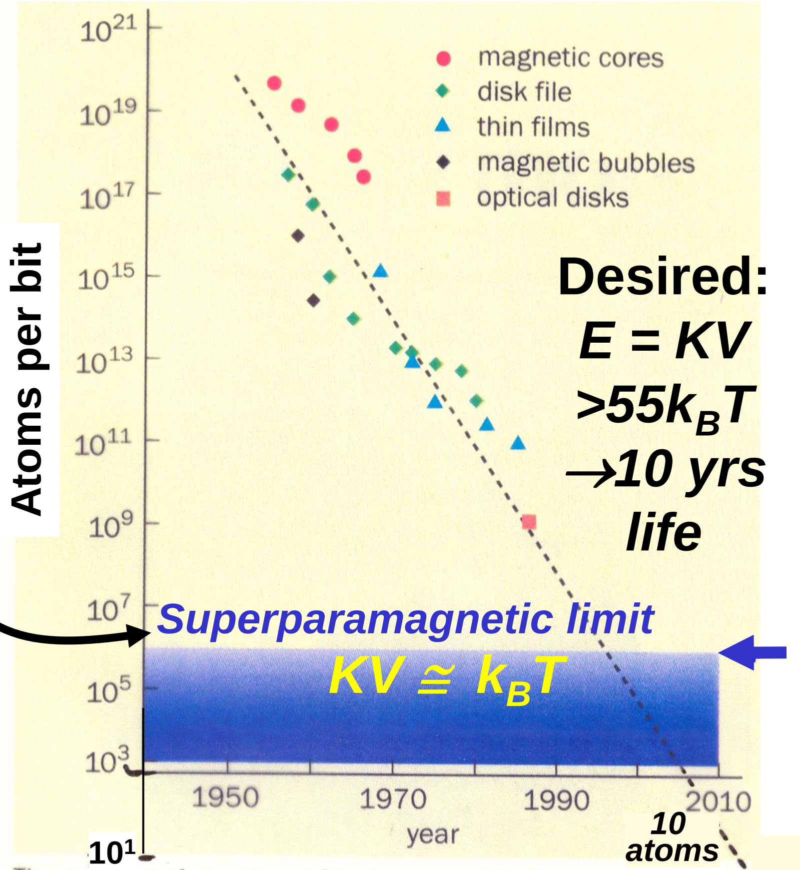
2015: 1.3 Tbits/in^2 = 150 Gbytes/in^2 ≈ 25 nm x 25 nm x 14 nm thick ≈ 400,000 atoms/bit, read at GHz rates with head at 5-7 nm above disc



Doubling every year!

http://www.research.ibm.com/journal/sj/422/grochowski.html

How for can we go?



Superparamagnetic limit

$KV \cong k_BT$

The number of atoms used to store one bit of information with different forms of magnetic or optical storage has reduced over the years. The blue region indicates the superparamagnetic regime, below which thermal fluctuations at room temperature could alter the orientation of magnetic bits.

Desired:

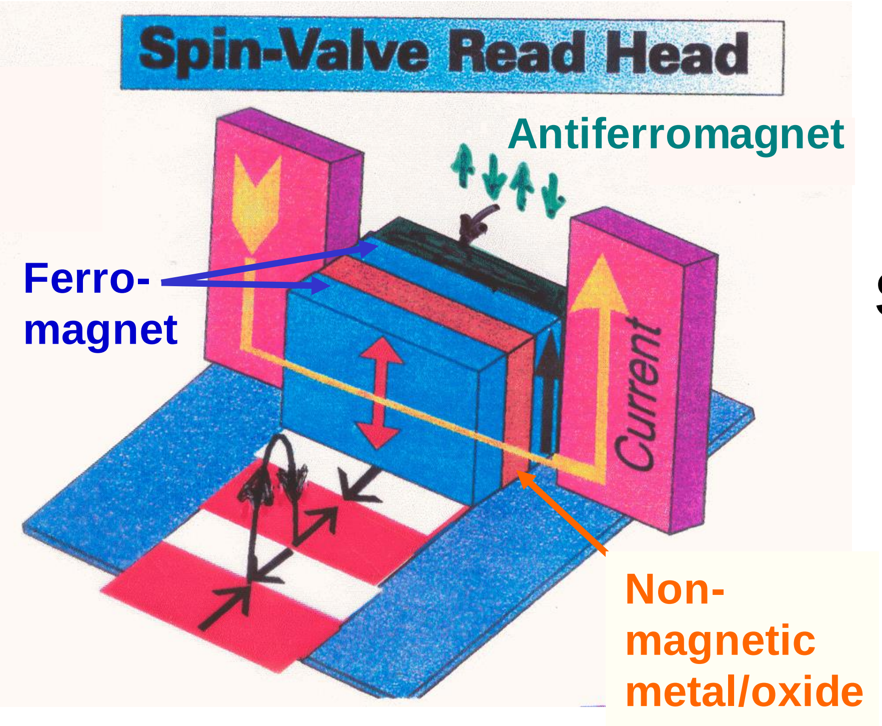
$E = KV$

$>55k_BT$

$\rightarrow$*10 yrs life*

Harris, Awschalom Physics World, Jan. '99

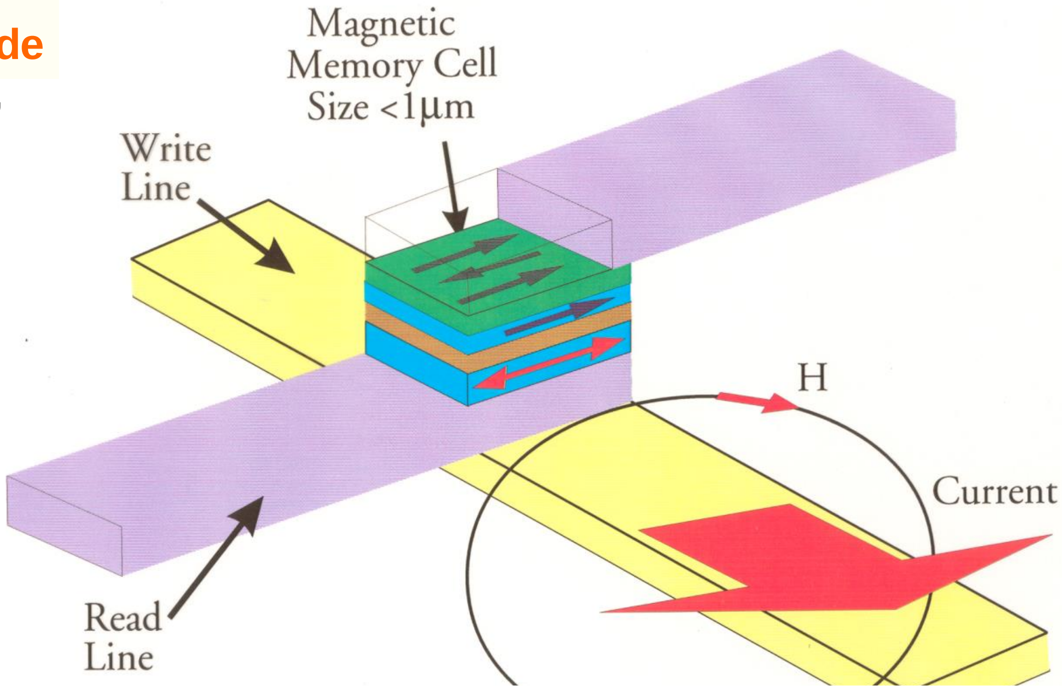
Some new directions with magnetic nanolayer structures--”spintronics”



Uses “giant magnetoresistance (GMR)” and “exchange bias” --in every high-speed read head now

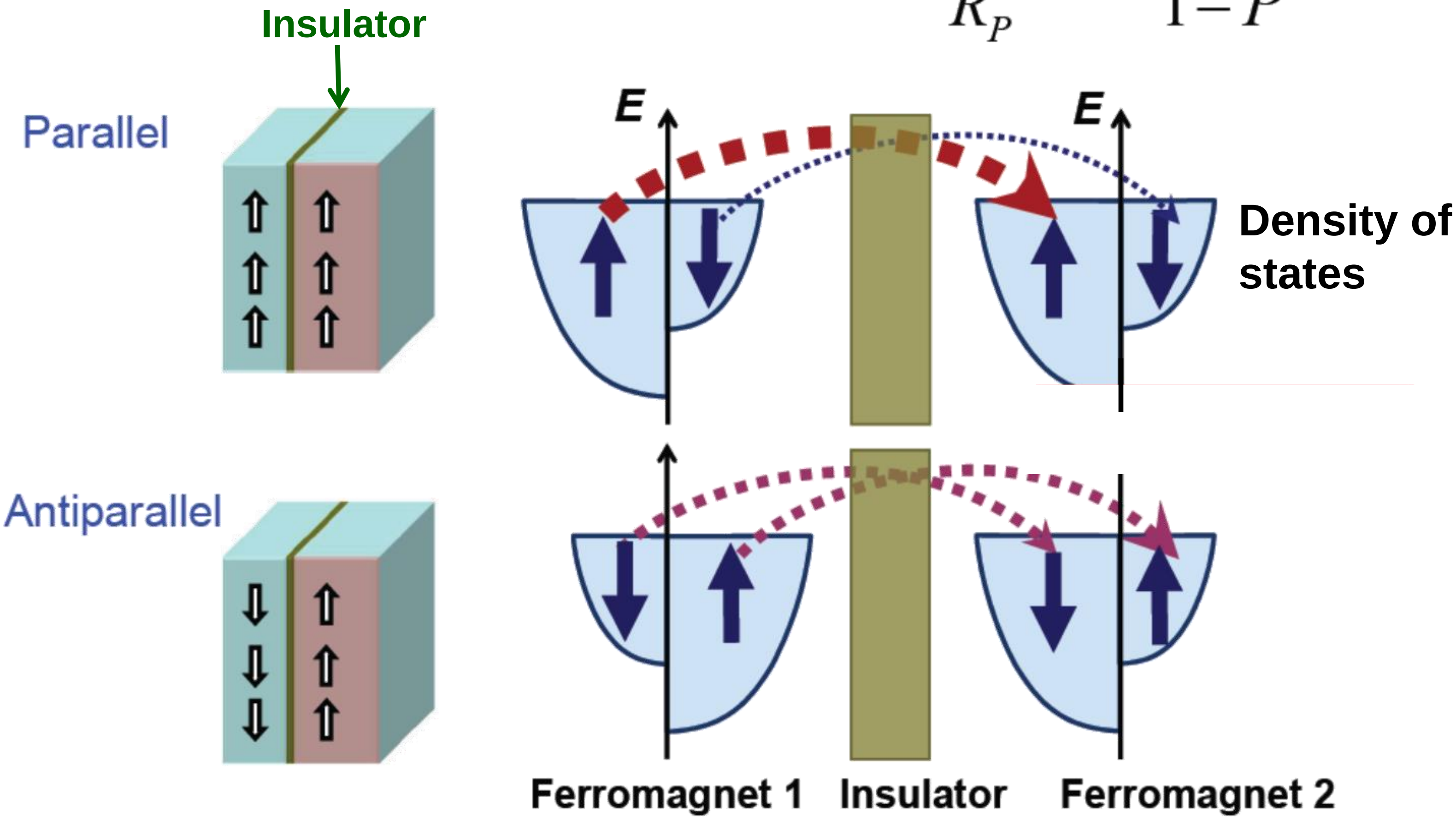
Crucial surfaces & buried interfaces everywhere, as well as complex materials (e.g. colossal magnetoresistance (CMR))

Magnetic Random Access Memory (MRAM-Non Volatile)



Up to 100 Mbit devices in R&D: applications to e.g. cell phone use

$$\text{Tunnel MagnetoResistance (TMR)} = \frac{R_{AP} - R_P}{R_P} = \frac{2P^2}{1 - P^2}$$



Room temperature TMR: Miyazaki and Tezuka (Tohoku U.), *J. Mag. Mag. Mat.* 1995 and Moodera *et al. Phys. Rev. Lett.* 1995.

H. Ohno

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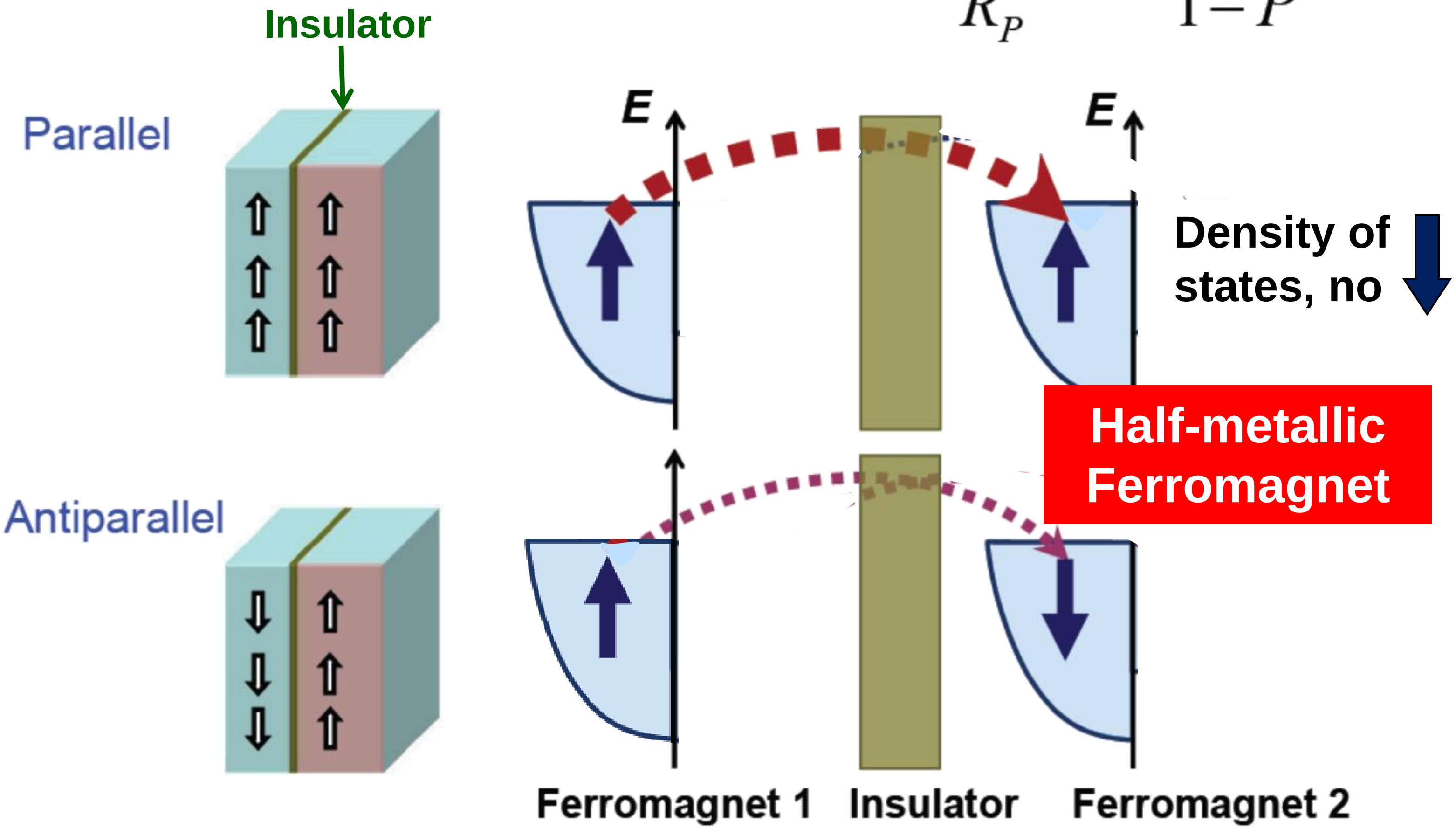


Insulator

Parallel

Antiparallel

Density of states, no ↓

Half-metallic Ferromagnet

Ferromagnet 1

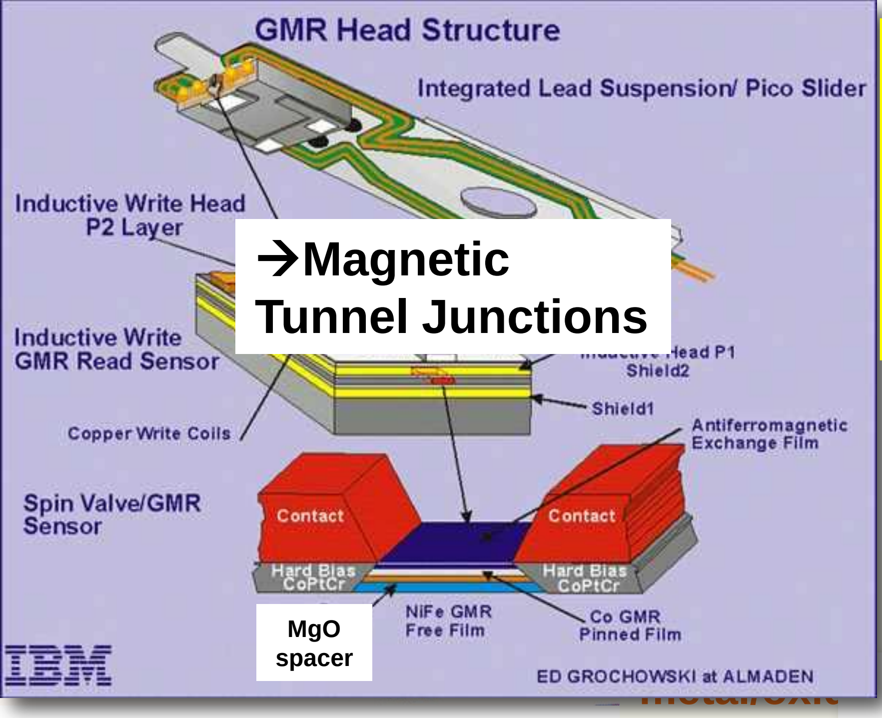
Insulator

Ferromagnet 2

Room temperature TMR: Miyazaki and Tezuka (Tohoku U.), *J. Mag. Mag. Mat.* 1995 and Moodera *et al. Phys. Rev. Lett.* 1995.

H. Ohno

Some key elements in Spintronics/Semiconductors/ Sensors—multilayer nanostructures



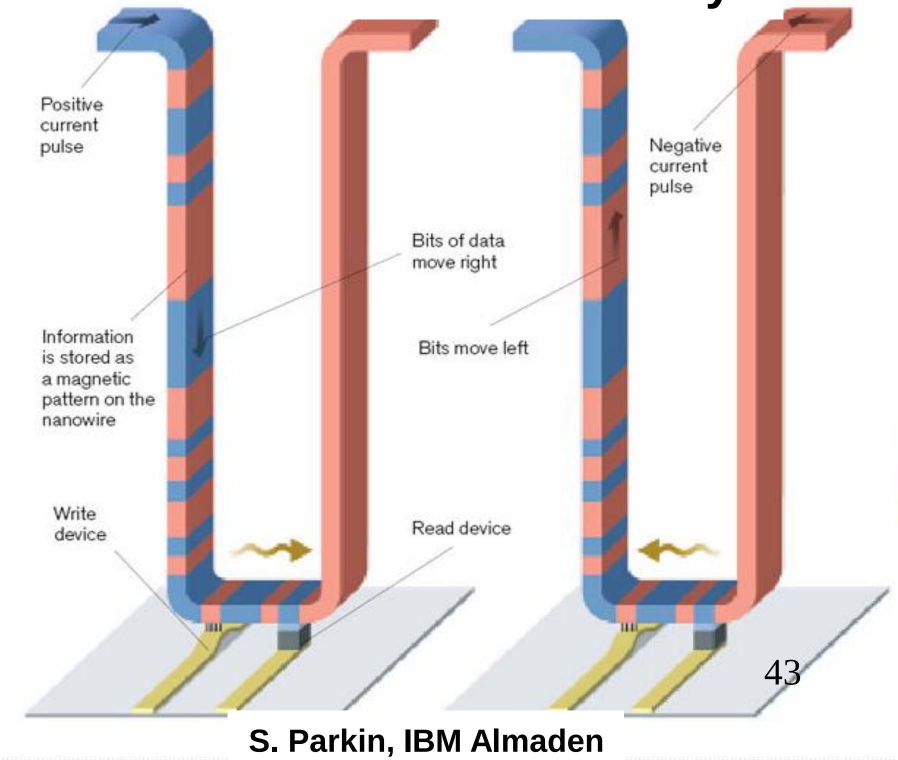
→Magnetic Tunnel Junctions

MgO spacer

Crucial buried functional layers & interfaces everywhere-

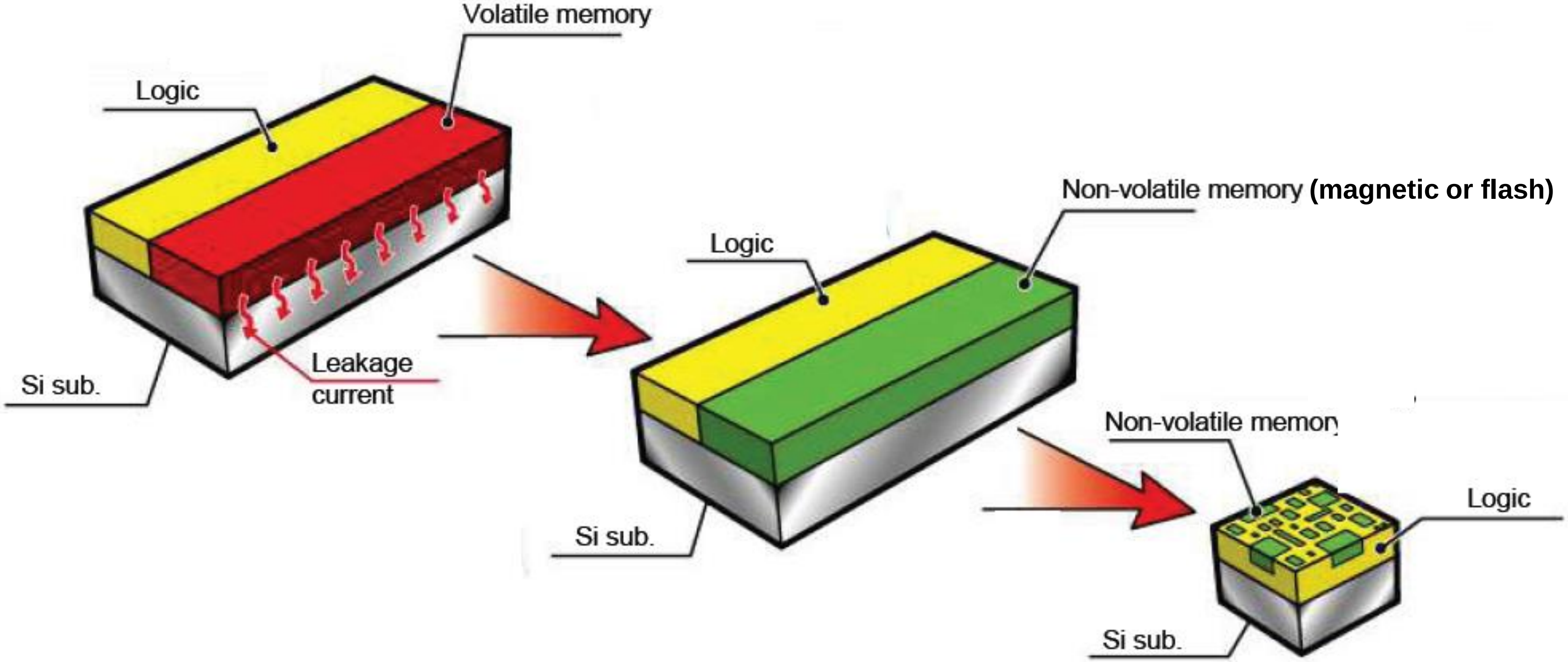
Magnetic Random Access Memory (MRAM-Non Volatile)

→Race Track Memory?



S. Parkin, IBM Almaden

Toward Nonvolatile CMOS VLSI

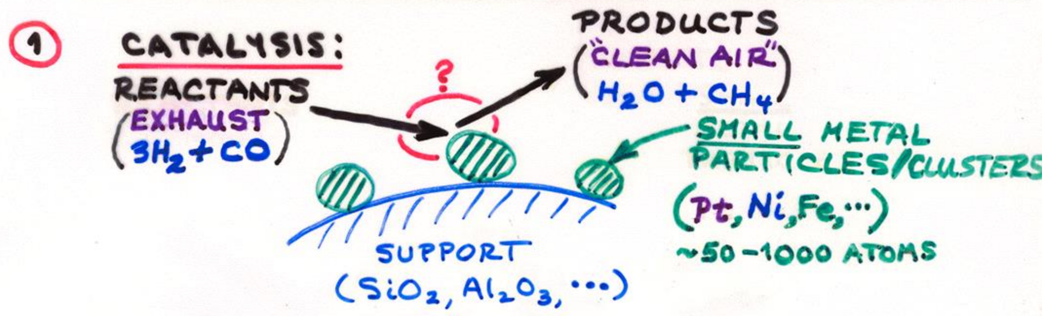


Hideo Ohno, Tohoku Univ.
IVC Conference, Busan, Korea, August, 2016

Scientific and technological areas related to surface/interface/nano science:

- **Integrated circuits—higher speed, higher density**
- **Magnetic storage—higher density, magnetic logic**
- **Catalysis—auto catalytic converter, petrochemical processing**

SOME AREAS OF APPLICATION: SURFACE SCIENCE



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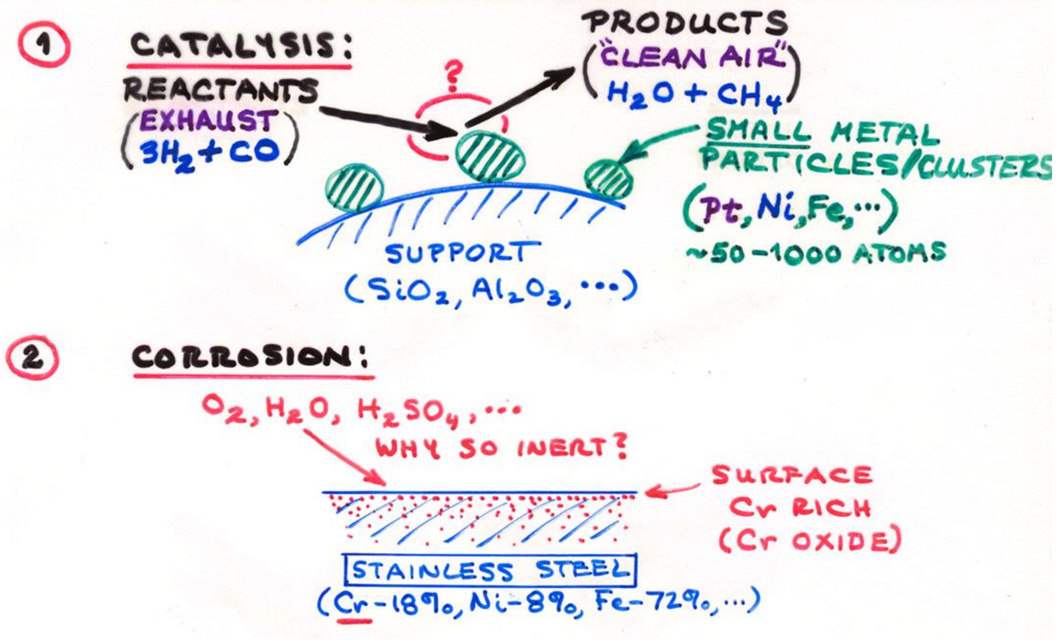

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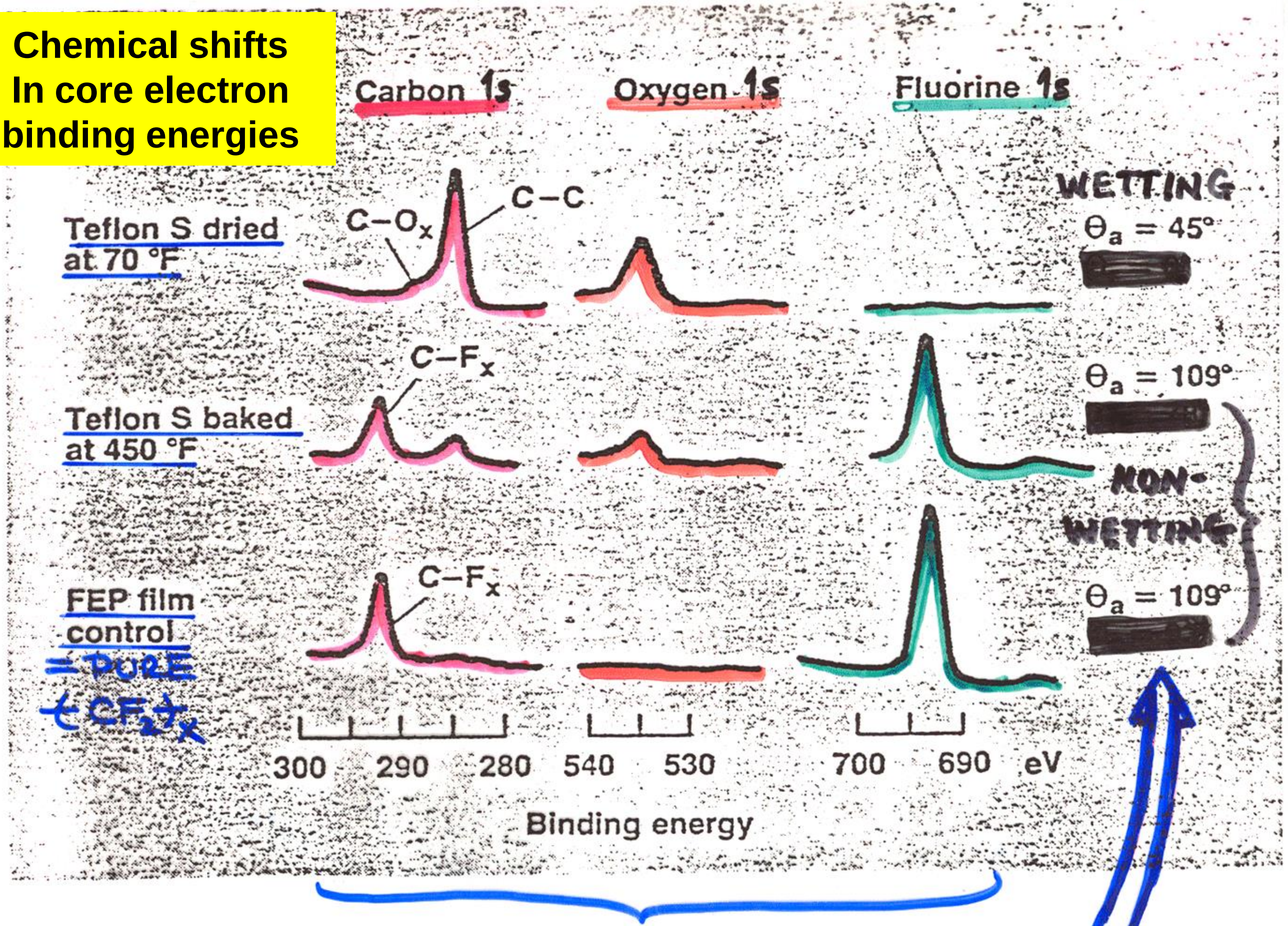
- **Corrosion—major annual economic cost**
- **Polymer surface modification—promote adhesion, fire resistance,…**

SURFACE TREATMENT OF A LOW-FRICTION POLYMERIC COATING FOR TOOLS

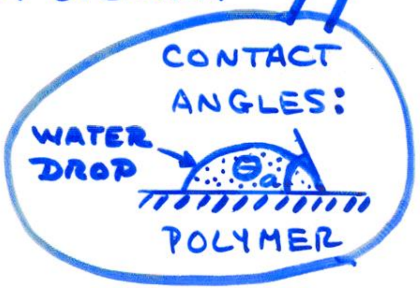
"TEFLON S" = A MIXTURE OF EPOXY AND $-(CF_2)-_x$

Chemical shifts In core electron binding energies



X-RAY PHOTOELECTRON SPECTRA

(D. DWIGHT, CHEMTECH, MARCH 1982)

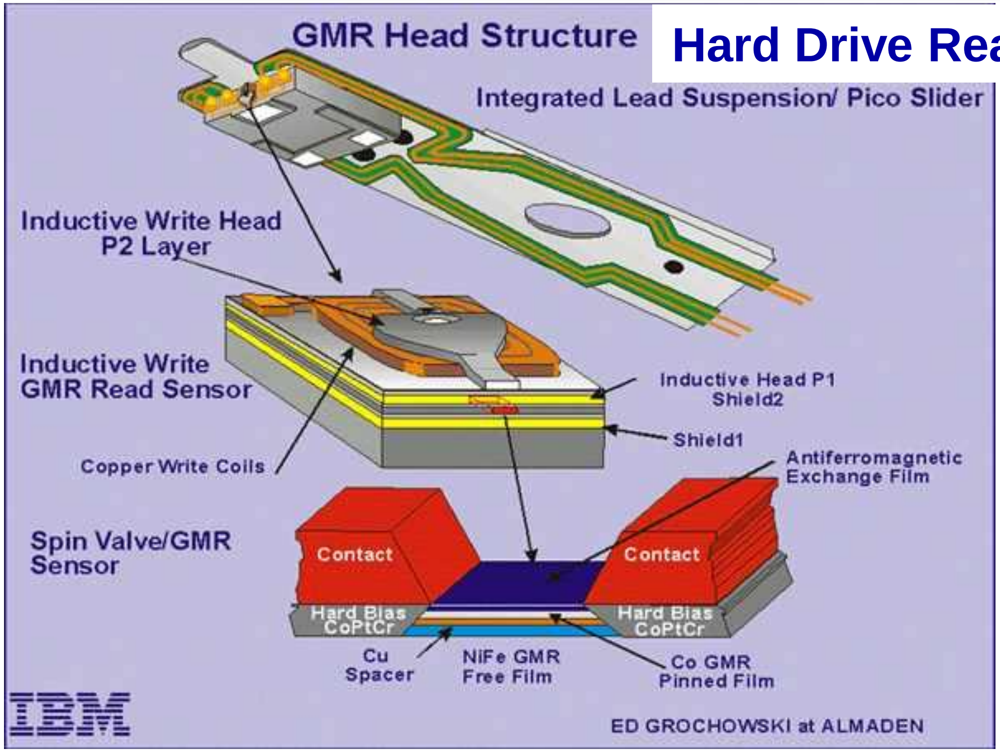


Scientific and technological areas related to surface/interface/nano science:

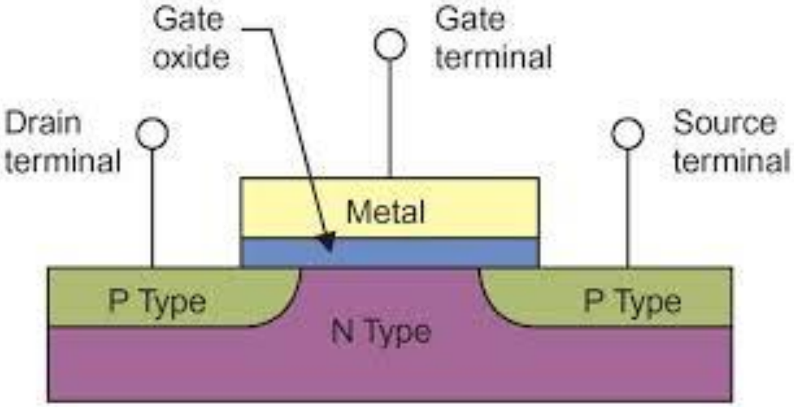
- Integrated circuits—higher speed, higher density
- Magnetic storage—higher density, magnetic logic
- Catalysis—auto catalytic converter, petrochemical processing
- Corrosion—major annual economic cost
- Polymer surface modification—promote adhesion, fire resistance,…
- Batteries, fuel cells, photovoltaic cells—the solar/hydrogen economy?

Interfaces in information and energy technology

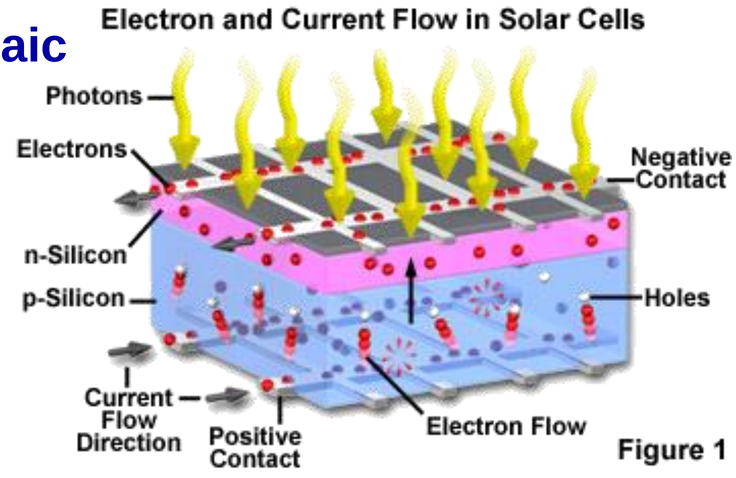
Hard Drive Read Head



Transistor

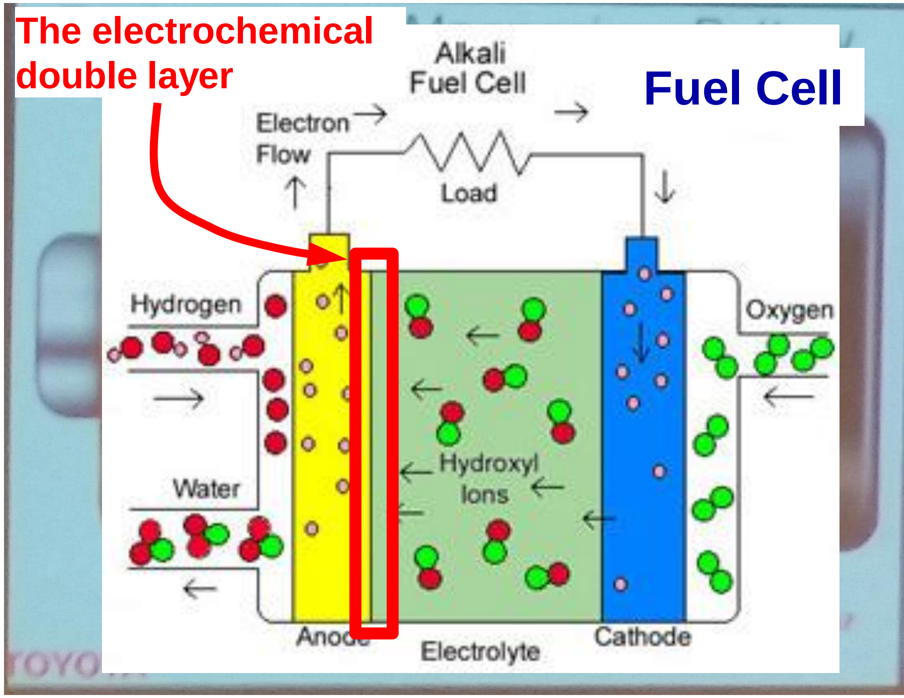


Photovoltaic Cell



The electrochemical double layer

Fuel Cell



Interfaces in information and energy technology

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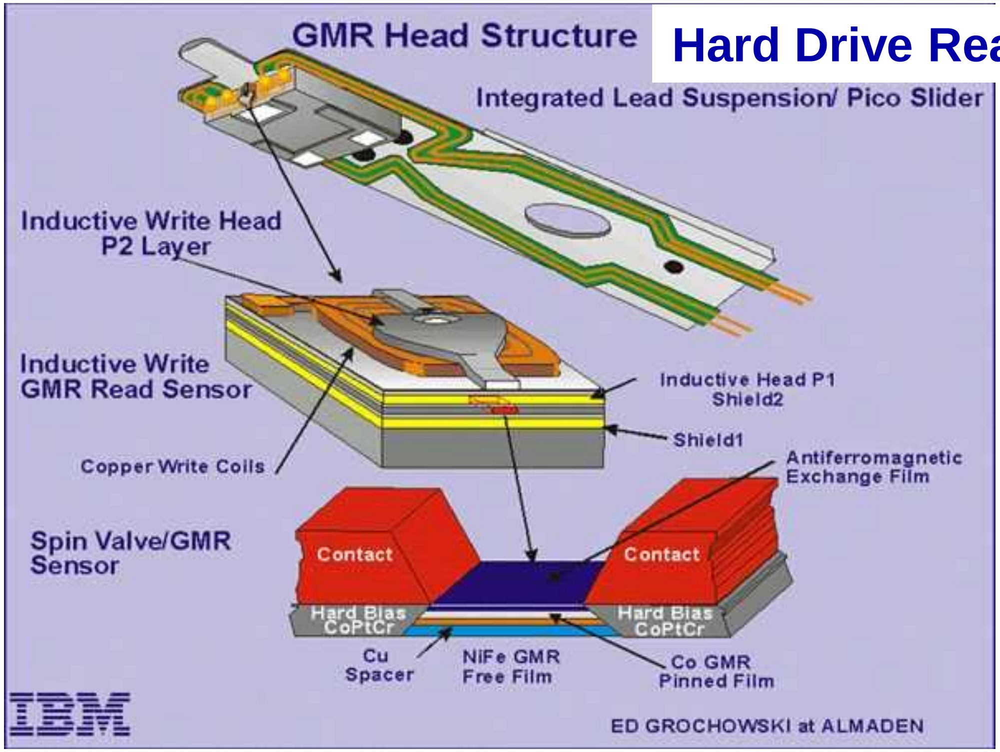
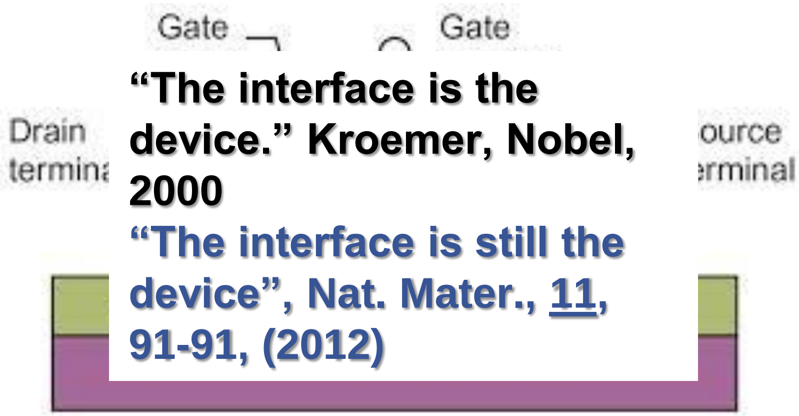


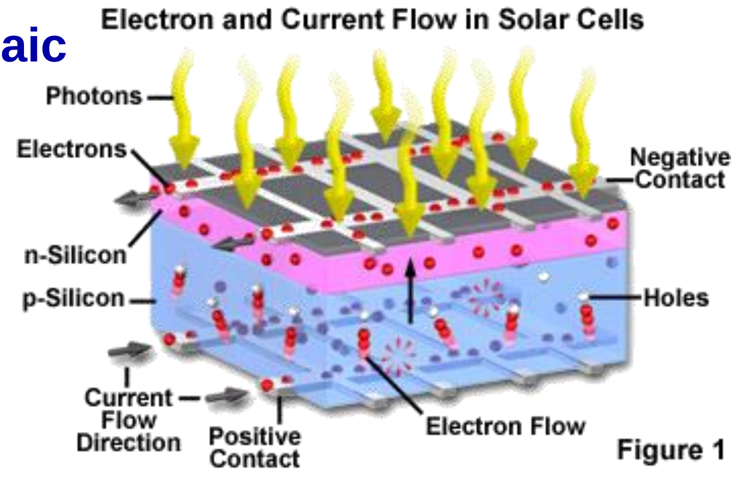
Transistor



"The interface is the device." Kroemer, Nobel, 2000

"The interface is still the device", Nat. Mater., 11, 91-91, (2012)

Photovoltaic Cell



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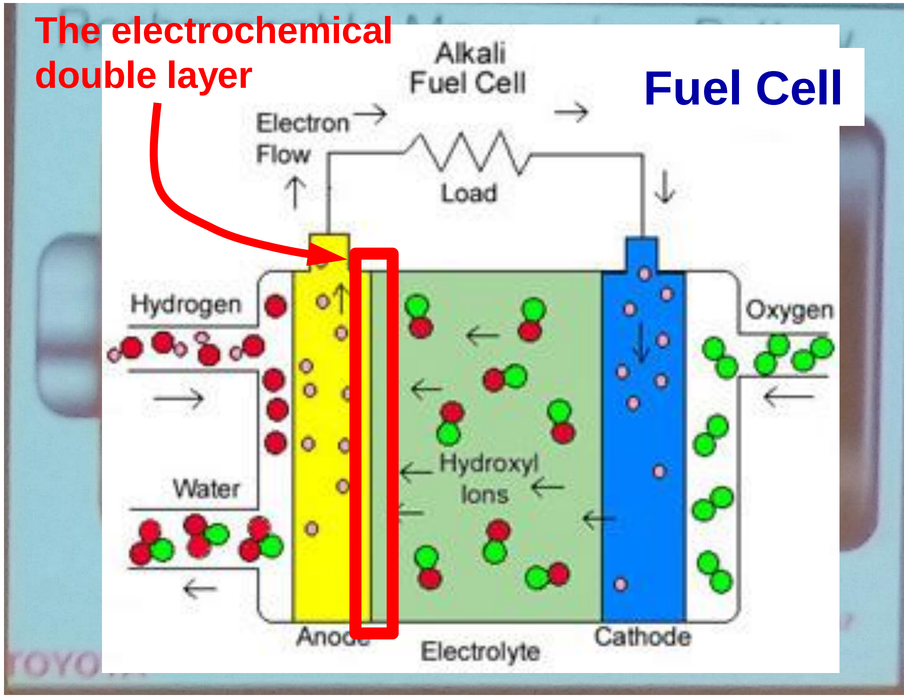

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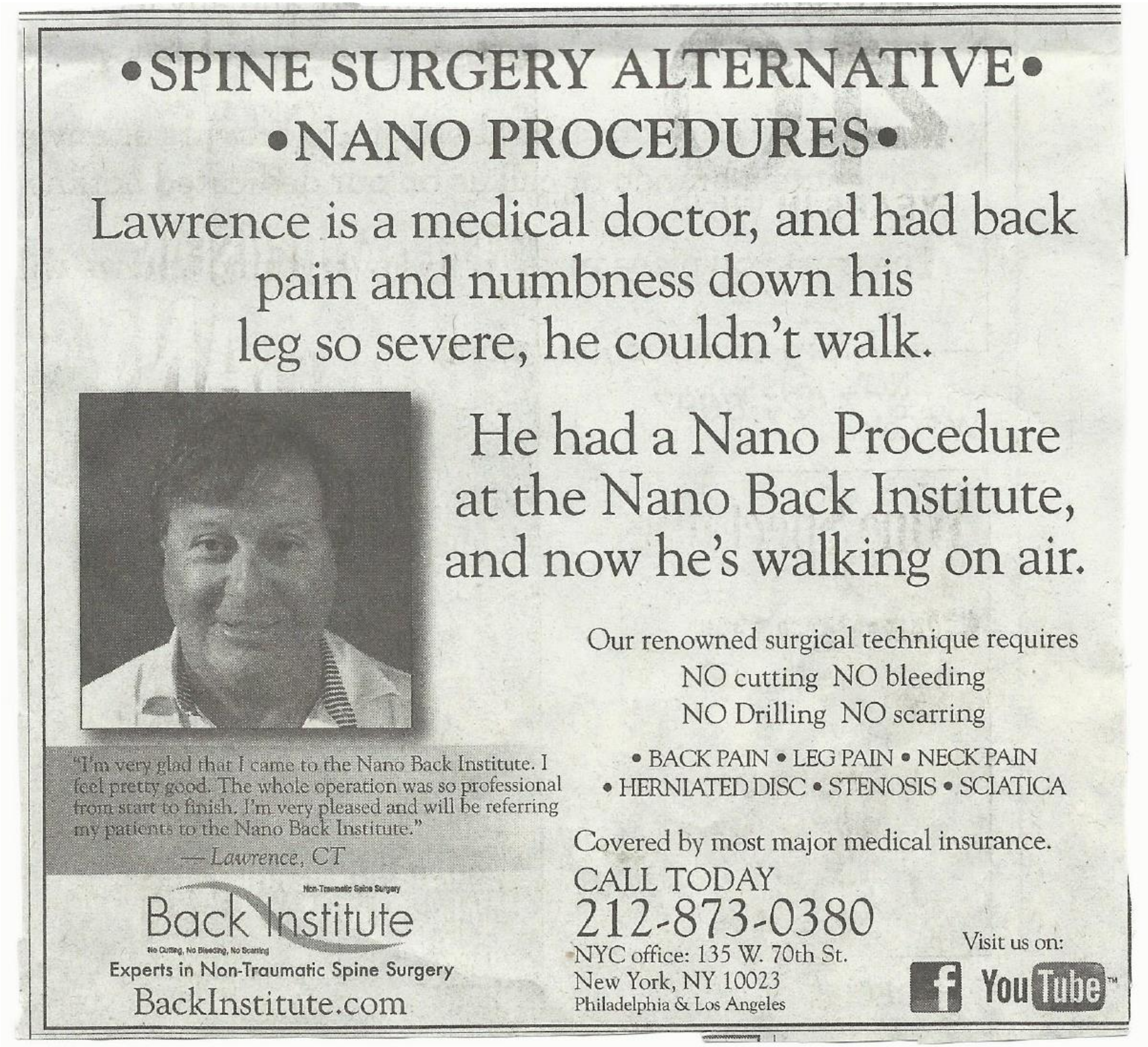
- **Corrosion—major annual economic cost**
- **Polymer surface modification—promote adhesion, fire resistance,…**
- **Batteries, fuel cells, photovoltaic cells—the solar/hydrogen economy?**
- **Lubrication (tribology)—nanometer-scale layers**
- **Atmospheric particulates—ice, carbonaceous,…**
- **Nuclear reactors and waste storage—how long-lasting?**
- **Environmental science—retention of contaminants in soil, reactions on atmospheric particles**
- **Biomaterials—compatibility through surface interactions**
- **Sensors—surface reactions→change in voltage, resistance**

And nano back surgery?!!



•SPINE SURGERY ALTERNATIVE•

•NANO PROCEDURES•

Lawrence is a medical doctor, and had back pain and numbness down his leg so severe, he couldn't walk.

He had a Nano Procedure at the Nano Back Institute, and now he's walking on air.

"I'm very glad that I came to the Nano Back Institute. I feel pretty good. The whole operation was so professional from start to finish. I'm very pleased and will be referring my patients to the Nano Back Institute."

—*Lawrence, CT*

Our renowned surgical technique requires

NO cutting NO bleeding

NO Drilling NO scarring

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• HERNIATED DISC • STENOSIS • SCIATICA

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No Cutting, No Bleeding, No Scarring

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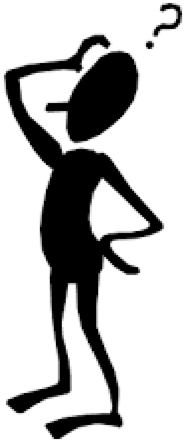
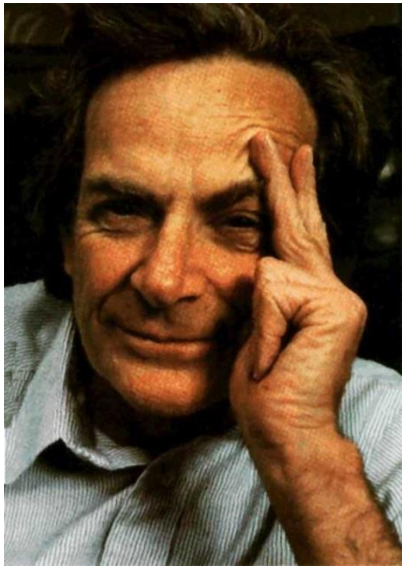




1959 — Richard P. Feynman “There’s plenty of room at the bottom”

“Why cannot we write the entire 24 volumes of the Encyclopedia Brittanica on the head of a pin?”

It would be possible if you could print it with dots (= bits) that are 8 nanometers or about 32 metal atoms across, containing about 1000 atoms

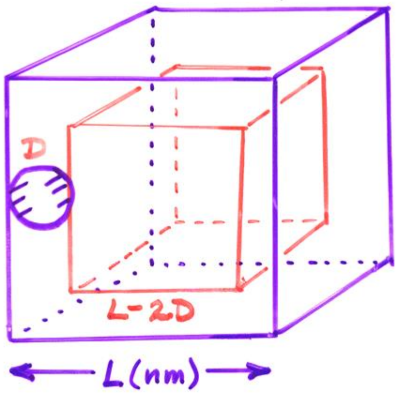
+ Many visionary ideas:

- ***Miniaturization of computers***
- ***Imaging and manipulation of single atoms or molecules →→***
  http://www.zyvex.com/nanotech/feynman.html

But information still stored with about 400,000 atoms, so we are still a long way from his vision

FRACTION OF ATOMS ON THE SURFACE OF A CUBE:

D = ATOMIC DIAM. ≈ 0.2 nm = 2 Å



$$\text{SURFACE FRACTION} = \frac{L^3-(L-2D)^3}{L^3}$$

L	FRACTION
1 µm = 1000 nm	0.001 ≈ 0.1%
0.1 µm = 100 nm	0.012 ≈ 1.2%
0.01 µm = 10 nm	0.115 ≈ 11.5%
0.001 µm = 1 nm	0.784 = 78.4%

➡ **Nanoscience is surface science**

SOME UNITS:

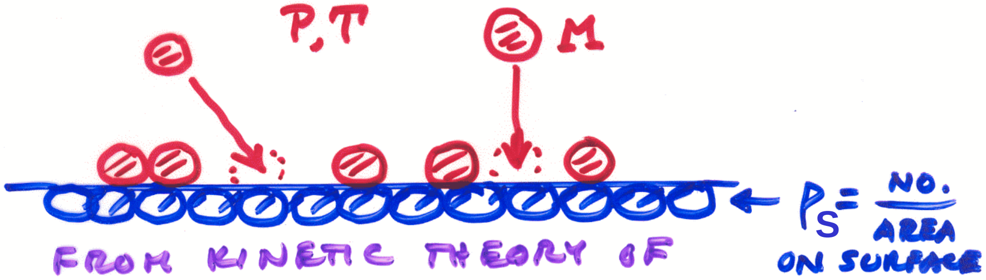
1 HAIR ≈ 50 microns

1 micron = 10^{-6} m = 1,000 nm = 10,000 Å
≈ 5,000 atoms

0.001 micron = 10^{-9} m = 1 nanometer = 1 nm = 10 Å
≈ 5 atoms

WHY IS ULTRAHIGH VACUUM IMPORTANT?

TIME TO BUILD UP A SINGLE ATOMIC/MOLECULAR LAYER = 1 MONOLAYER ≡ 1 ML IF EACH ATOM/MOLECULE FROM GAS PHASE HITTING SURFACE STICKS: τ_1



FROM KINETIC THEORY OF GASES:

$$\tau_1\ (\text{sec}) = 2.84 \times 10^{-23}[T(K)M]^{1/2}\rho_S(\text{cm}^{-2})/P(\text{torr})$$

N_2, CO O_2
↓ ↓

WITH TYPICAL NOS. FOR $M = 28, 32$

$T = 298K$

$\rho_S = 1-2 \times 10^{15}\ \text{cm}^{-2}$
↑
METALS, SEMICOND.

	τ_1	P
	1 s	10^{-6} torr
	100 s ~2 min	10^{-8} ..
	~15 min	10^{-9} ..
TYPICAL [	~2.8 hr	10^{-10} ..
	~27.8 hr	10^{-11} ..

→ **Need to work at ~10^{-10}-10^{-11} torr to have clean surfaces**

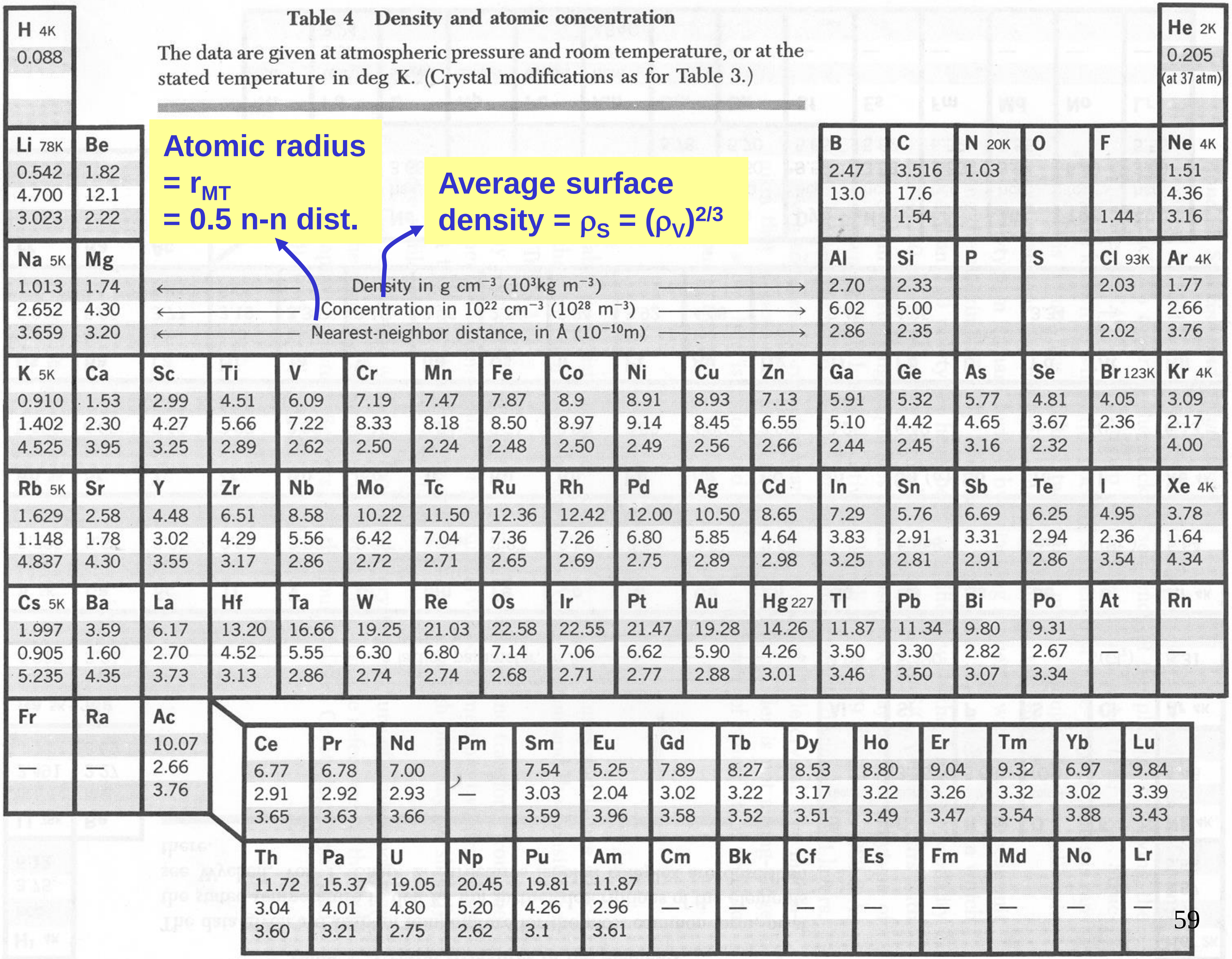


Table 4 Density and atomic concentration

The data are given at atmospheric pressure and room temperature, or at the stated temperature in deg K. (Crystal modifications as for Table 3.)

H 4K 0.088																	**He** 2K 0.205 (at 37 atm)
Li 78K 0.542 4.700 3.023	**Be** 1.82 12.1 2.22											**B** 2.47 13.0	**C** 3.516 17.6 1.54	**N** 20K 1.03	**O**	**F** 1.44	**Ne** 4K 1.51 4.36 3.16
Na 5K 1.013 2.652 3.659	**Mg** 1.74 4.30 3.20											**Al** 2.70 6.02 2.86	**Si** 2.33 5.00 2.35	**P**	**S**	**Cl** 93K 2.03 2.02	**Ar** 4K 1.77 2.66 3.76
K 5K 0.910 1.402 4.525	**Ca** 1.53 2.30 3.95	**Sc** 2.99 4.27 3.25	**Ti** 4.51 5.66 2.89	**V** 6.09 7.22 2.62	**Cr** 7.19 8.33 2.50	**Mn** 7.47 8.18 2.24	**Fe** 7.87 8.50 2.48	**Co** 8.9 8.97 2.50	**Ni** 8.91 9.14 2.49	**Cu** 8.93 8.45 2.56	**Zn** 7.13 6.55 2.66	**Ga** 5.91 5.10 2.44	**Ge** 5.32 4.42 2.45	**As** 5.77 4.65 3.16	**Se** 4.81 3.67 2.32	**Br** 123K 4.05 2.36	**Kr** 4K 3.09 2.17 4.00
Rb 5K 1.629 1.148 4.837	**Sr** 2.58 1.78 4.30	**Y** 4.48 3.02 3.55	**Zr** 6.51 4.29 3.17	**Nb** 8.58 5.56 2.86	**Mo** 10.22 6.42 2.72	**Tc** 11.50 7.04 2.71	**Ru** 12.36 7.36 2.65	**Rh** 12.42 7.26 2.69	**Pd** 12.00 6.80 2.75	**Ag** 10.50 5.85 2.89	**Cd** 8.65 4.64 2.98	**In** 7.29 3.83 3.25	**Sn** 5.76 2.91 2.81	**Sb** 6.69 3.31 2.91	**Te** 6.25 2.94 2.86	**I** 4.95 2.36 3.54	**Xe** 4K 3.78 1.64 4.34
Cs 5K 1.997 0.905 5.235	**Ba** 3.59 1.60 4.35	**La** 6.17 2.70 3.73	**Hf** 13.20 4.52 3.13	**Ta** 16.66 5.55 2.86	**W** 19.25 6.30 2.74	**Re** 21.03 6.80 2.74	**Os** 22.58 7.14 2.68	**Ir** 22.55 7.06 2.71	**Pt** 21.47 6.62 2.77	**Au** 19.28 5.90 2.88	**Hg** 227 14.26 4.26 3.01	**Tl** 11.87 3.50 3.46	**Pb** 11.34 3.30 3.50	**Bi** 9.80 2.82 3.07	**Po** 9.31 2.67 3.34	**At** —	**Rn** —
Fr —	**Ra** —	**Ac** 10.07 2.66 3.76															

Ce 6.77 2.91 3.65	**Pr** 6.78 2.92 3.63	**Nd** 7.00 2.93 3.66	**Pm** —	**Sm** 7.54 3.03 3.59	**Eu** 5.25 2.04 3.96	**Gd** 7.89 3.02 3.58	**Tb** 8.27 3.22 3.52	**Dy** 8.53 3.17 3.51	**Ho** 8.80 3.22 3.49	**Er** 9.04 3.26 3.47	**Tm** 9.32 3.32 3.54	**Yb** 6.97 3.02 3.88	**Lu** 9.84 3.39 3.43
Th 11.72 3.04 3.60	**Pa** 15.37 4.01 3.21	**U** 19.05 4.80 2.75	**Np** 20.45 5.20 2.62	**Pu** 19.81 4.26 3.1	**Am** 11.87 2.96 3.61	**Cm** —	**Bk** —	**Cf** —	**Es** —	**Fm** —	**Md** —	**No** —	**Lr** —

← Density in g cm^{-3} (10^3kg m^{-3}) →

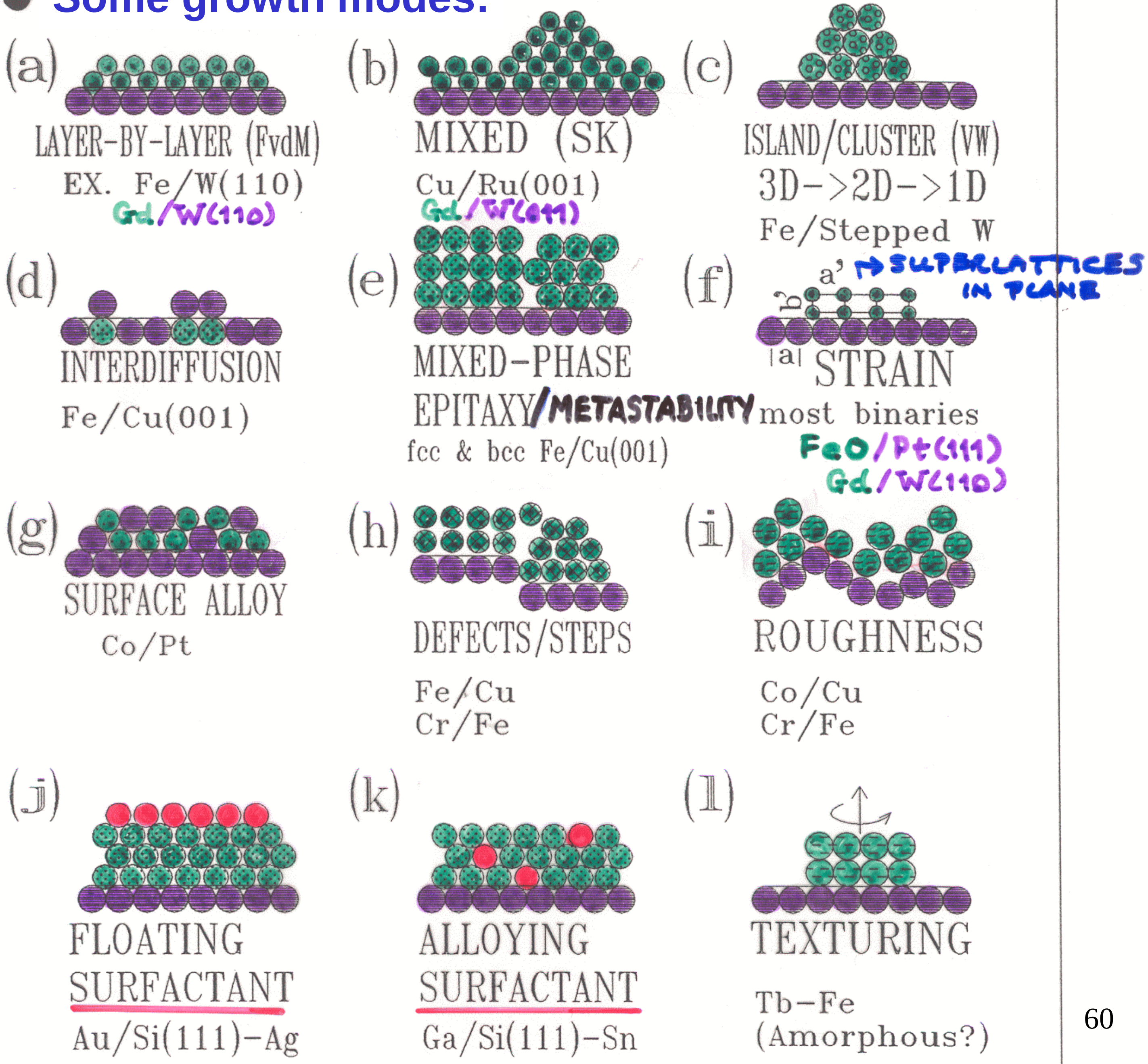
← Concentration in 10^{22} cm^{-3} (10^{28} m^{-3}) →

← Nearest-neighbor distance, in Å (10^{-10}m) →

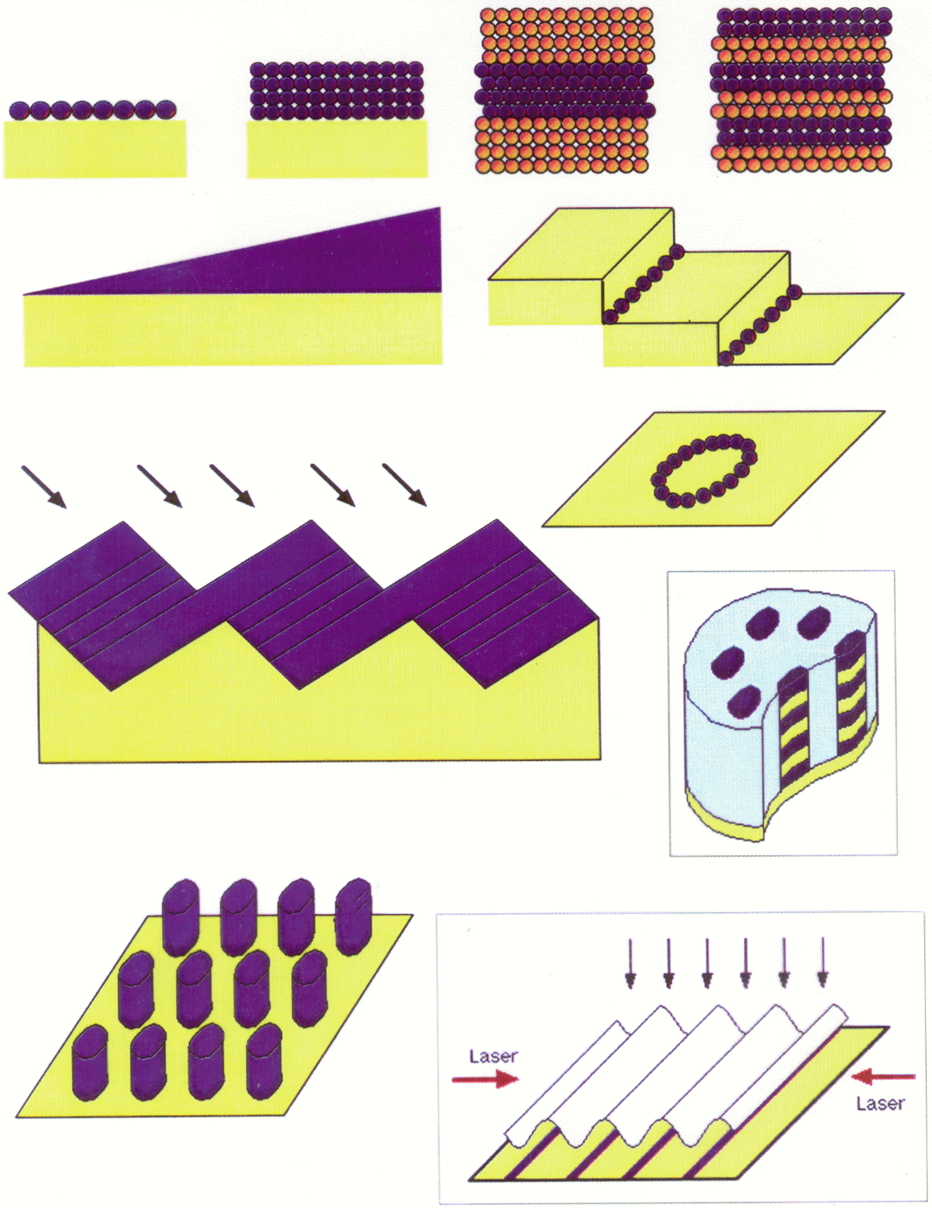
Atomic radius = r_{MT} = 0.5 n-n dist.

Average surface density = $\rho_S = (\rho_V)^{2/3}$

- **Some growth modes:**



Some possible structures in surface/interface/nanoscience



KORTRIGHT
ET AL., J.M.M.
207, 44('99')

TRANSLATIONAL SYMMETRY IN BULK SOLIDS: 14 basic types

Good websites/downloads for simple structures:

http://www.dawgsdk.org/crystal/en/library/fcc#0002

http://demonstrations.wolfram.com/CrystalViewer/

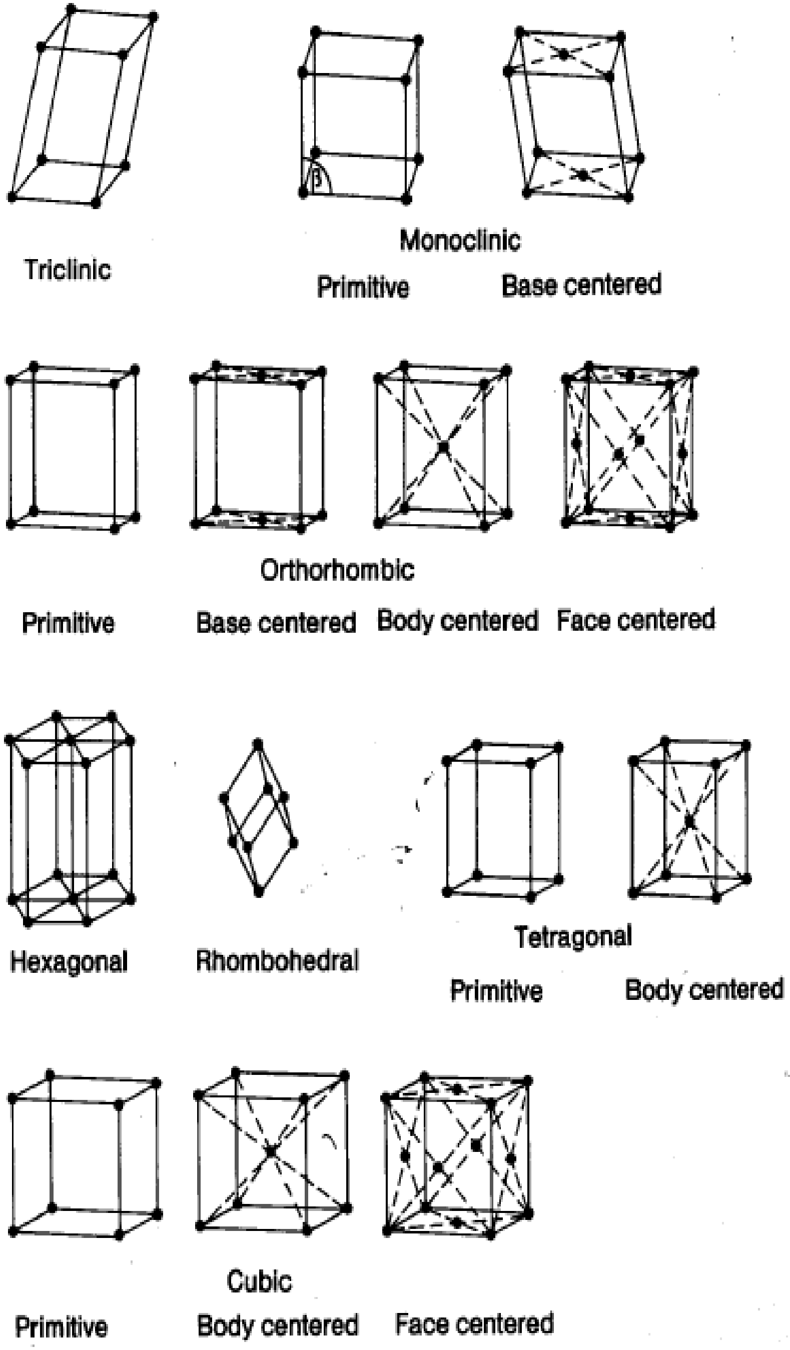


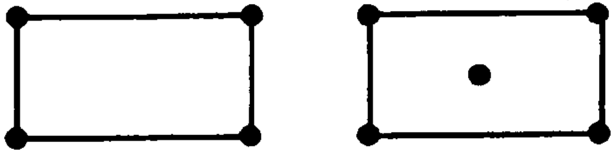
Fig. 2.3. The 14 three-dimensional Bravais lattices. The hexagonal lattice and the two centered cubic lattices are particularly important in solid state physics

TRANSLATIONAL SYMMETRY AT SURFACES: 5 basic types

Table 2.1. *The five two-dimensional Bravais nets*

Shape of unit mesh	Mesh symbol	Conventional rule for choice of axes	Nature of axes and angles	Name
General parallelogram	p	None	$a \neq b$ $\gamma \neq 90°$	Oblique
Rectangle	p c	Two shortest, mutually perpendicular vectors	$a \neq b$ $\gamma = 90°$	Rectangular
Square	p	Two shortest, mutually perpendicular vectors	$a = b$ $\gamma = 90°$	Square
60° angle rhombus	p	Two shortest vectors at 120° to each other	$a = b$ $\gamma = 120°$	Hexagonal

Oblique



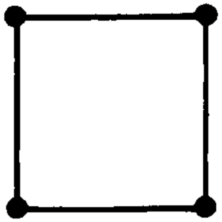
p

c

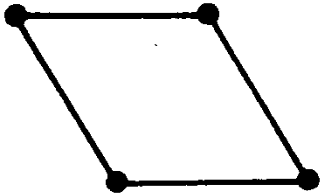
Rectangular

p = primitive

c = centered



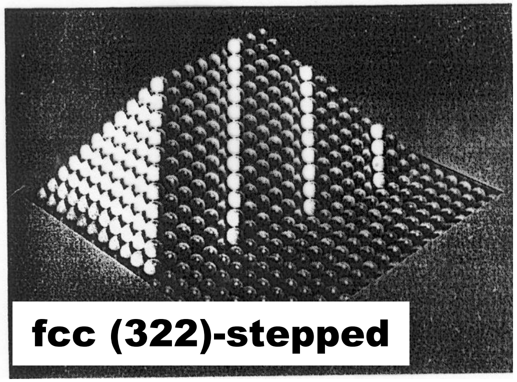
Square



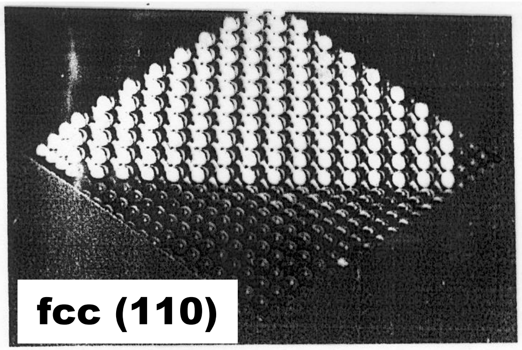
Hexagonal

+ Various visualizations of crystal surfaces at: http://www.fhi-berlin.mpg.de/~hermann/Balsac/pictures.html

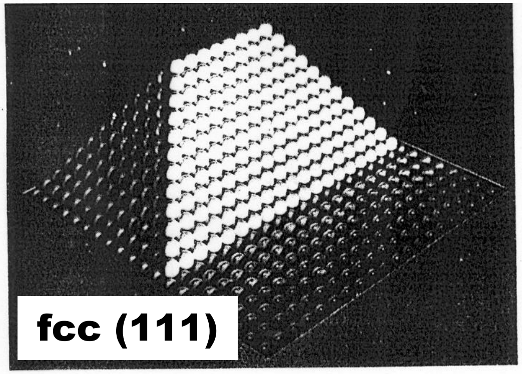
WHAT DO SURFACES LOOK LIKE? SOME fcc AND bcc SURFACES



fcc (322)-stepped



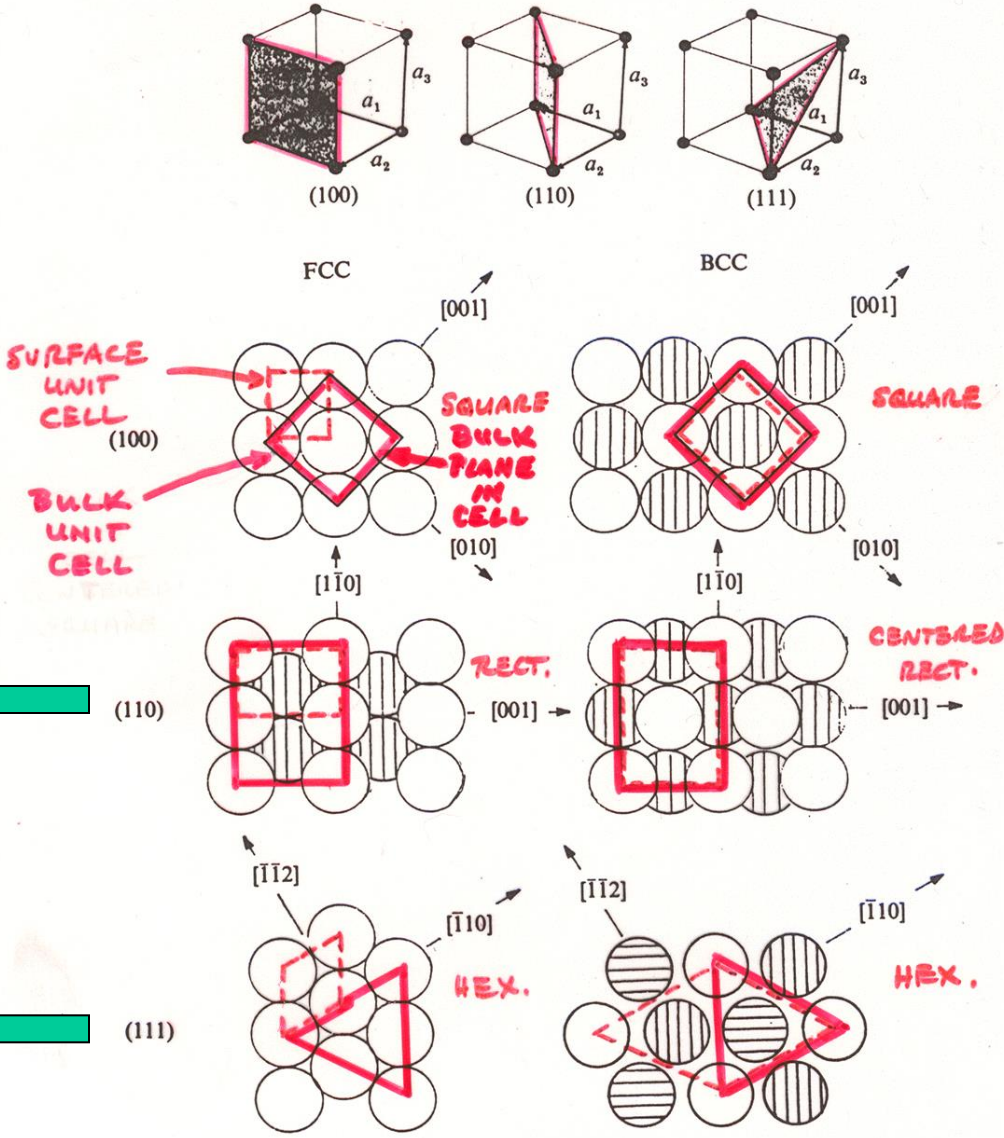
fcc (110)



fcc (111)

+ Various visualizations of crystal surfaces at: http://www.fhi-berlin.mpg.de/~hermann/Balsac/pictures.html

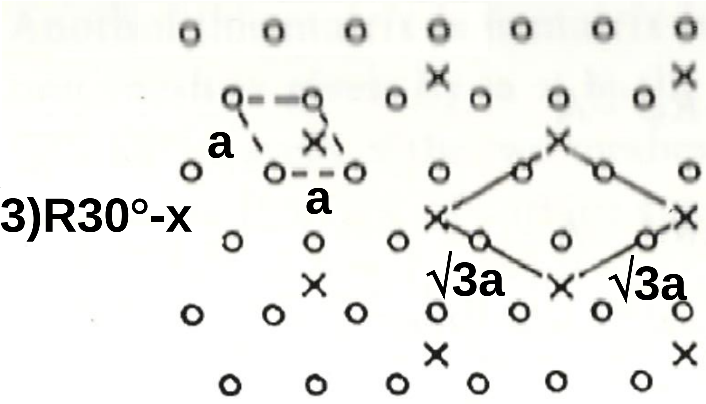
Fig. 3.2. Low-index ideal surfaces of a hard-sphere cubic crystal. Vertical and horizontal markings indicate the second and third atom layers, respectively. Cube face is indicated for (100) to set the scale (Nicholas, 1965).



HOW TO DESCRIBE DIFFERENT (hkℓ) SURFACES OF X WITH ORDERED ADSORBATE STRUCTURES OF x ON THEM? WOOD NOTATION:

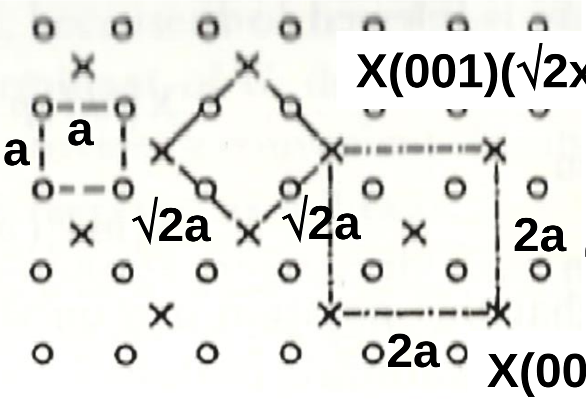
X(hkℓ)(p x q)Rϕ°-x (Woodruff, pp. 22-23)

Hexagonal surface of X



X(111)(√3x√3)R30°-x

Square surface of X

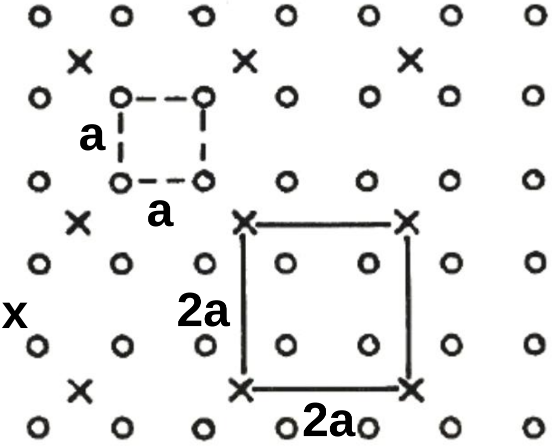


X(001)(√2x√2)R45°-x

"centered"

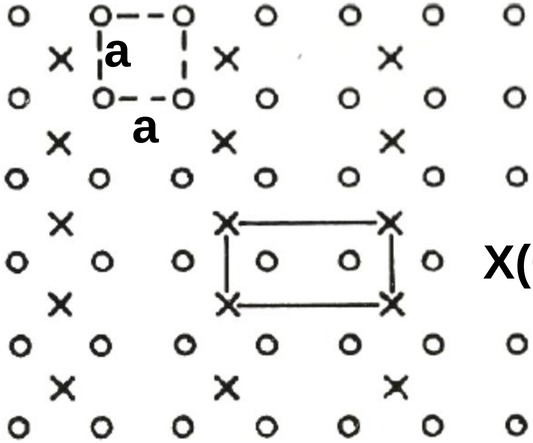
X(001)c(2X2)-x

Square surface of X



X(001)(2X2)-x

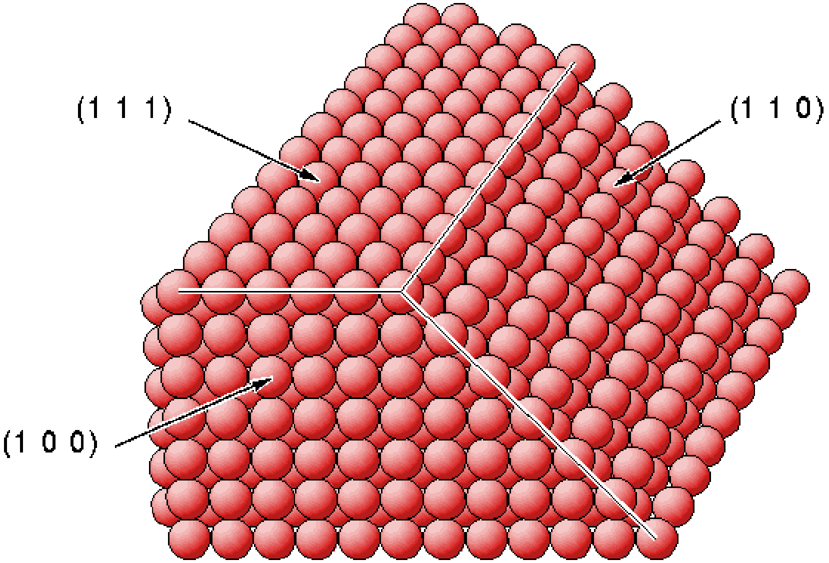
Square surface of X



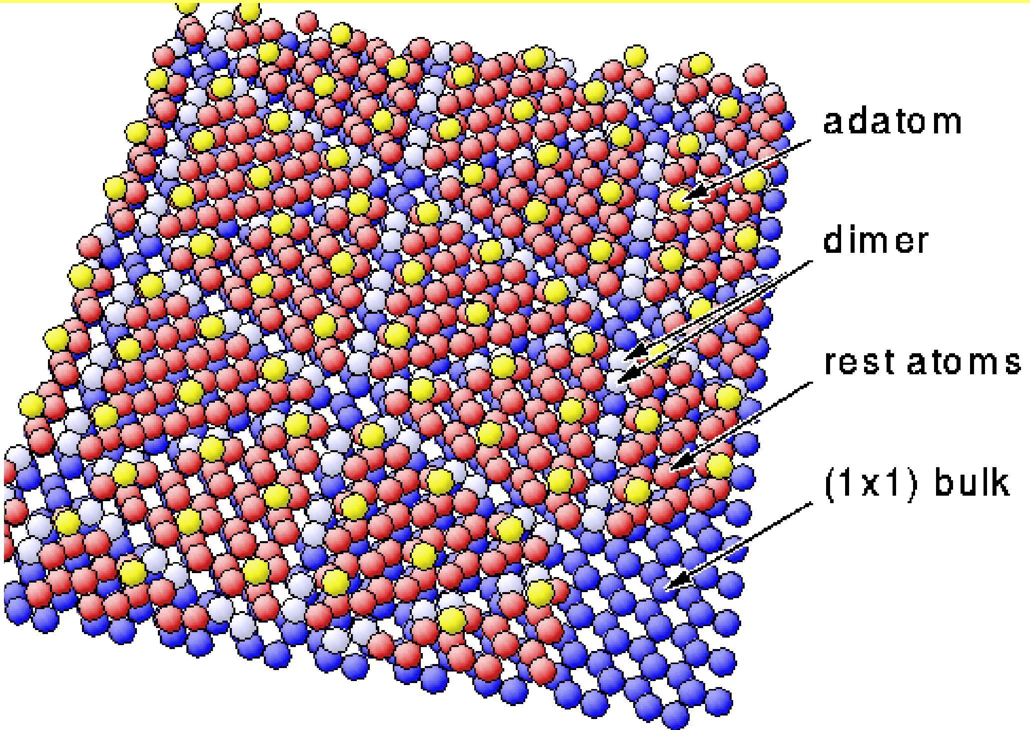
X(001)(2X1)-x

Notation: **(hkℓ) = definite set of planes**
{hkℓ} = set of planes with h,k,ℓ in all permutations
[hkℓ] = definite direction, ⊥ (hkℓ) planes
<hkℓ> = set of directions with h,k,ℓ in all permutations

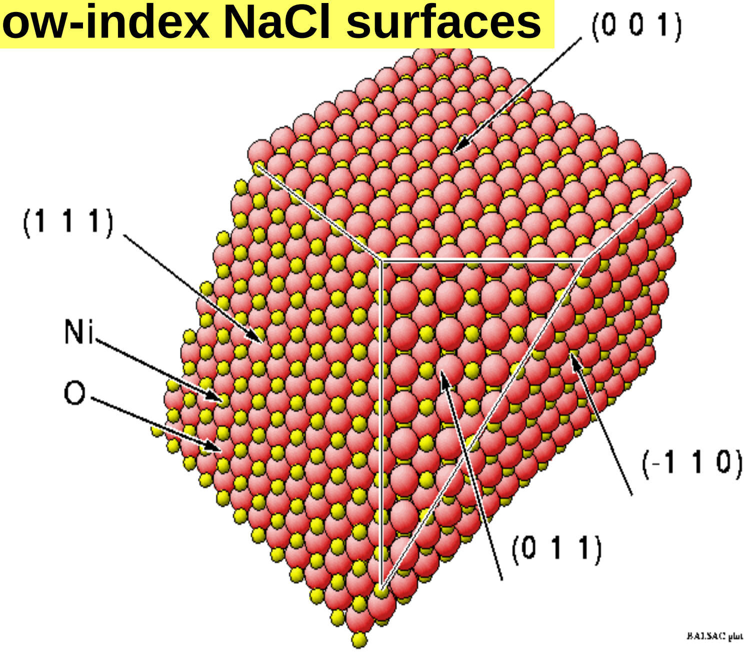
Low-index fcc metal surfaces



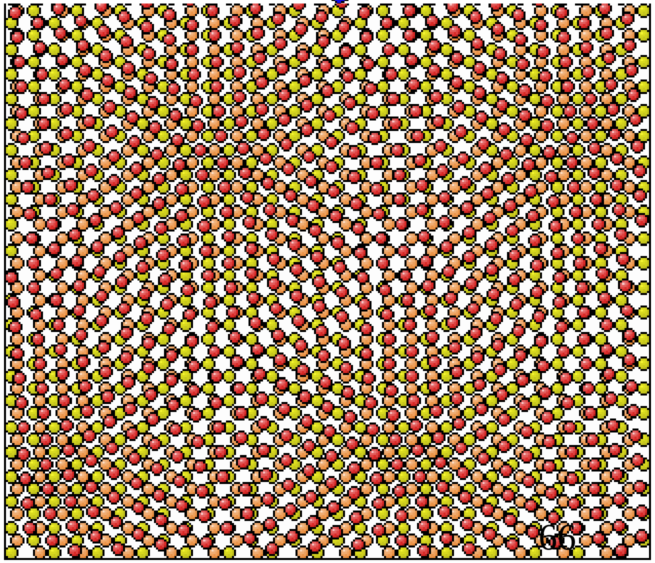
Si(111)-(7x7)—Dimer-adatom-stacking fault model



Low-index NaCl surfaces

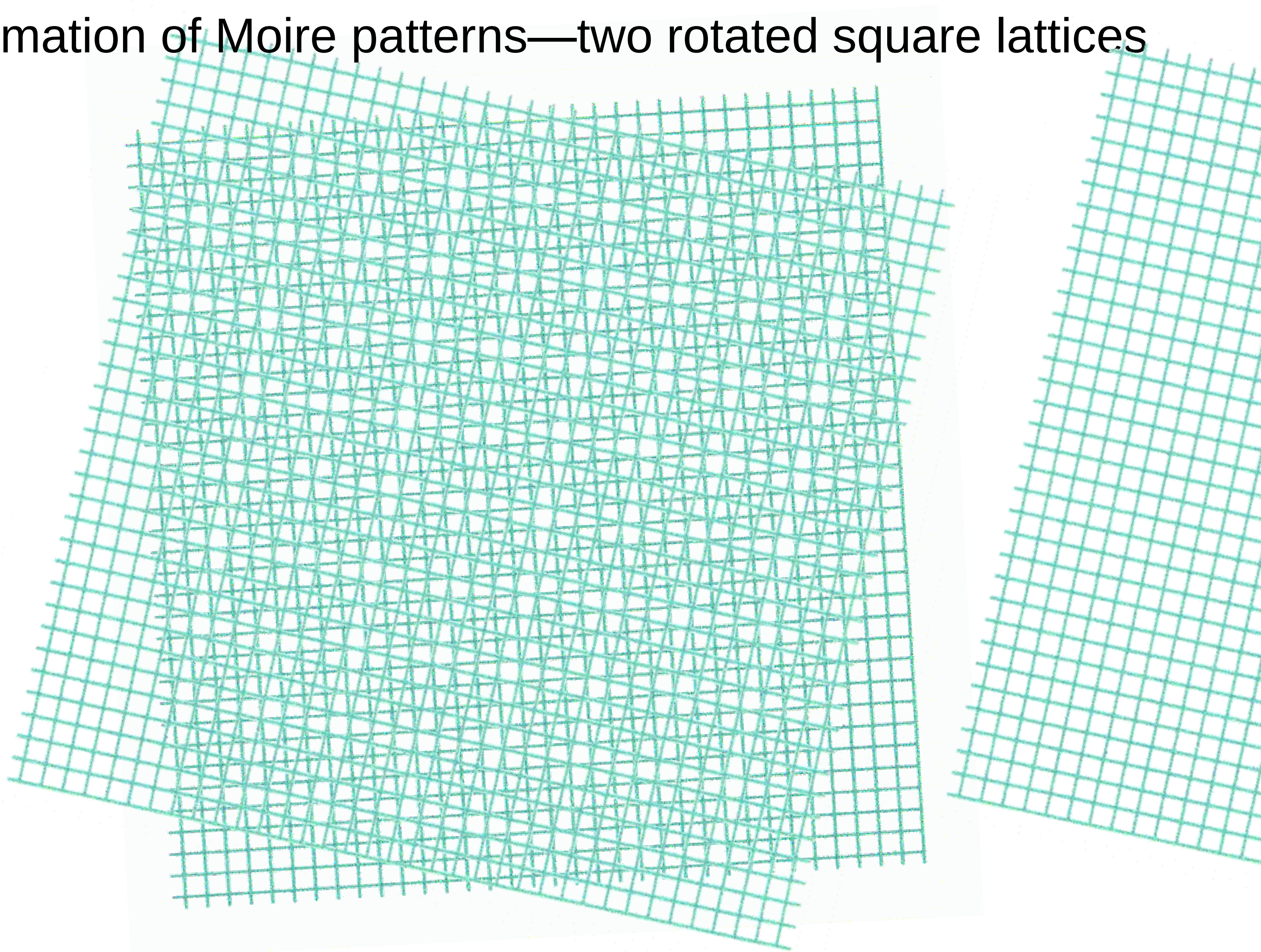


Fcc(111) super-lattice = a Moiré pattern: 4 degree rot'n.



http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/pictures.html

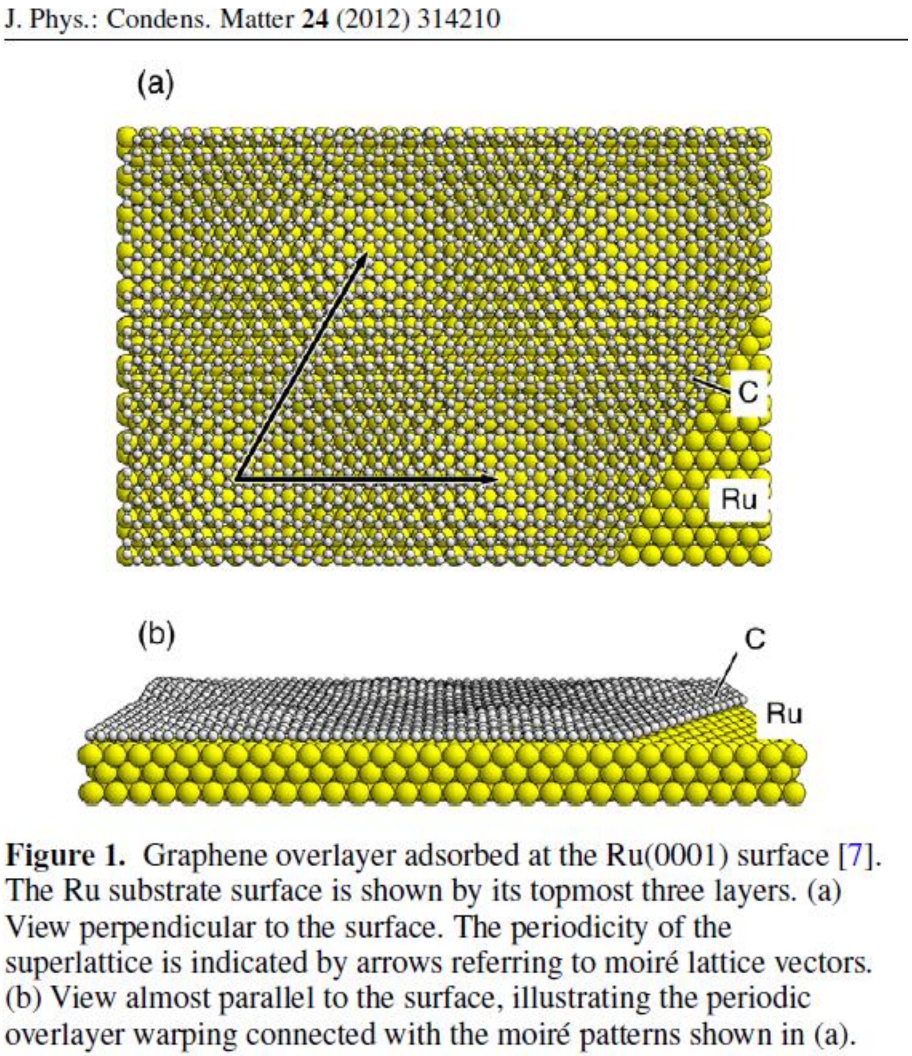
Formation of Moire patterns—two rotated square lattices



Plus demo with two crossed-axis diffraction gratings and laser

Moiré patterns in the growth of graphene

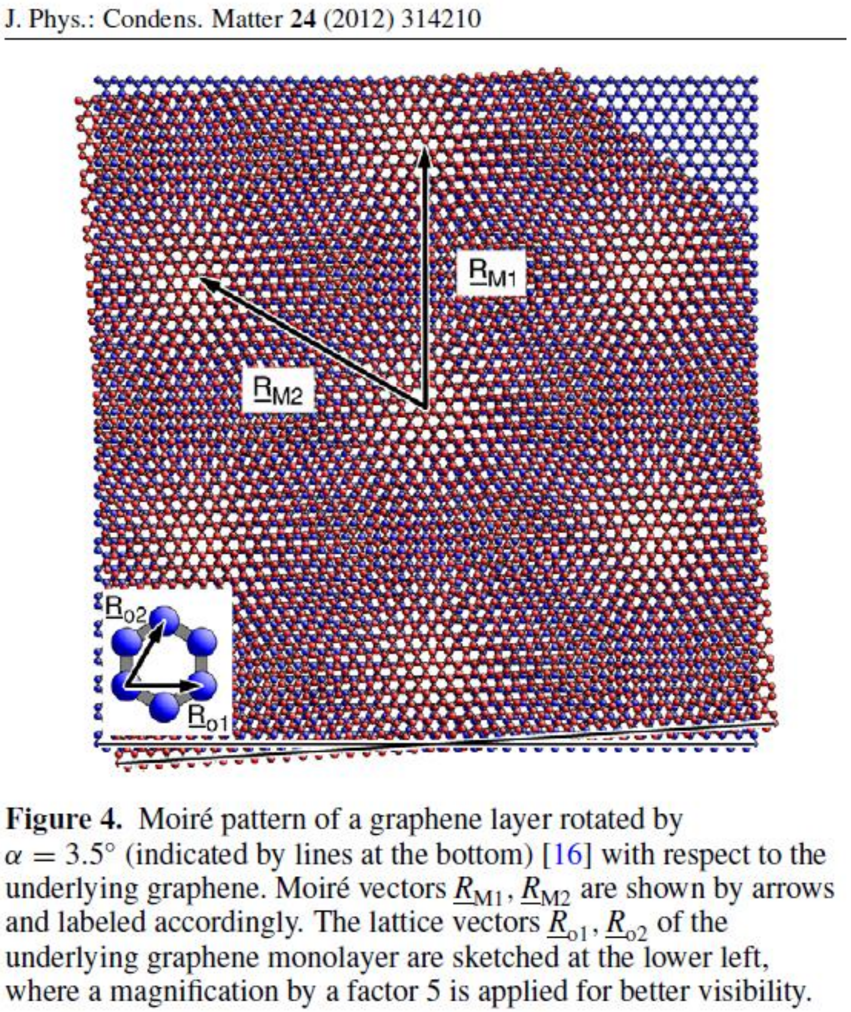
Graphene on Ru(0001)-no rotation



J. Phys.: Condens. Matter **24** (2012) 314210

Figure 1. Graphene overlayer adsorbed at the Ru(0001) surface [7]. The Ru substrate surface is shown by its topmost three layers. (a) View perpendicular to the surface. The periodicity of the superlattice is indicated by arrows referring to moiré lattice vectors. (b) View almost parallel to the surface, illustrating the periodic overlayer warping connected with the moiré patterns shown in (a).

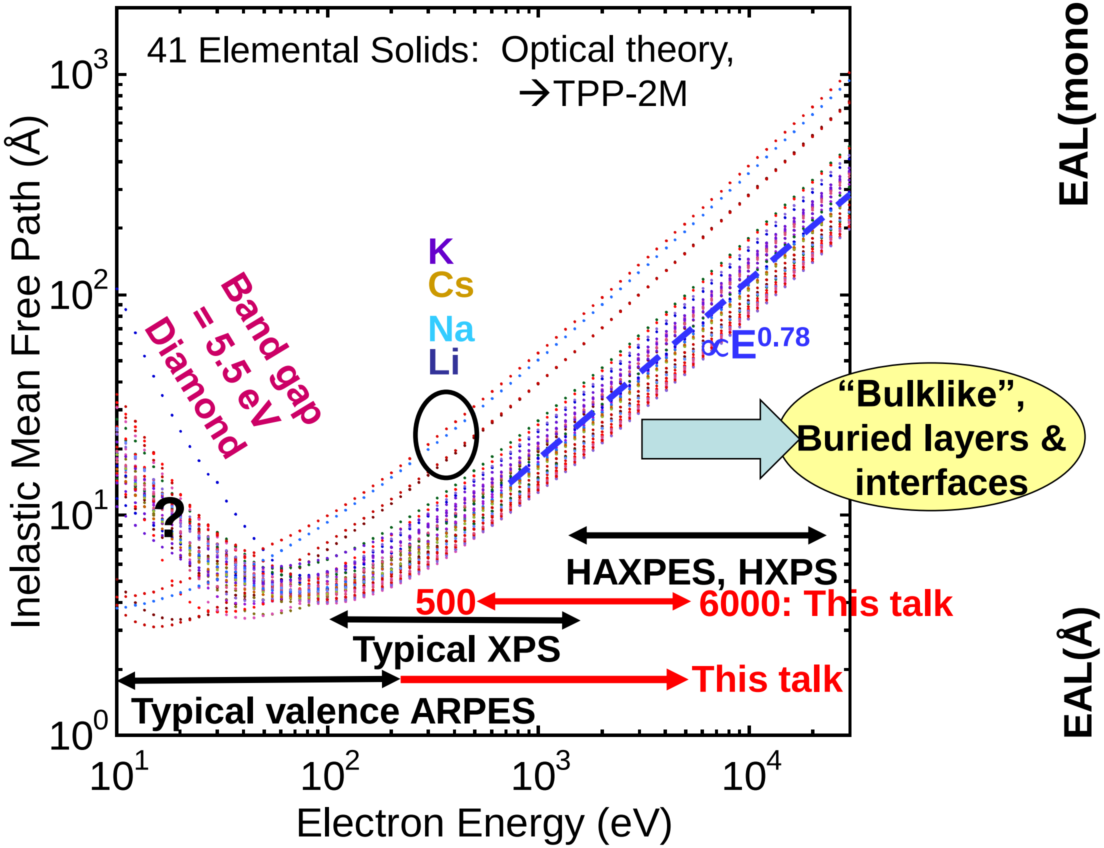
Graphene on graphene-3.5° rotation



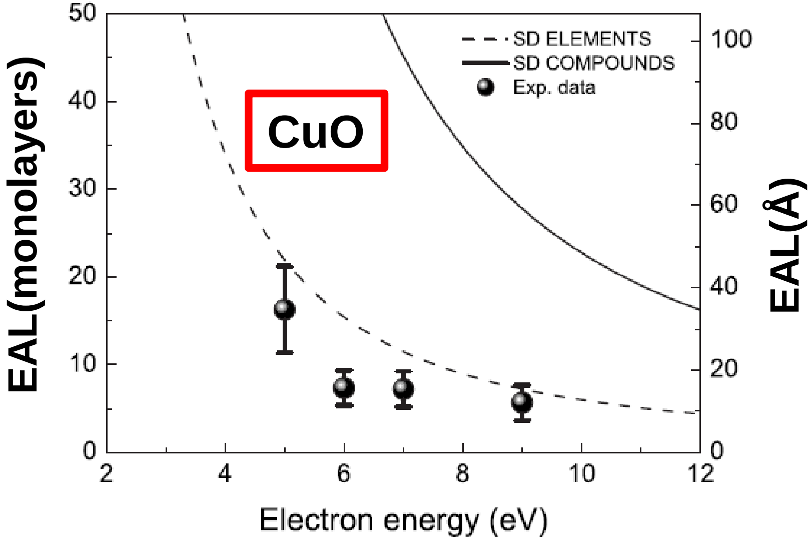
J. Phys.: Condens. Matter **24** (2012) 314210

Figure 4. Moiré pattern of a graphene layer rotated by $\alpha = 3.5^\circ$ (indicated by lines at the bottom) [16] with respect to the underlying graphene. Moiré vectors $\underline{R}_{M1}$, $\underline{R}_{M2}$ are shown by arrows and labeled accordingly. The lattice vectors $\underline{R}_{o1}$, $\underline{R}_{o2}$ of the underlying graphene monolayer are sketched at the lower left, where a magnification by a factor 5 is applied for better visibility.

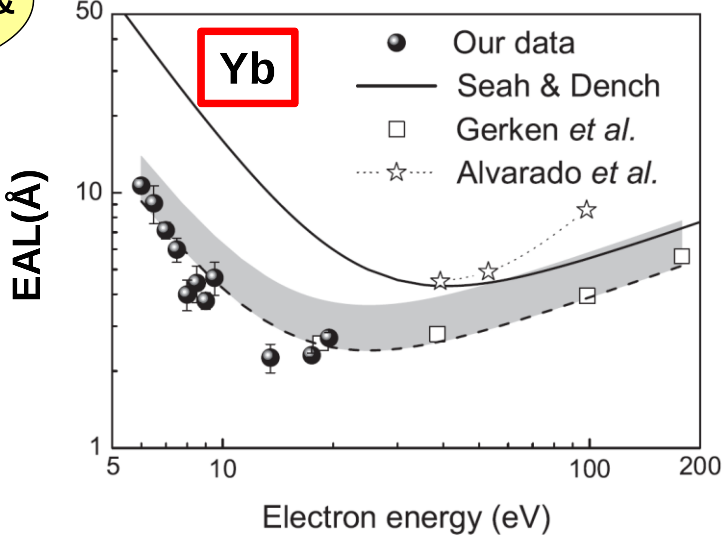
Electrons as probes of surface and bulk properties



Tanuma, Powell, Penn, Surf. and Interf. Anal. 43, 689 (2011)



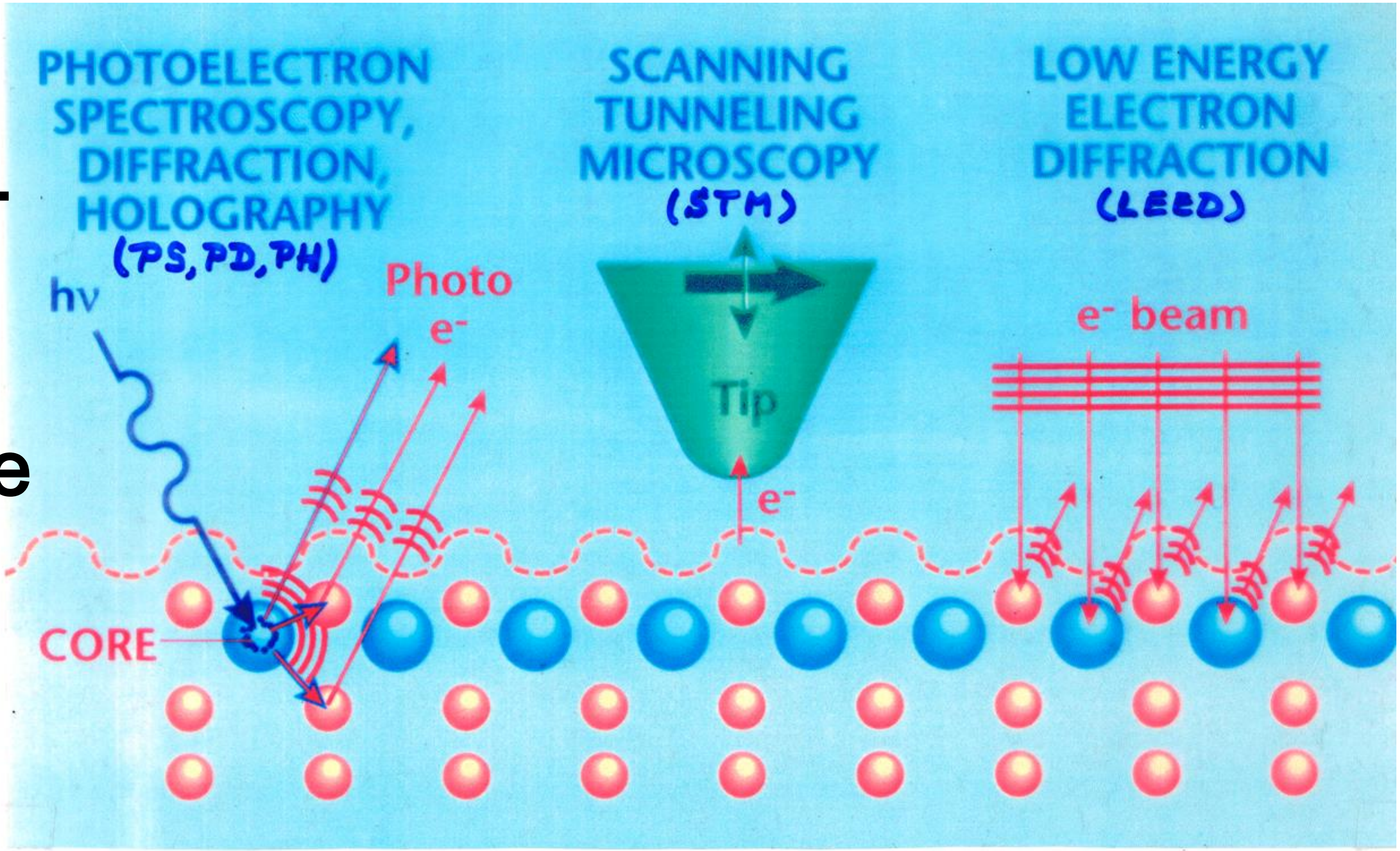
Offi et al., PRB 77, 201101R (2008)



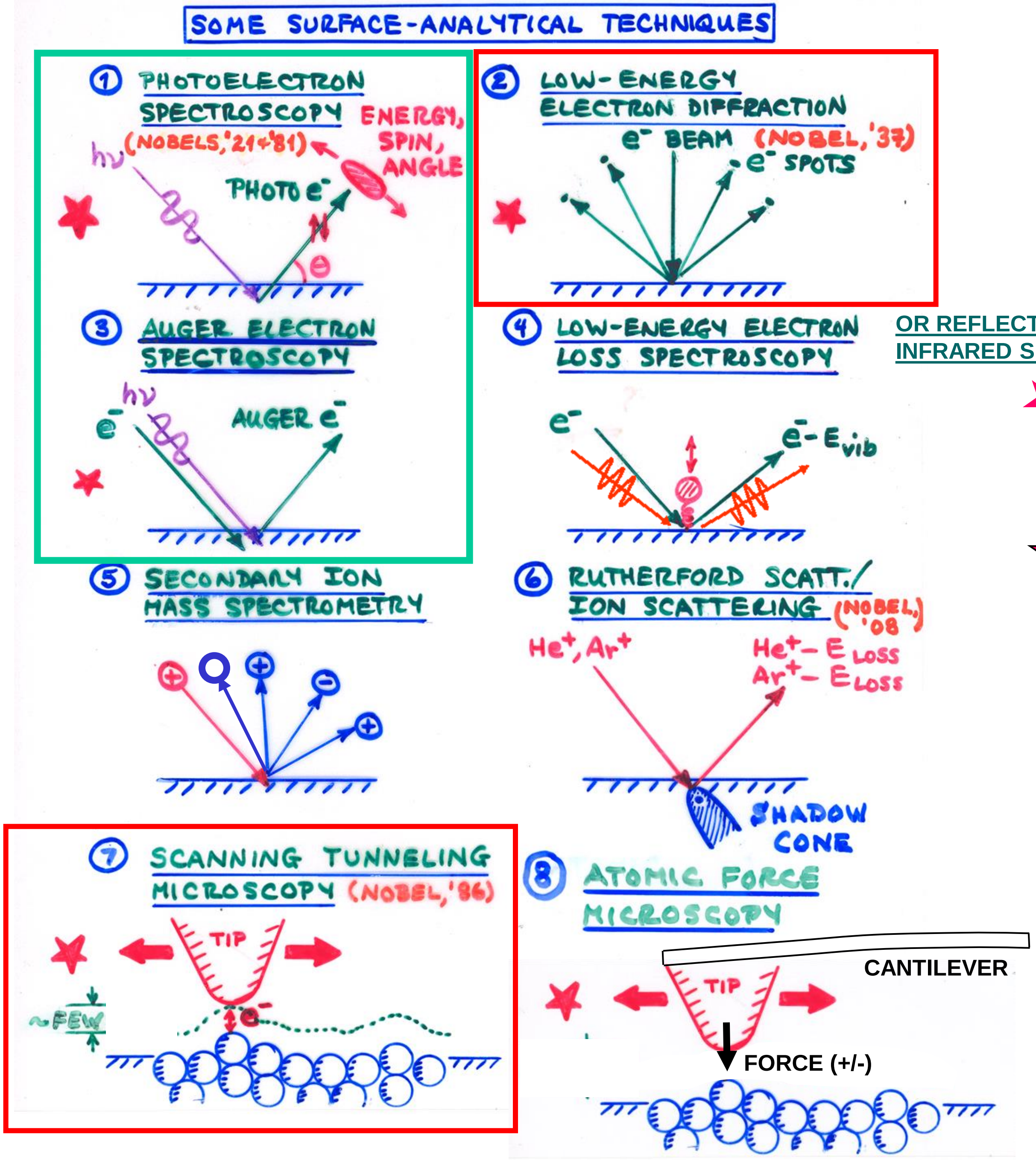
Offi et al., J. Phys.: Cond. Matt. 22 (2010) 305002

→The only certain way to obtain more bulk sensitivity

Some Complementary Surface Structure Probes



-Type of order:	Short (< 10Å)	Short, long and disorder	Long (> 100Å)
-Atom & site specific:	Yes	No	No
-Sensing depth:	5-40Å	Mostly surface D.O.S.	5-20Å
-Lateral resolution:	1 mm^2 to (300Å)^2	Single atom	1 mm^2 to 1 micron^2



CANTILEVER

FORCE (+/-)

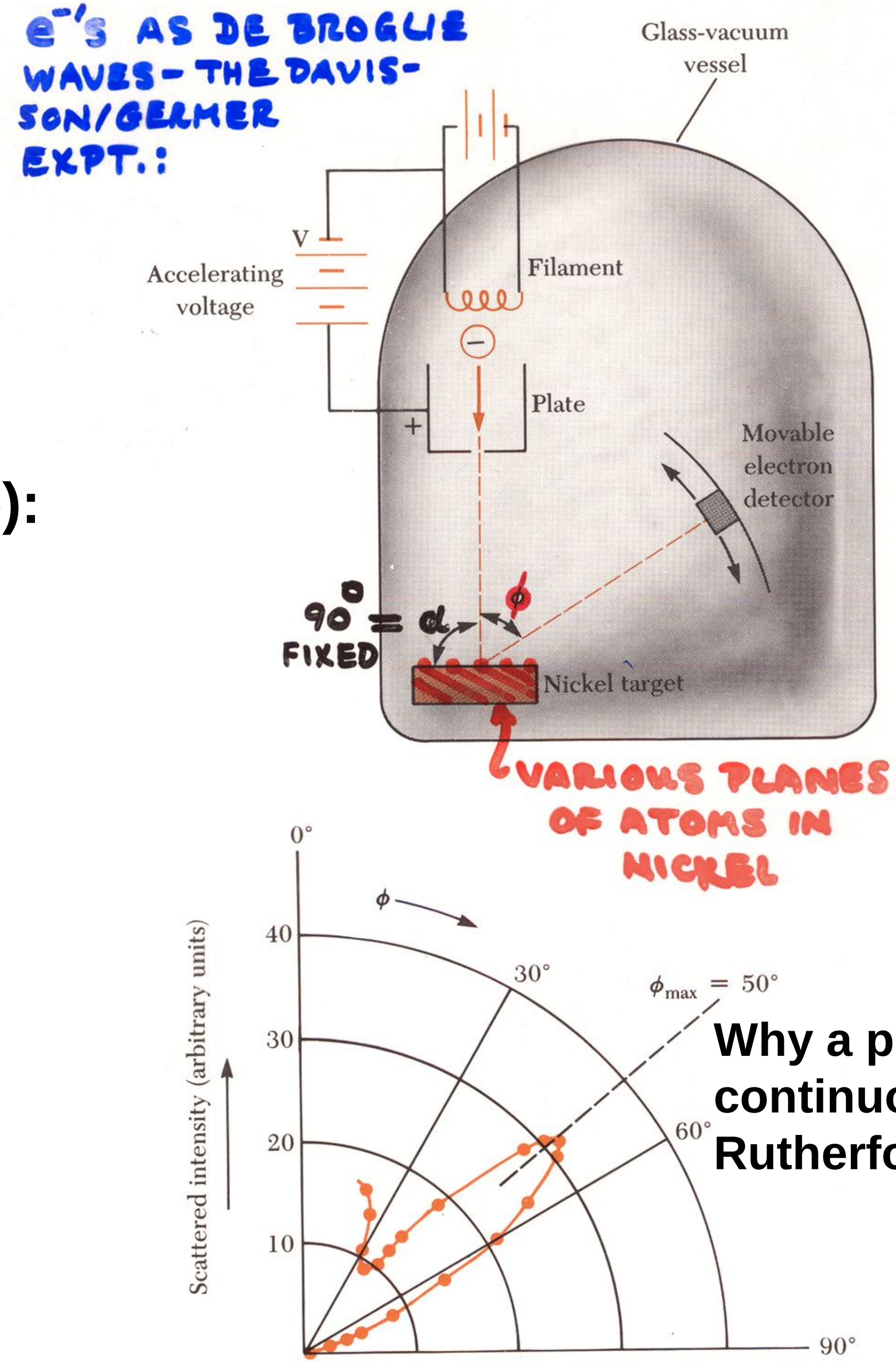
OR REFLECTION/ABSORPTION INFRARED SPECTROSCOPY

★ **= AT UC DAVIS Profs. Chiang, da Silva Neto, Fadley, Hamidian,…**

Low Energy Electron Diffraction (See Woodruff, Sections 2.6-2.7

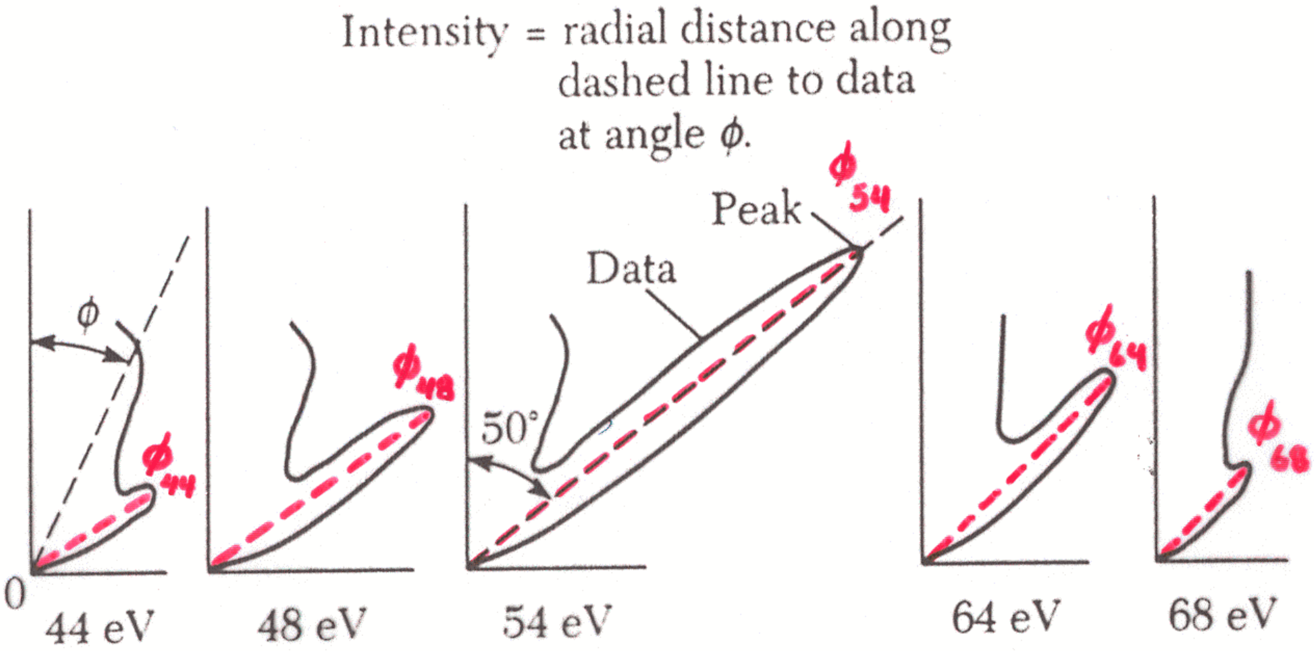
Particles behaving as waves (de Broglie):

$$\lambda = h/p$$



Why a peak and not continuous as in Rutherford scattering?

The Davison-Germer Experiment: Details



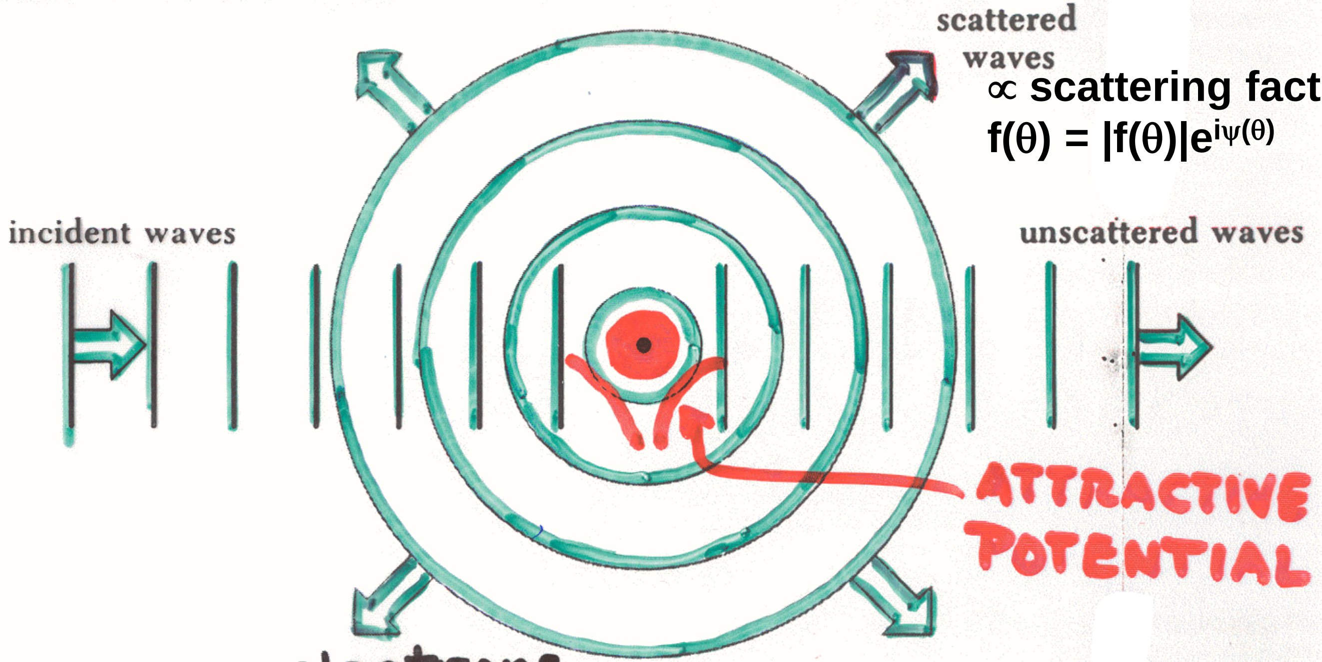
Intensity = radial distance along dashed line to data at angle ϕ.

INT. = STRONG MAXIMUM

$\phi_{44} > \phi_{48} > \phi_{54} > \phi_{64} > \phi_{68}$

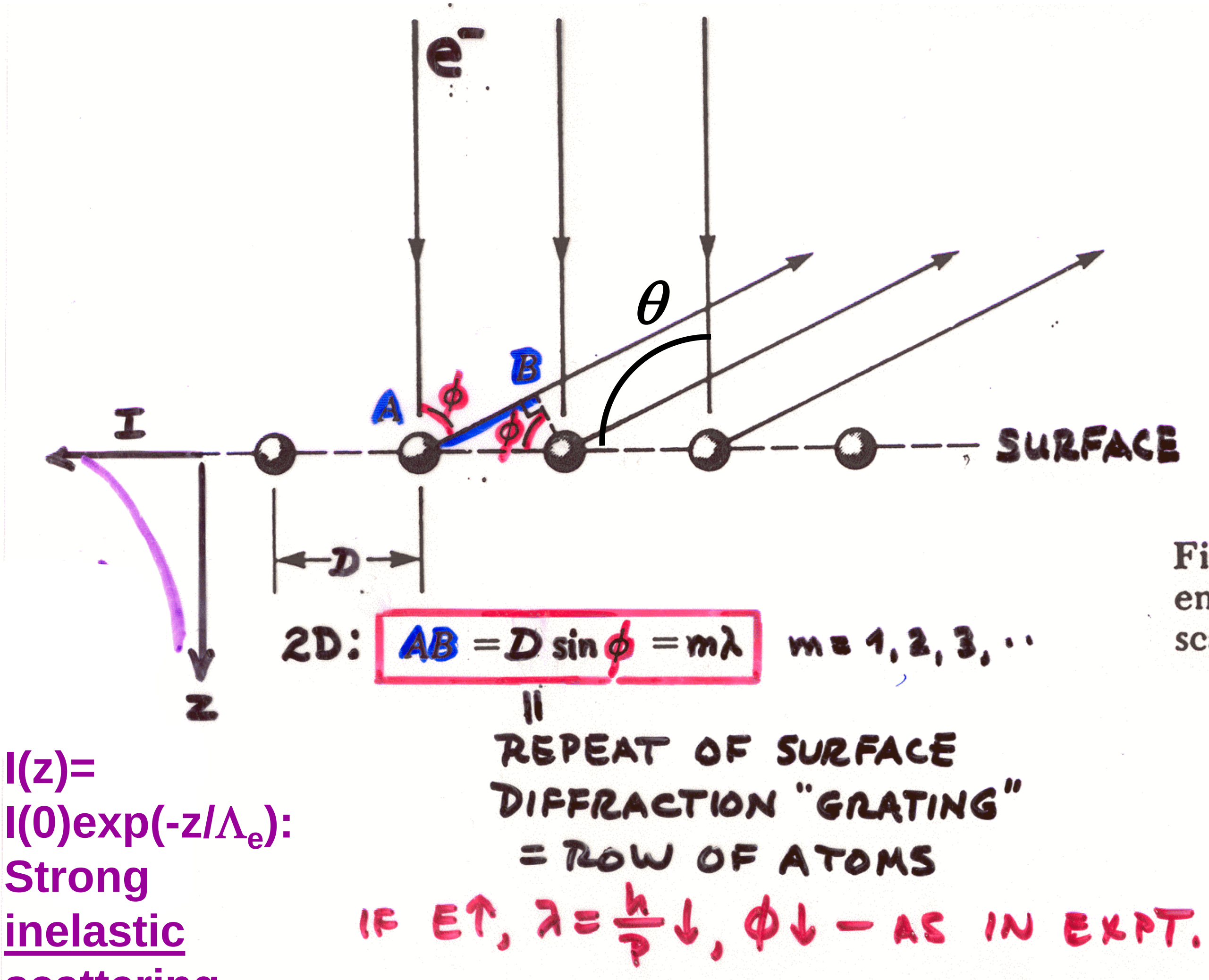
ϕ decreasing →

SCATTERING OF AN e^- BY AN ATOM:



$\propto$ **scattering factor =**
$f(\theta) = |f(\theta)|e^{i\psi(\theta)}$

FIGURE 2.15 The scattering of ~~electromagnetic radiation~~ electrons by a group of atoms. Incident plane waves are reemitted as spherical waves.



2D: $\boxed{AB = D \sin\phi = m\lambda}$ m = 1, 2, 3, ..

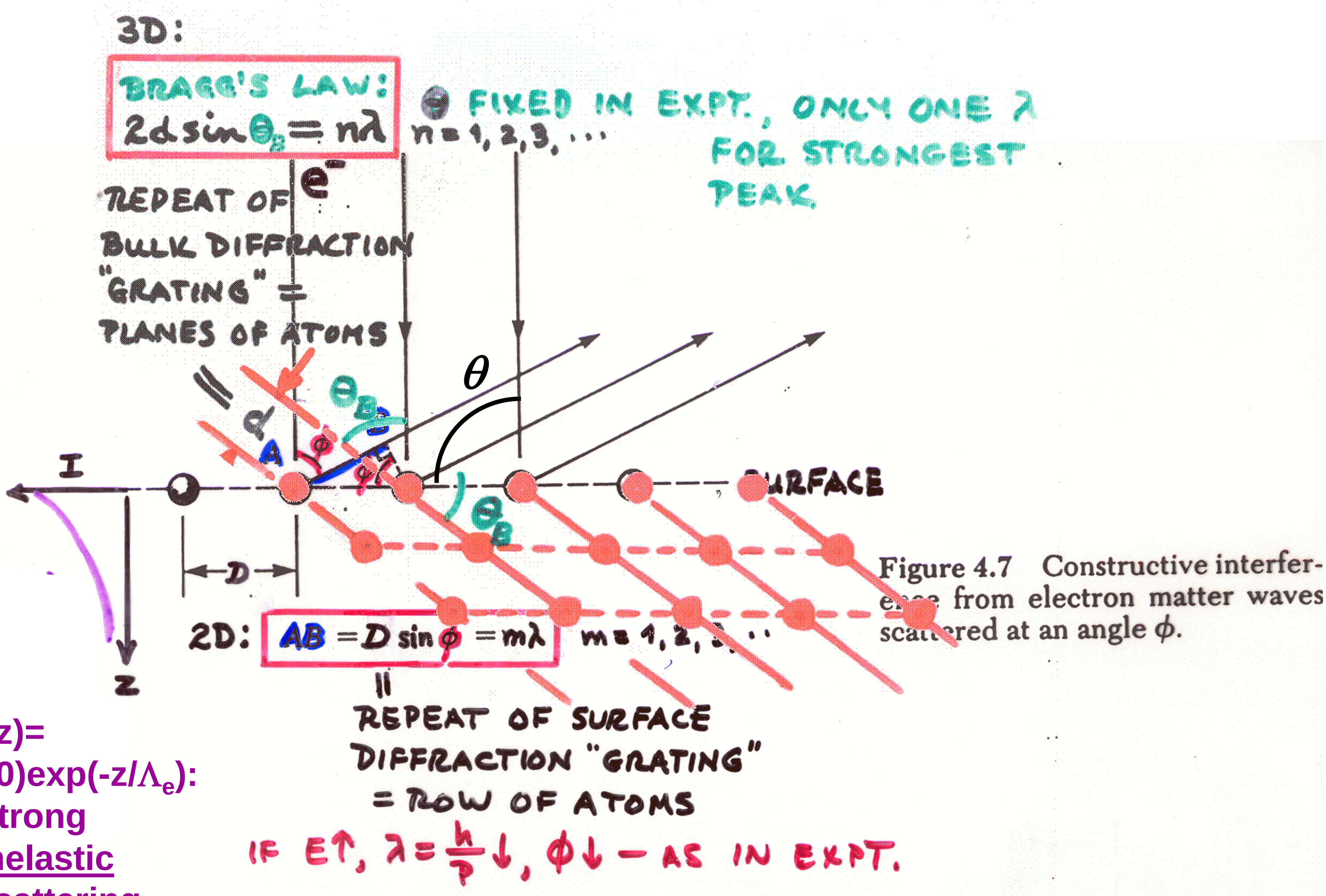
$\parallel$

REPEAT OF SURFACE DIFFRACTION "GRATING" = ROW OF ATOMS

IF E↑, $\lambda = \frac{h}{p}$↓, φ↓ — AS IN EXPT.

Figure 4.7 Constructive interference from electron matter waves scattered at an angle ϕ.

$I(z) = I(0)\exp(-z/\Lambda_e)$: Strong <u>inelastic</u> scattering attenuation



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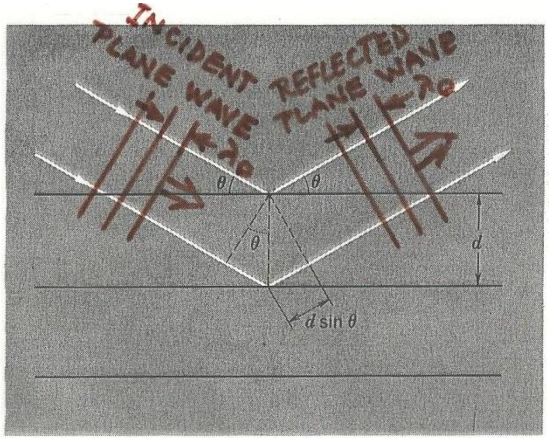
$I(z) = I(0)\exp(-z/\Lambda_e)$: Strong <u>inelastic</u> scattering attenuation

Bragg's Law in 3D and crystal planes



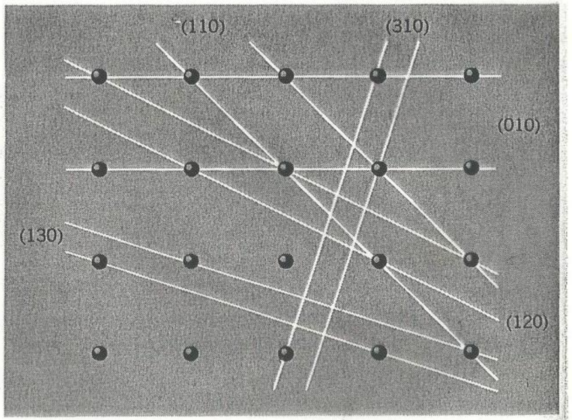


Figure 2 Derivation of the Bragg equation $2d\sin\theta = n\lambda$; here d is the spacing of parallel atomic planes and $2n\pi$ is the difference in phase between reflections from successive planes. What do we mean by a set of parallel reflecting planes? Any set of parallel planes will do, provided each plane passes through at least three non-colinear lattice points! See Fig. 3 for several examples. *The reflecting planes have nothing to do with the surface planes bounding the particular specimen,* because the x-rays or neutrons see all!

Figure 3 Several types of reflecting planes in a simple cubic crystal lattice. The planes shown are labeled by their Miller indices. We have shown in each case a set of two parallel planes. The closest distance between parallel planes tends to decrease as the indices increase; thus high index reflections require shorter wavelengths. In principle the number of different types of reflecting planes is unlimited if the crystal is infinite.

CONSTRUCTIVE INTERFERENCE
BETWEEN PLANES FOR:

$$\boxed{\underset{1,2,3,\dots}{n}\lambda_0 = 2\underset{d_{hkl}}{d}\sin\theta}$$ — BRAGG'S LAW

$$\lambda_0 \leq 2d$$

TRANSLATIONAL SYMMETRY IN BULK SOLIDS: 14 basic types

Good websites/downloads for simple structures:

http://www.dawgsdk.org/crystal/en/library/fcc#0002

http://demonstrations.wolfram.com/CrystalViewer/

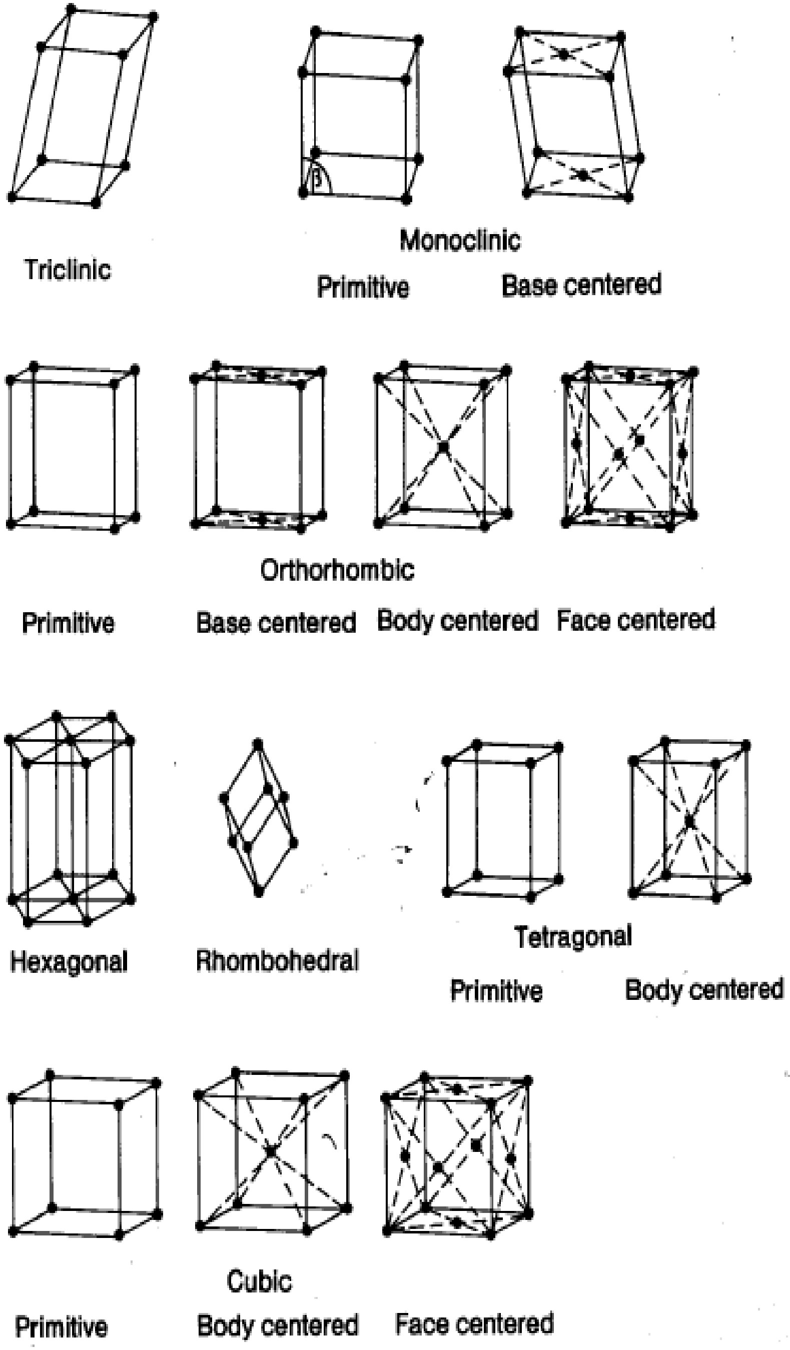
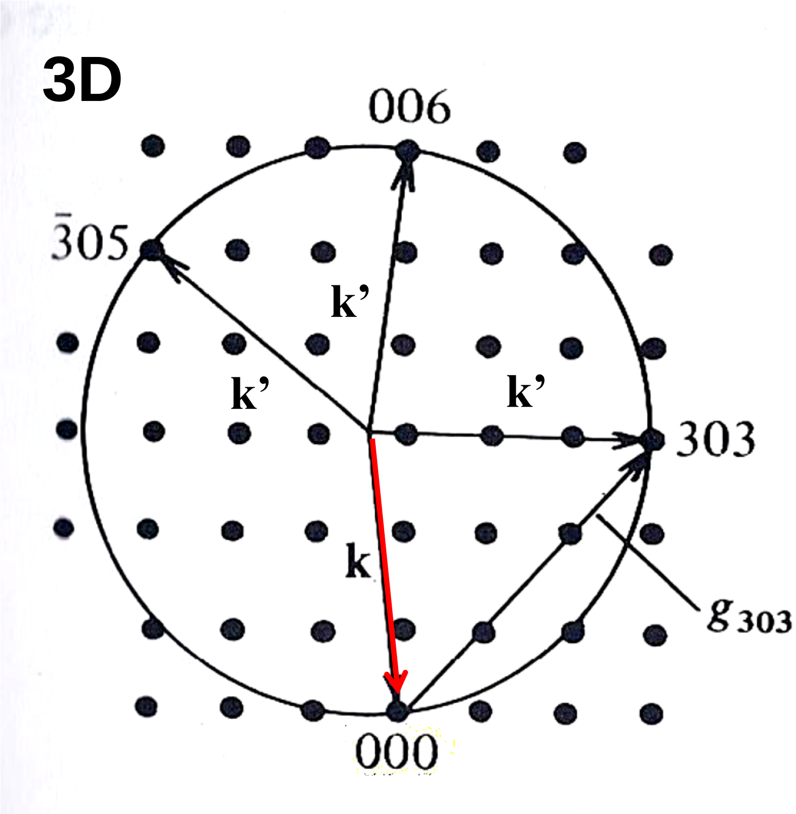


Fig. 2.3. The 14 three-dimensional Bravais lattices. The hexagonal lattice and the two centered cubic lattices are particularly important in solid state physics

Bragg’s Law, the Reciprocal Lattice and the Ewald Sphere Construction in 3D and 2D



$\vec{a}, \vec{b}$, and $\vec{c}$ are primitive (non-centered) unit cell vectors

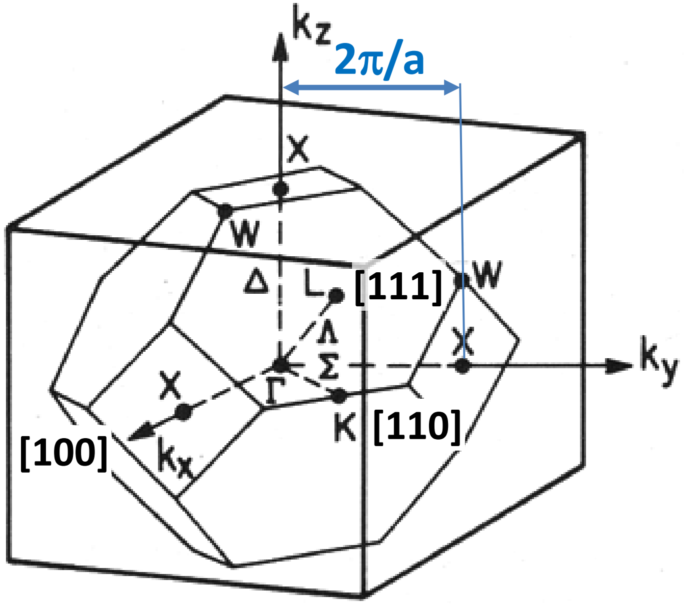
Elastic scattering: $|\vec{k}'| = |\vec{k}|$

$\vec{k}' = \vec{k} + \vec{g}_{hkl}$, with

$\bar{g}_{hkl} = h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^*$

$\vec{a}^* = 2\pi \frac{\vec{b}x\vec{c}}{V}$, $b^* = 2\pi \frac{\vec{c}x\vec{a}}{V}$, $c^* = 2\pi \frac{\vec{a}x\vec{b}}{V}$, $V = \vec{a} \bullet \vec{b} x \vec{c}$

Reciprocal lattice vectors and 1st Brillouin zone for the bulk fcc lattice: Bounded by planes halfway to nearest recip. lattice point

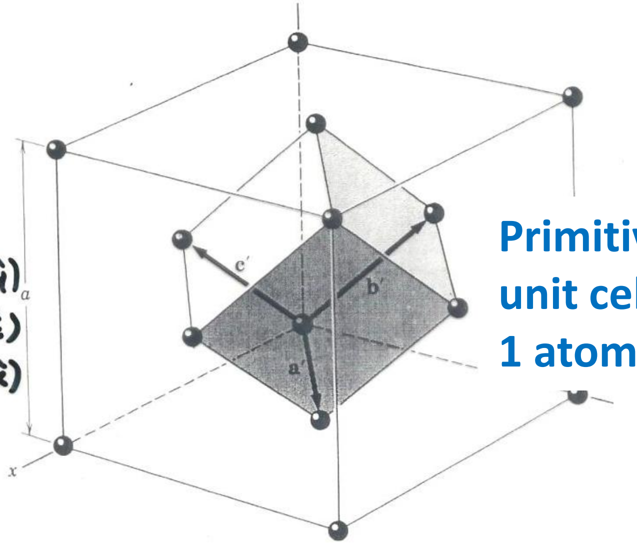


PRIMITIVE

$\bar{a}' = \frac{1}{2}a(\hat{x}+\hat{y})$

$\bar{b}' = \frac{1}{2}a(\hat{y}+\hat{z})$

$\bar{c}' = \frac{1}{2}a(\hat{z}+\hat{x})$



Real fcc

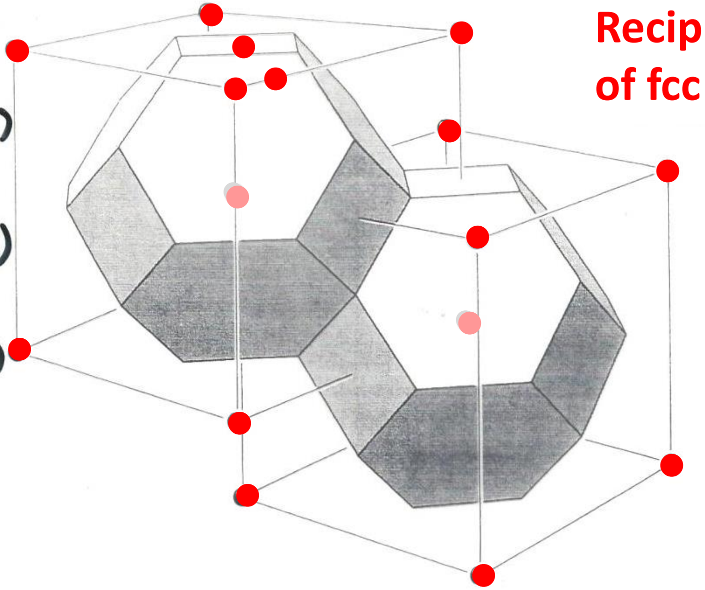
Primitive unit cell: 1 atom

PRIMITIVE

$\bar{a}^* =$
$\frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

$\bar{b}^* =$
$\frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$

$\bar{c}^* =$
$\frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$



Reciprocal of fcc = bcc

Figure 28 Brillouin zones of the face-centered cubic lattice. The cells are in reciprocal space, and the reciprocal lattice is body-centered, as drawn.

TRANSLATIONAL SYMMETRY AT SURFACES: 5 basic types

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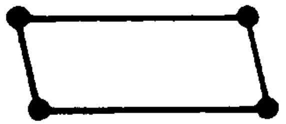
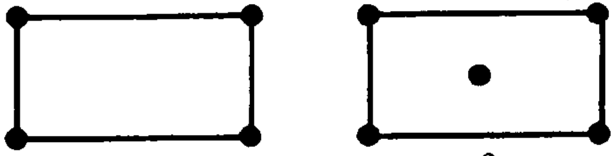
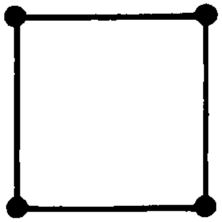

Oblique

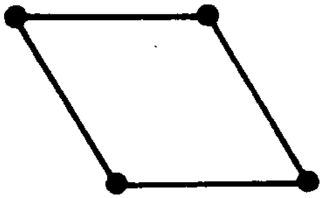


Rectangular

p = primitive

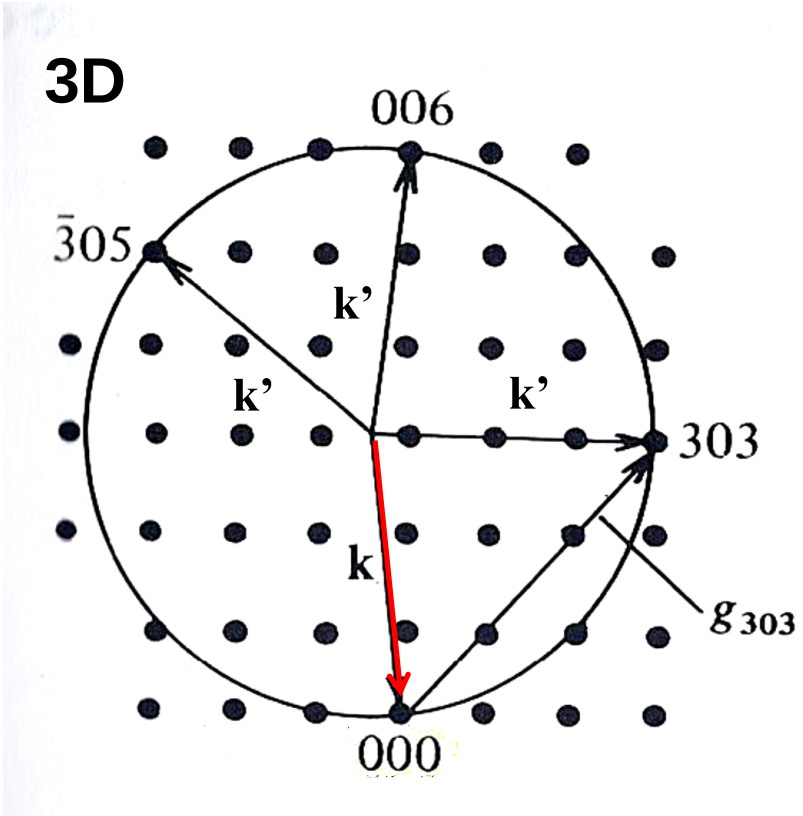
c = centered


Square


Hexagonal

+ Various visualizations of crystal surfaces at: http://www.fhi-berlin.mpg.de/~hermann/Balsac/pictures.html

Bragg's Law, the Reciprocal Lattice and the Ewald Sphere Construction in 3D and 2D



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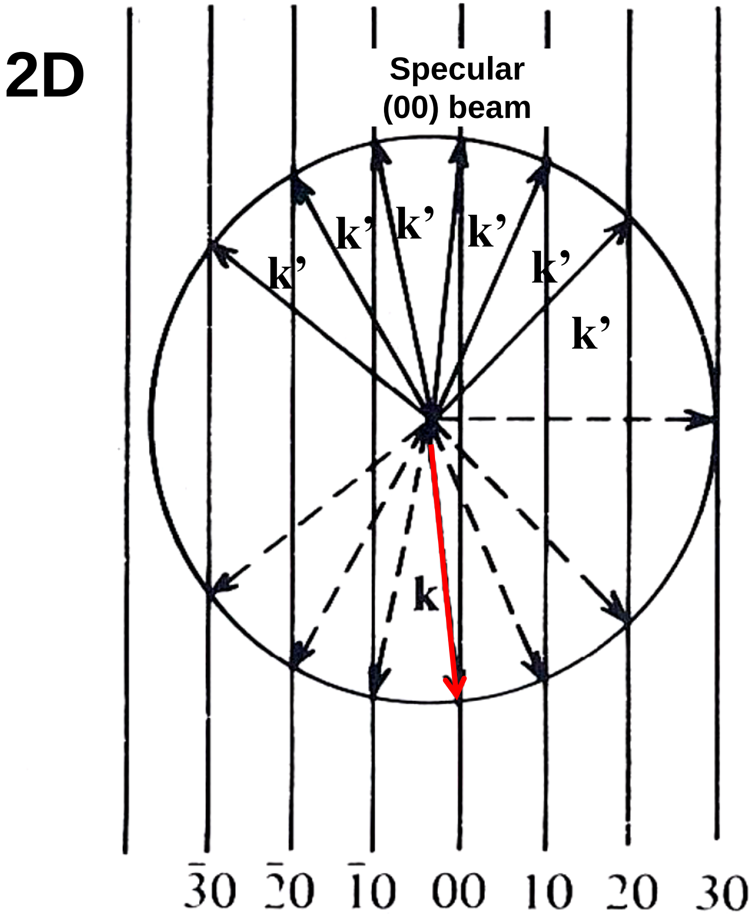
$\vec{k}' = \vec{k} + \vec{g}_{hkl}$, with

$\vec{g}_{hkl} = h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^*$

$$\vec{a}^*=2\pi\frac{\vec{b}x\vec{c}}{V},\ b^*=2\pi\frac{\vec{c}x\vec{a}}{V},c^*=2\pi\frac{\vec{a}x\vec{b}}{V}\ ,\ V=\vec{a}\bullet\vec{b}x\vec{c}$$



$\vec{a}$ and $\vec{b}$ are primitive (non-centered) unit cell vectors

$\hat{n}$ is unit vector along surface normal

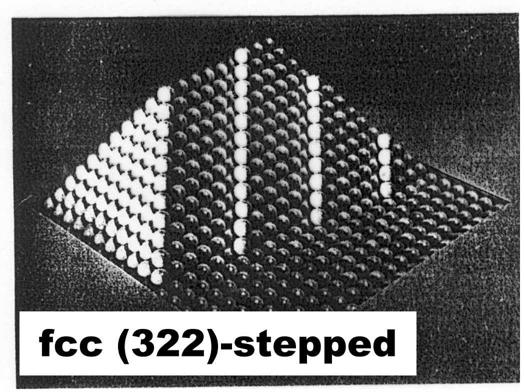
Elastic scattering: $|\vec{k}'|=|\vec{k}|$

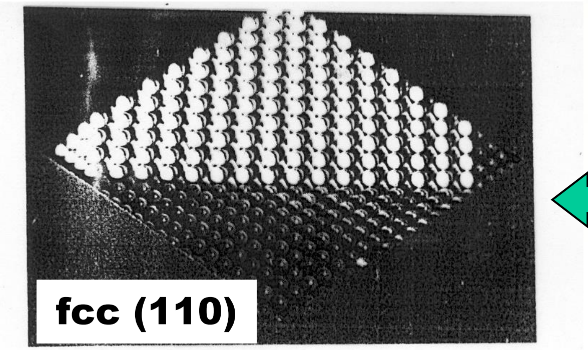
$\vec{k}_{\parallel}' = \vec{k}_{\parallel} + \vec{g}_{hk}$, with

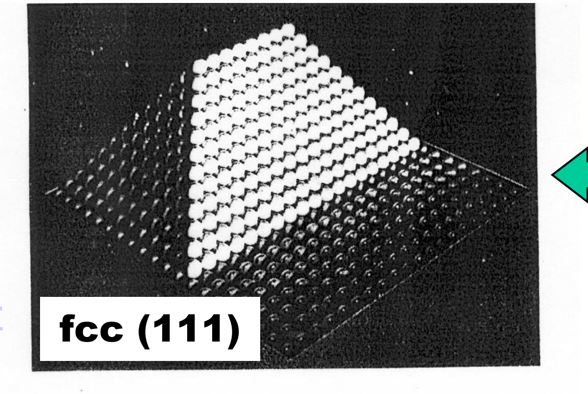
$\vec{g}_{hk} = h\vec{a}^* + k\vec{b}^*$

$$\vec{a}^*=2\pi\frac{\vec{b}\ x\ \hat{n}}{A},\ \vec{b}^*=2\pi\frac{\hat{n}\ x\ \vec{a}}{A},\ A=\vec{a}\bullet\vec{b}\ x\ \hat{n}$$

WHAT DO SURFACES LOOK LIKE?
SOME fcc AND bcc SURFACES

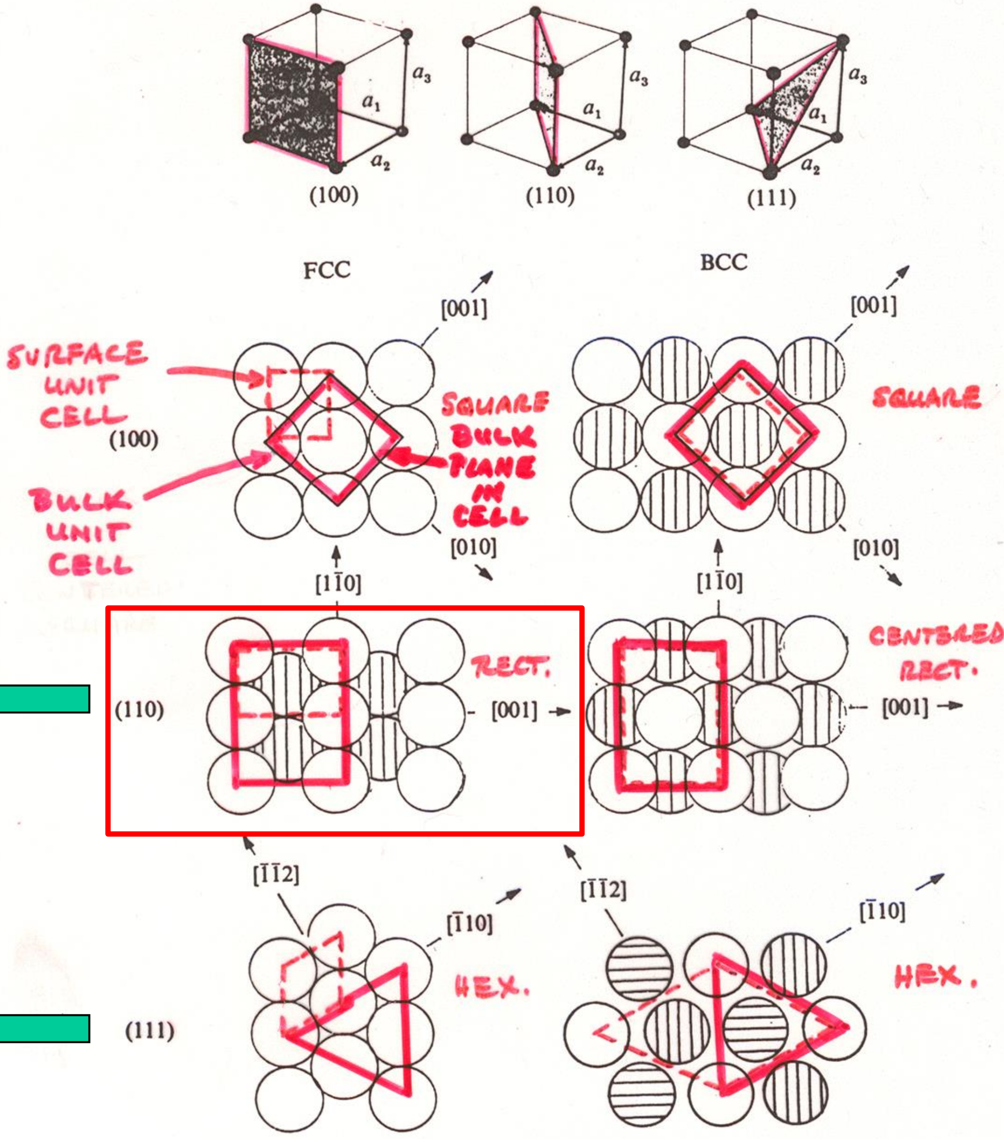

fcc (322)-stepped


fcc (110)

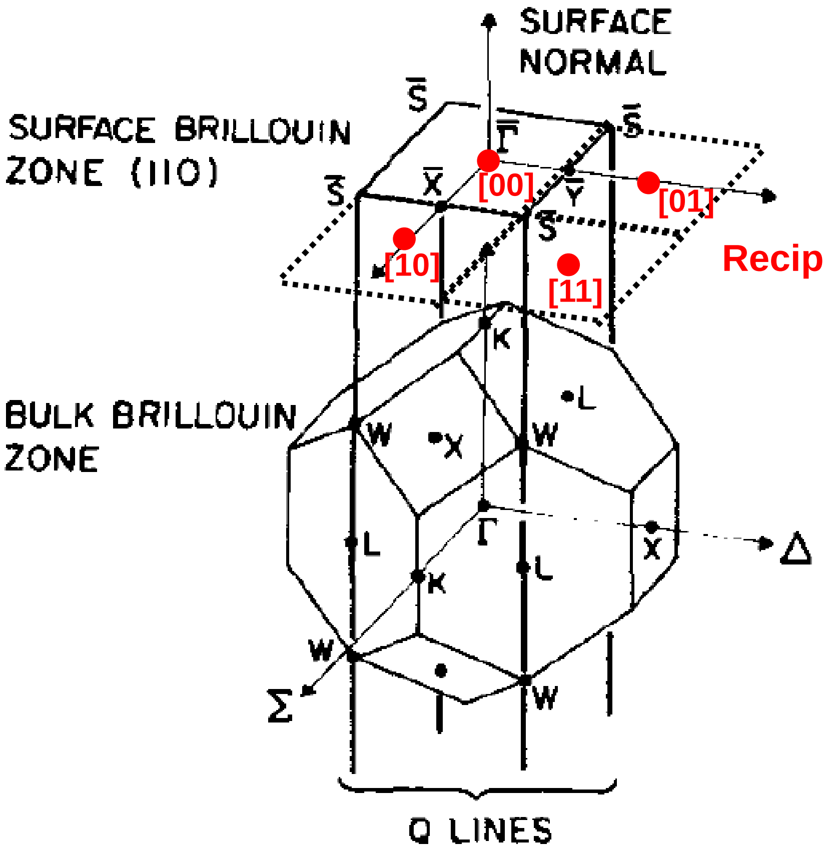

fcc (111)

+ Various visualizations of crystal surfaces at: http://www.fhi-berlin.mpg.de/~hermann/Balsac/pictures.html

Fig. 3.2. Low-index ideal surfaces of a hard-sphere cubic crystal. Vertical and horizontal markings indicate the second and third atom layers, respectively. Cube face is indicated for (100) to set the scale (Nicholas, 1965).



Reciprocal lattice vectors and 1st Brillouin zone for the bulk and (110) fcc lattice



Reciprocal lattice vectors

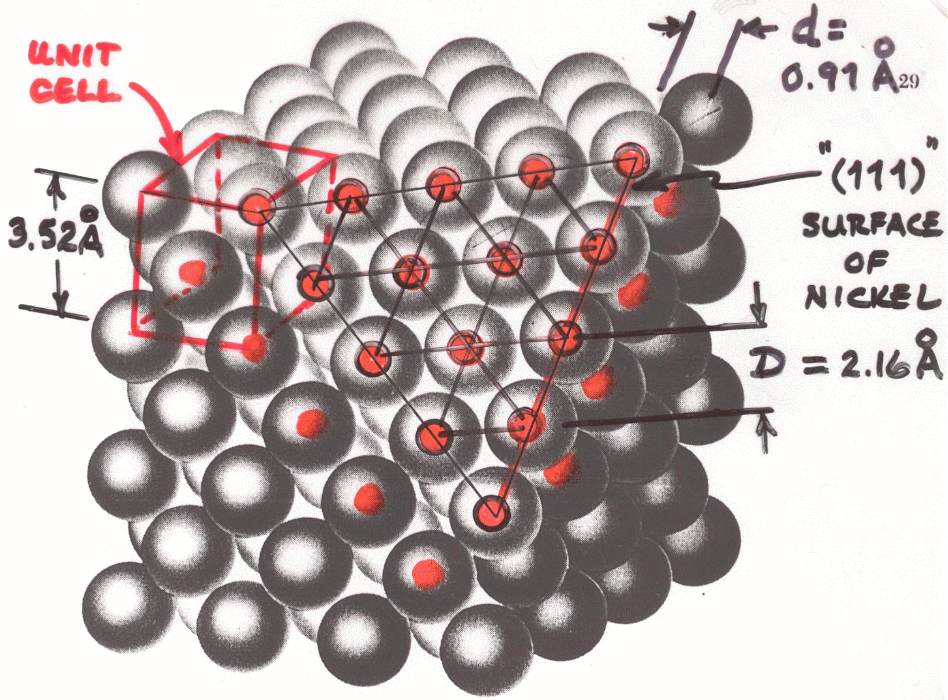


Figure 27b The fcc structure with one corner sliced off to expose a (111) plane. The (111) planes are close-packed layers of spheres. (After W. G. Moffatt, G. W. Pearsall, and J. Wulff, *Structure*, Vol. 1 of *Structure and properties of materials*, Wiley, 1964.)

E.G.: e^-'s @ 54eV

$$\lambda = \frac{h}{p} = 1.67\,\text{Å}$$

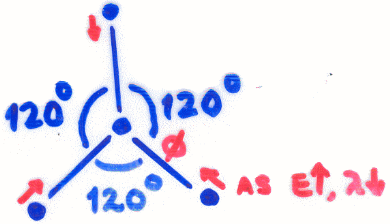
3D: $$\sin\theta_B = \frac{\lambda}{2d} = \frac{1.67}{2(0.91)}$$

$$\theta_B = 66.6°$$

$$\phi = \pi - 2\theta_B = 46.8°$$

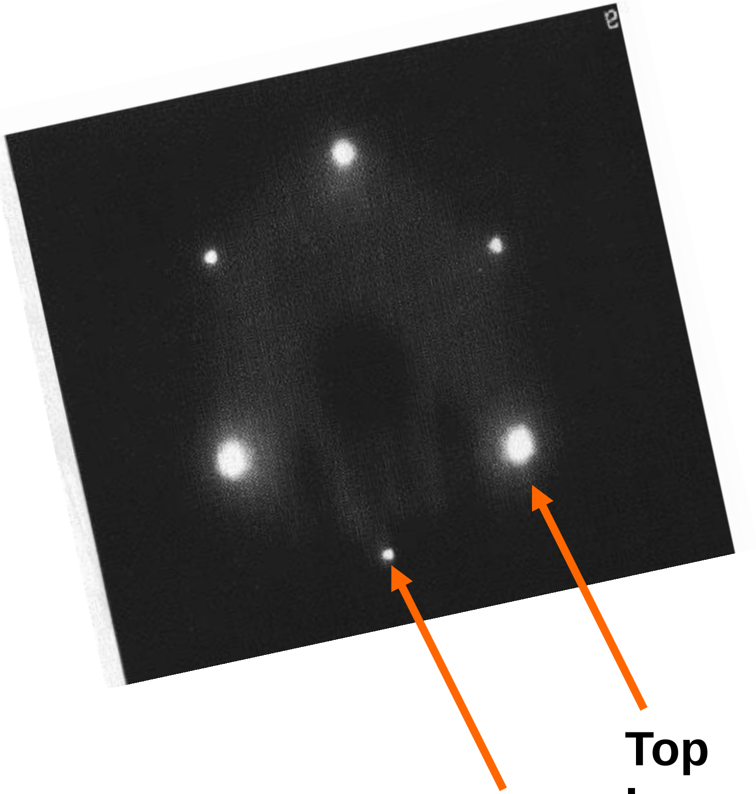
$$\approx 50° \text{ (EXPT.)}$$

⇓ IN DAVISSON-GERMER EXPT.



3 SETS OF ROWS "D" GIVE 3 SETS OF 2D MAXIMA

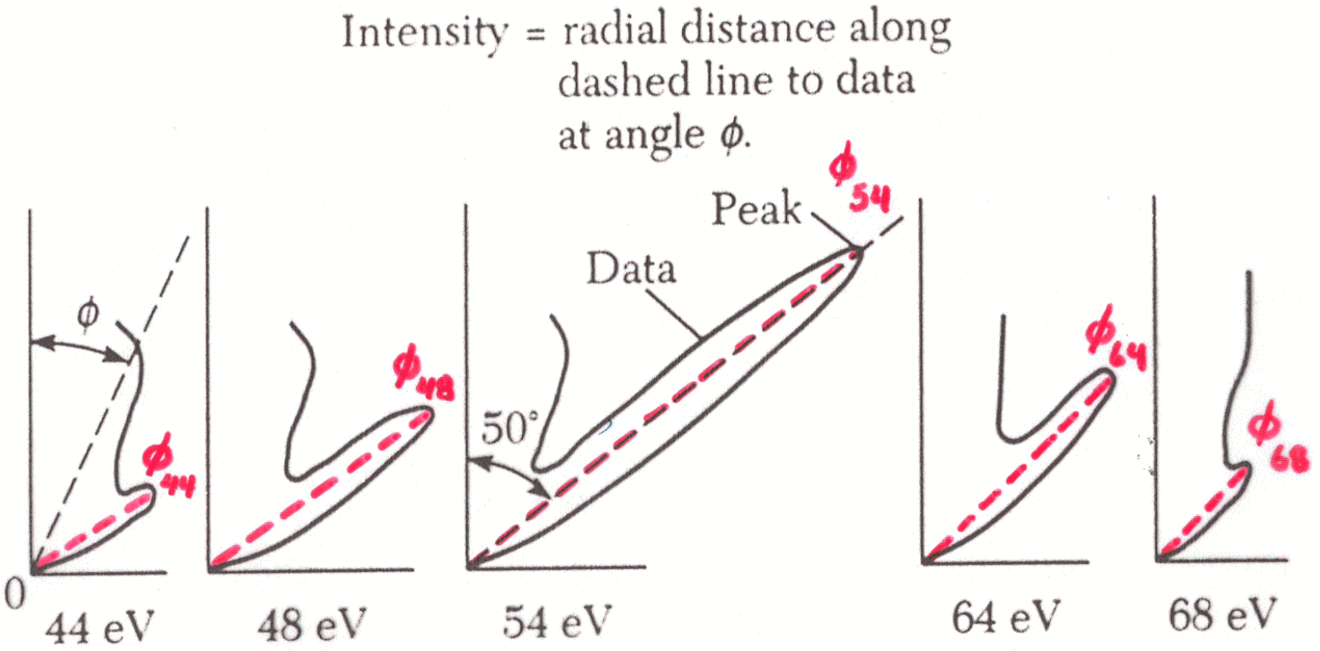
The experimental pattern from Ni(111)



Second layer rows (attenuated)

Top layer rows

The Davison-Germer Experiment: Details Explained



INT. = STRONG MAXIMUM

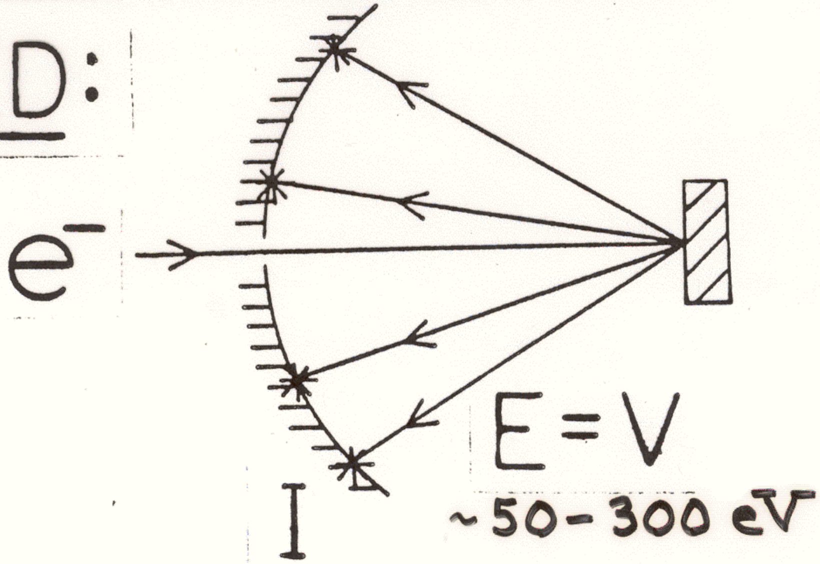
3D: $2d\sin\theta_B = n\lambda$ -

2D: $d_s\sin\phi = m\lambda$ - $\phi_{44} > \phi_{48} > \phi_{54} > \phi_{64} > \phi_{68}$

$(n=1,\ m=1)$

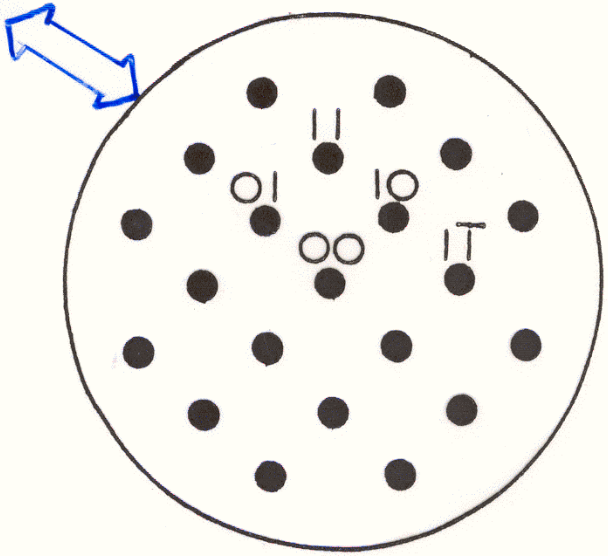
LOW ENERGY ELECTRON DIFFRACTION =

LEED:

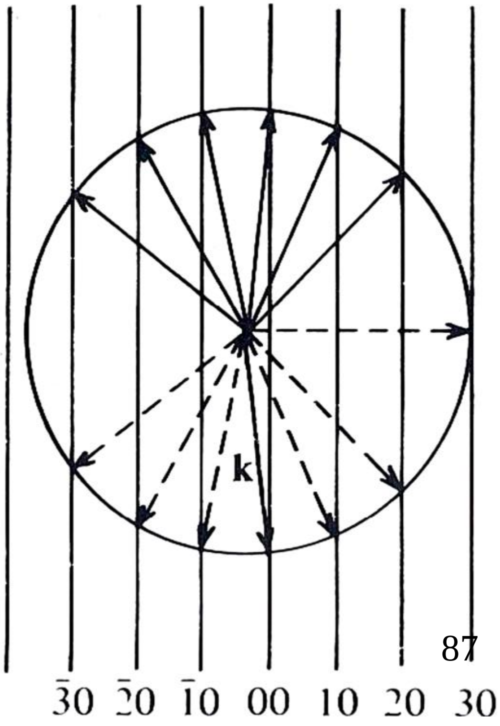


~50-300 eV

TWO-DIMENSIONAL SURFACE RECIPROCAL LATTICE

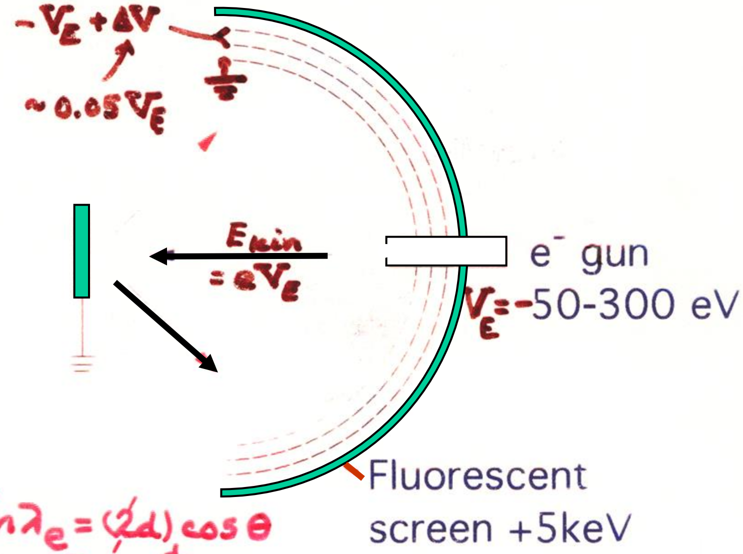


LONG-RANGE ORDER REQUIRED OVER ≳ 100Å.



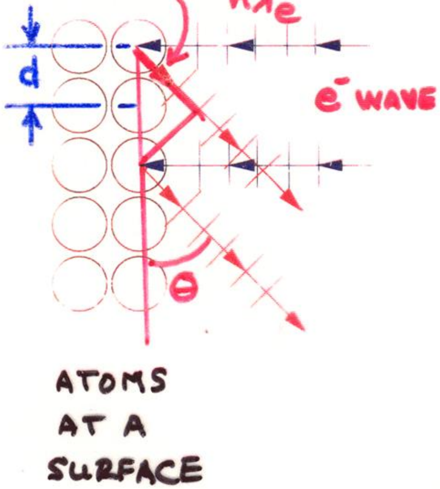
Low Energy Electron Diffraction

DAVISSON & GERMER REVISITED



$\cancel{2}n\lambda_e = (\cancel{2}d)\cos\theta$

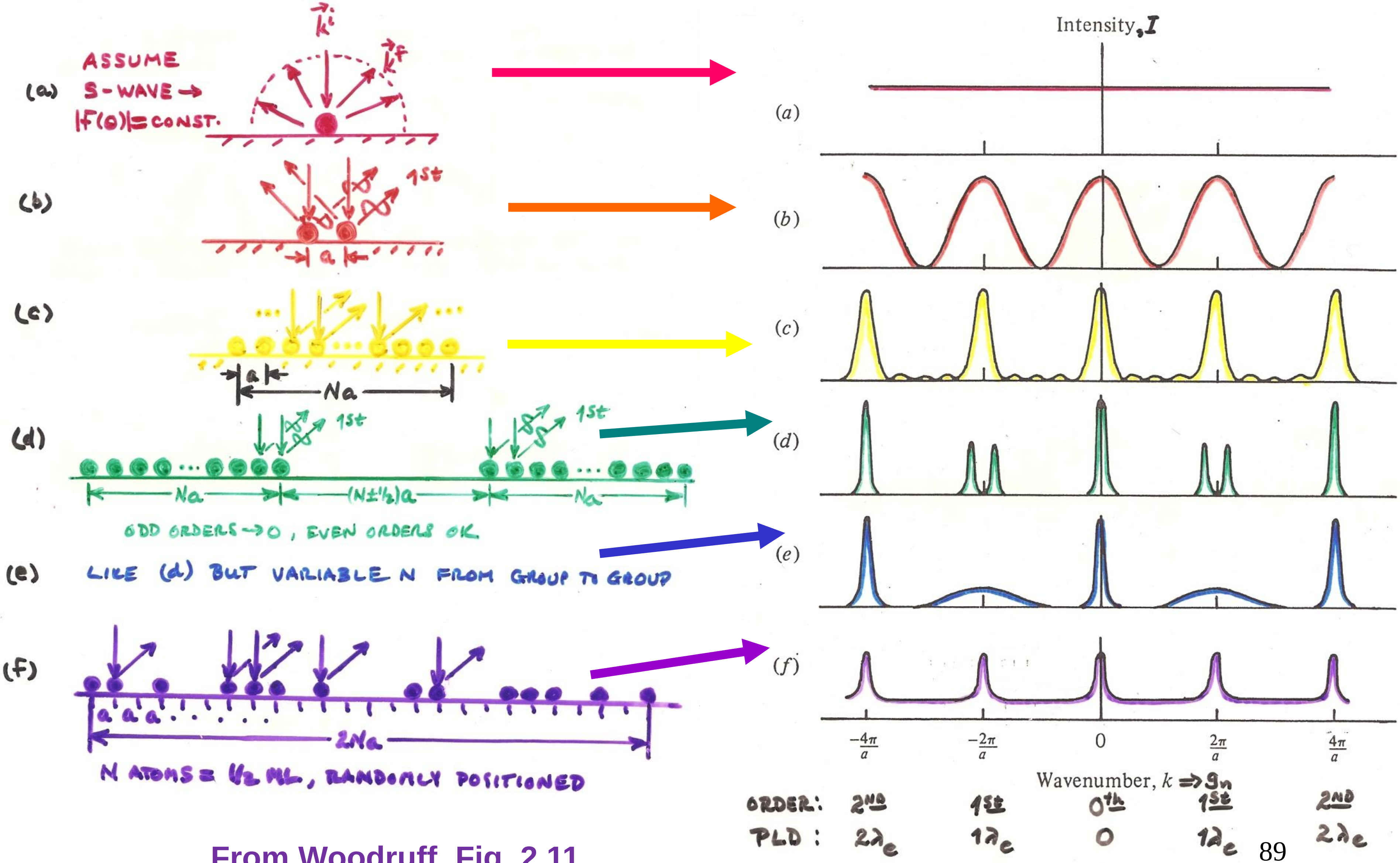
$\cos\theta = \frac{d}{n\lambda_e}$



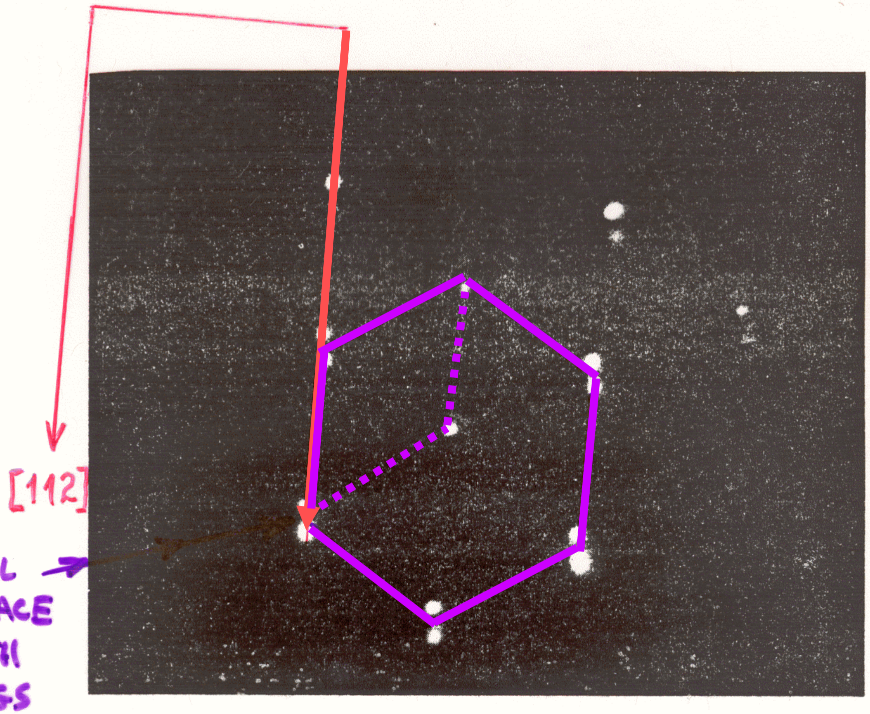
λ_e = 1.7 - 0.7 Å $= \frac{h}{P}$

LEED yields two-dimensional surface reciprocal lattice = two-dimensional atomic diffraction gratings – usually requires long-range order ≳ 100 Å

ELECTRON DIFFRACTION IN 2D FROM LINEAR (1D) ARRAYS OF ATOMS:



From Woodruff, Fig. 2.11



HEXAGONAL (111) TERRACE SPOTS WITH SPLITTINGS DUE TO LONG-PERIOD STEPS

Figure 1.36. *Diffraction pattern of a platinum crystal face that was cut 6°27′ with respect to the (111) crystal face in the direction of the (110) face. Note the doubling of the diffraction spots.*

Pt(stepped) – 5(111) × (100)

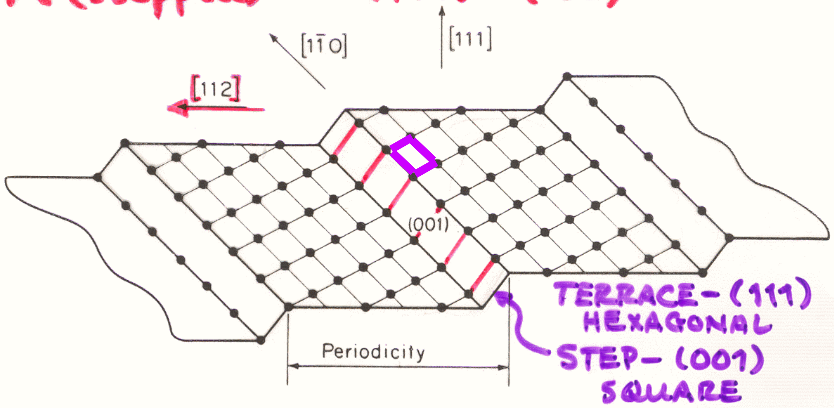
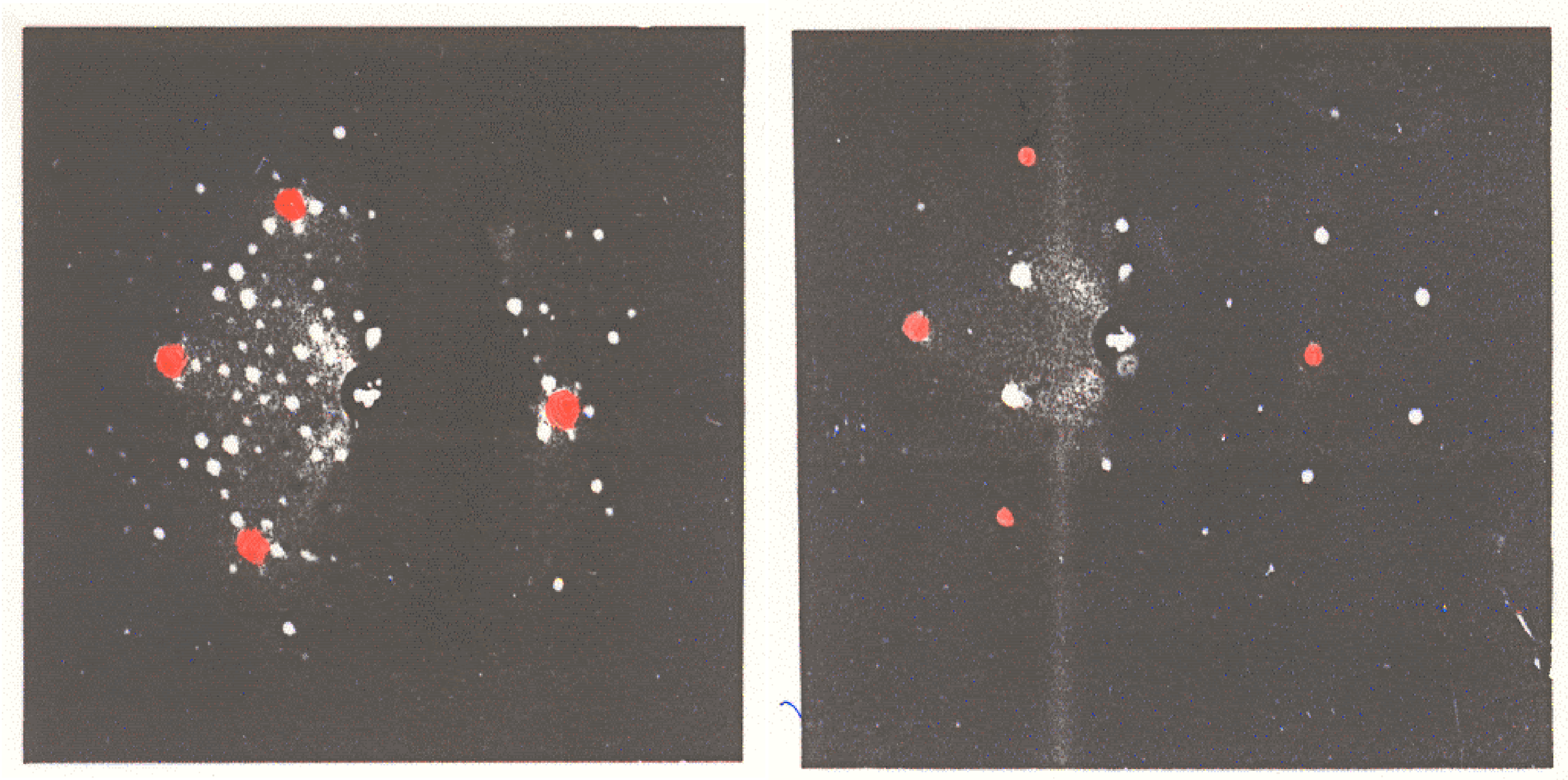


Figure 1.37. *Schematic representation of the platinum surface that exhibits ordered atomic steps.*

SOME TYPICAL LEED PATTERNS:

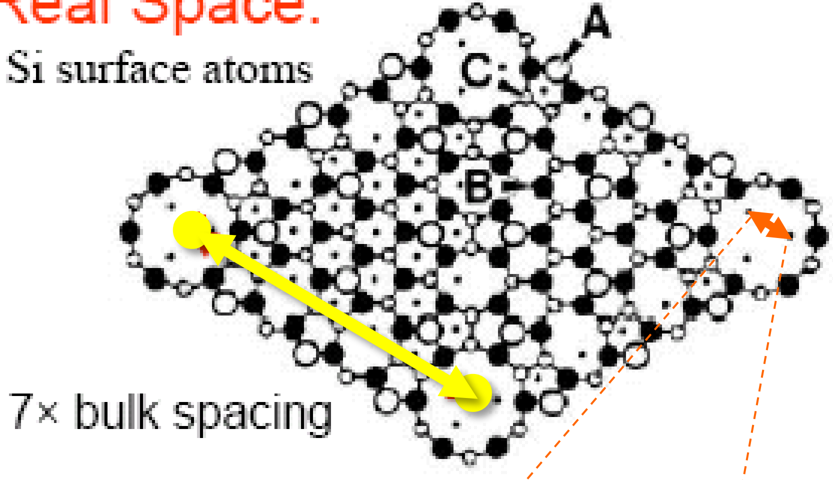


Si(111)-(7x7) (√3 x √3)R30° Ag/Si(111)

● = spots seen without any reconstruction or adsorption of simple Si(111) surface

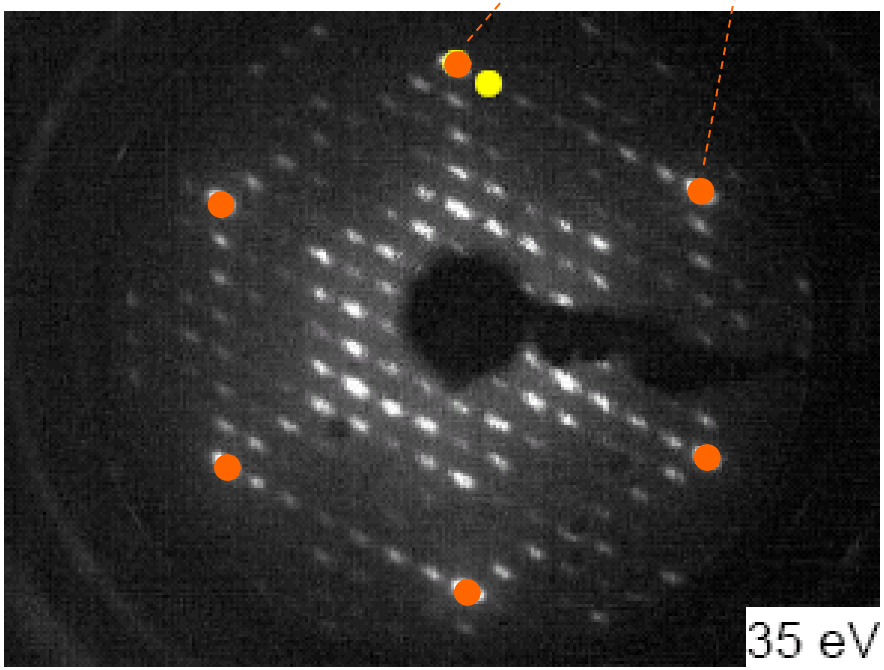
LEED: Si(111)7x7

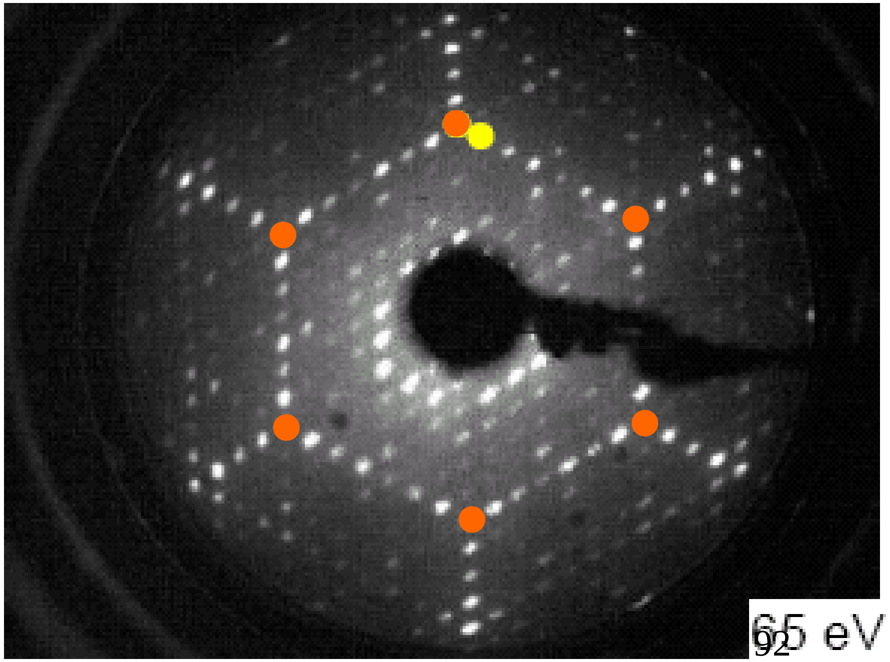
Real Space:



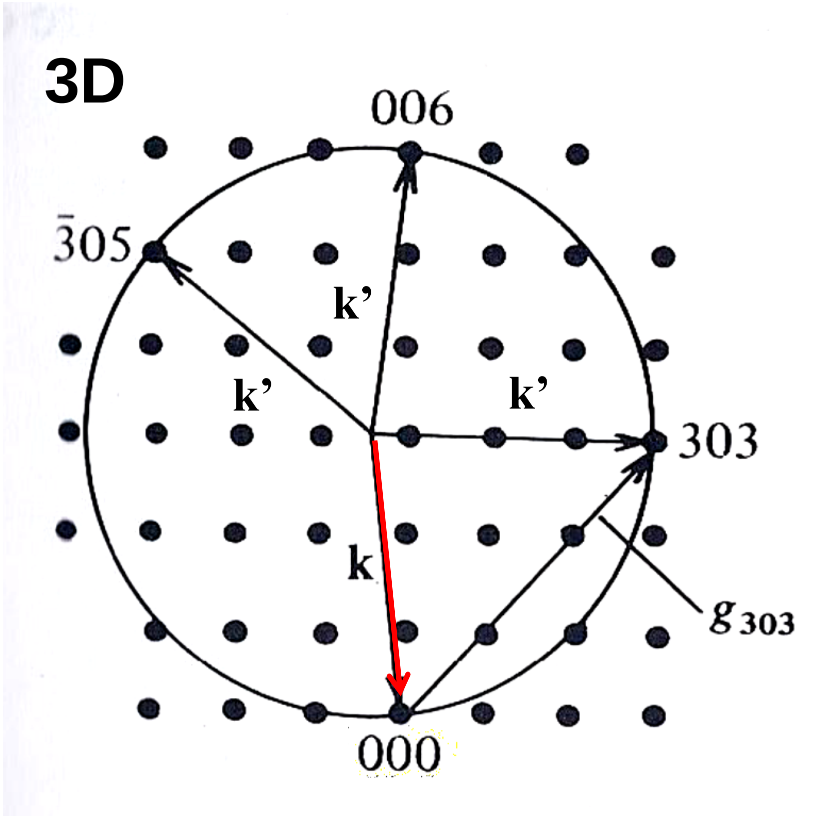
- Longer periodicities in real space give closer spots in k-space.
- Higher energy LEED images show spots closer together.

K-Space





Bragg's Law, the Reciprocal Lattice and the Ewald Sphere Construction in 3D and 2D



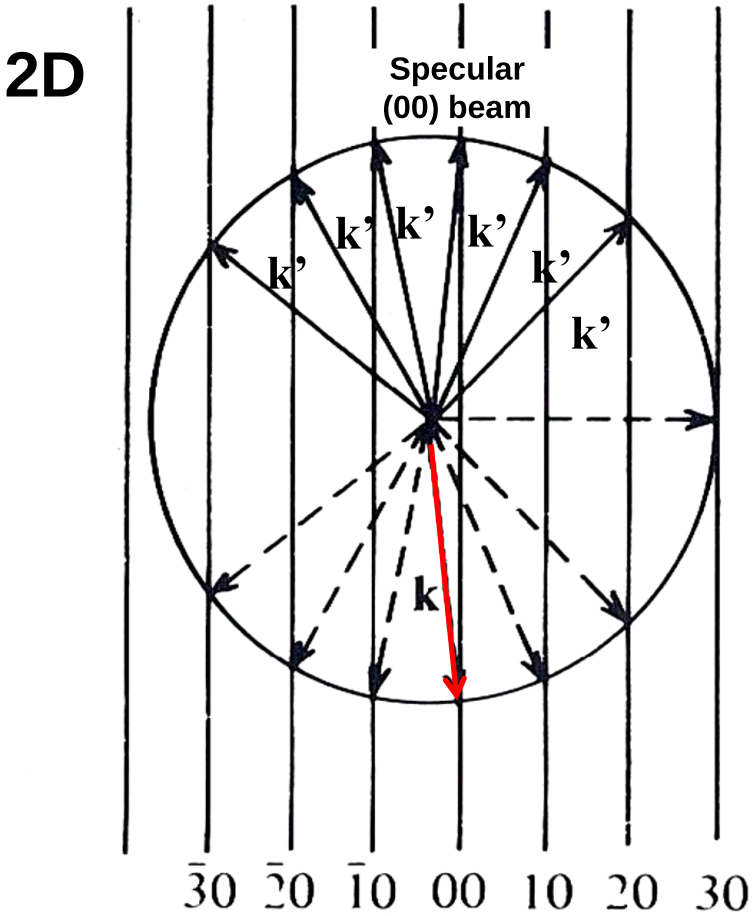
$\vec{a}, \vec{b}$, and $\vec{c}$ are primitive (non-centered) unit cell vectors

Elastic scattering: $|\vec{k}'|=|\vec{k}|$

$\vec{k}' = \vec{k} + \vec{g}_{hkl}$***, with***

$\vec{g}_{hkl} = h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^*$

$\vec{a}^* = 2\pi\frac{\vec{b}x\vec{c}}{V}$, $b^* = 2\pi\frac{\vec{c}x\vec{a}}{V}$, $c^* = 2\pi\frac{\vec{a}x\vec{b}}{V}$, $V=\vec{a}\bullet\vec{b}x\vec{c}$



$\vec{a}$ and $\vec{b}$ are primitive (non-centered) unit cell vectors

$\hat{n}$ is unit vector along surface normal

Elastic scattering: $|\vec{k}'|=|\vec{k}|$

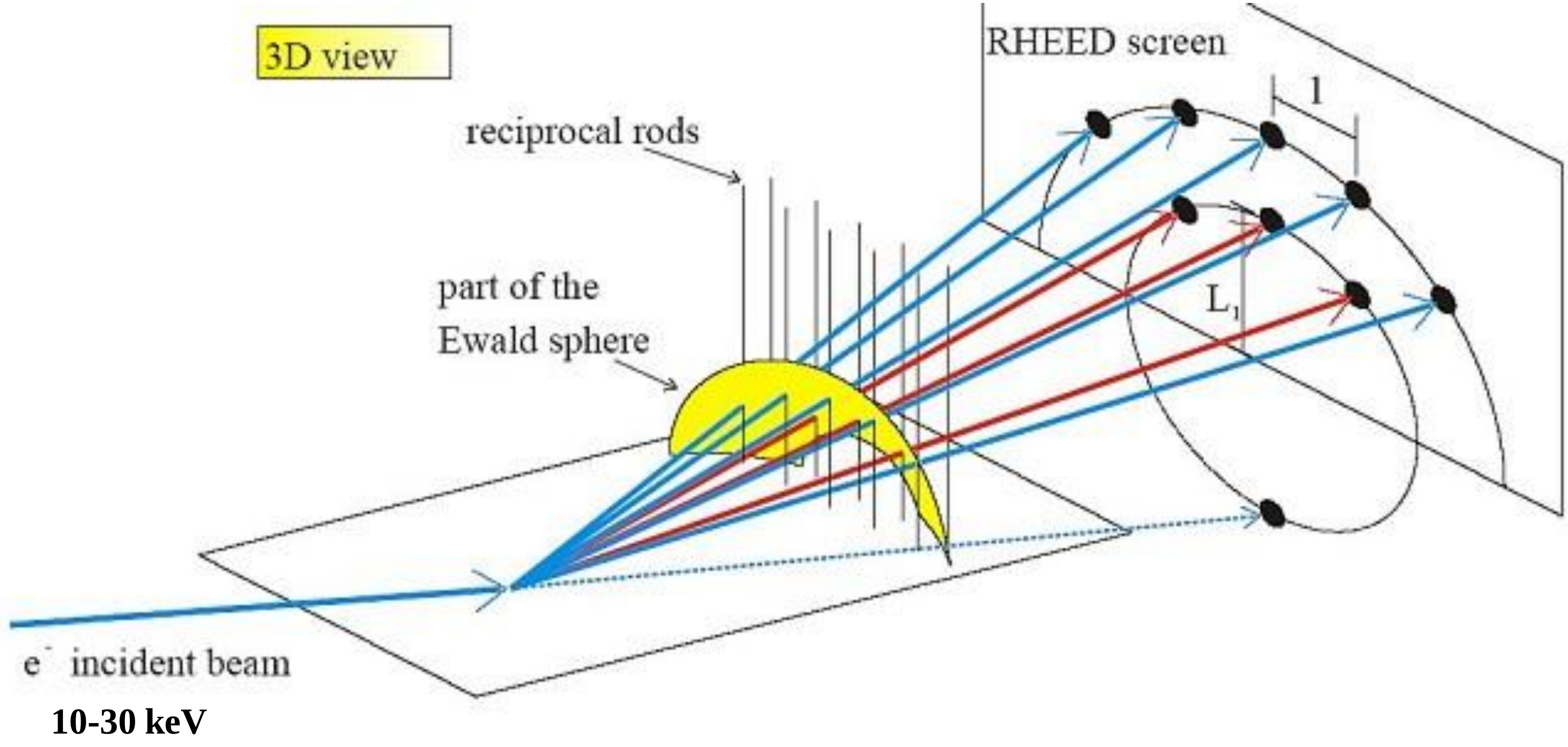
$\vec{k}_{\|}' = \vec{k}_{\|} + \vec{g}_{hk}$***, with***

$\vec{g}_{hk} = h\vec{a}^* + k\vec{b}^*$

$\vec{a}^* = 2\pi\frac{\vec{b}\,x\,\hat{n}}{A}$, $\vec{b}^* = 2\pi\frac{\hat{n}\,x\,\vec{a}}{A}$, $A=\vec{a}\bullet\vec{b}\,x\,\hat{n}$

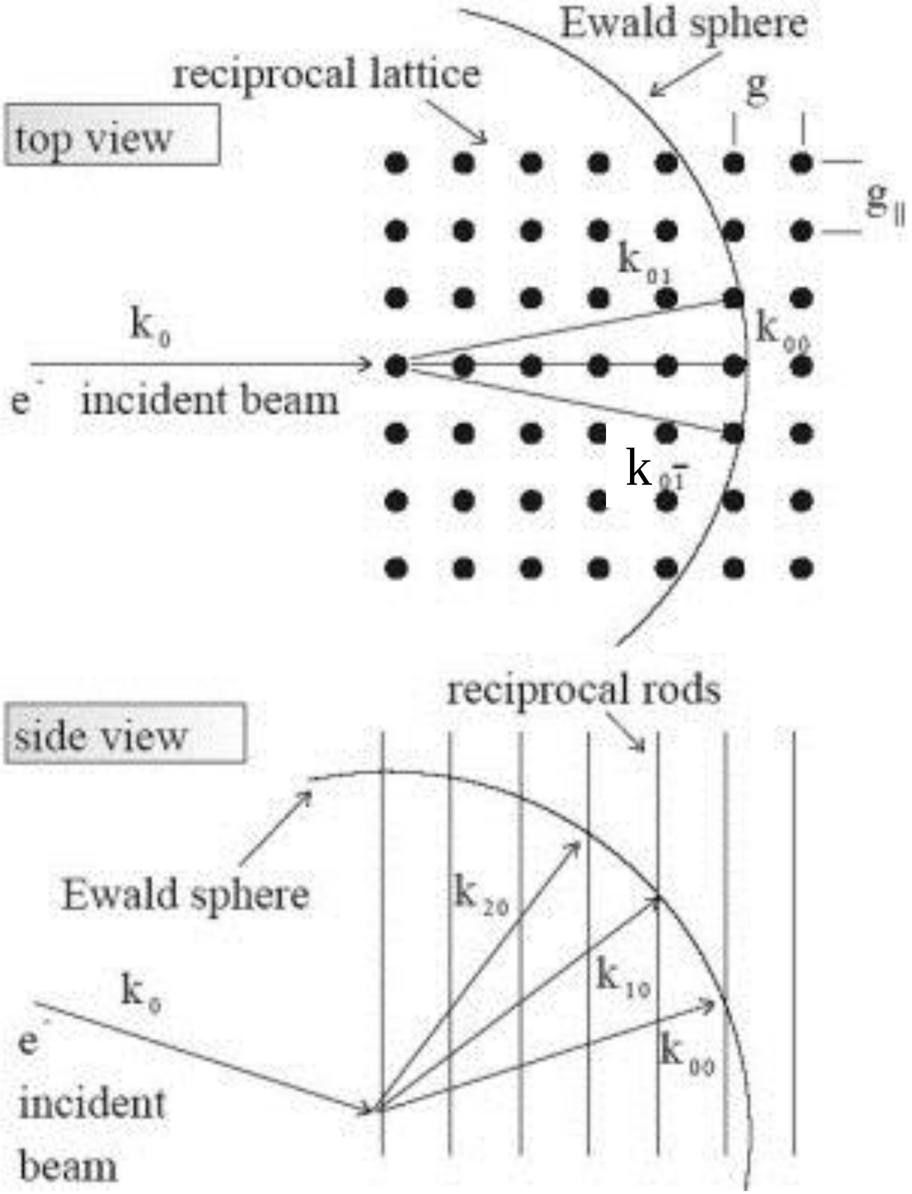
Reflection High-Energy Electron Diffraction (RHEED)

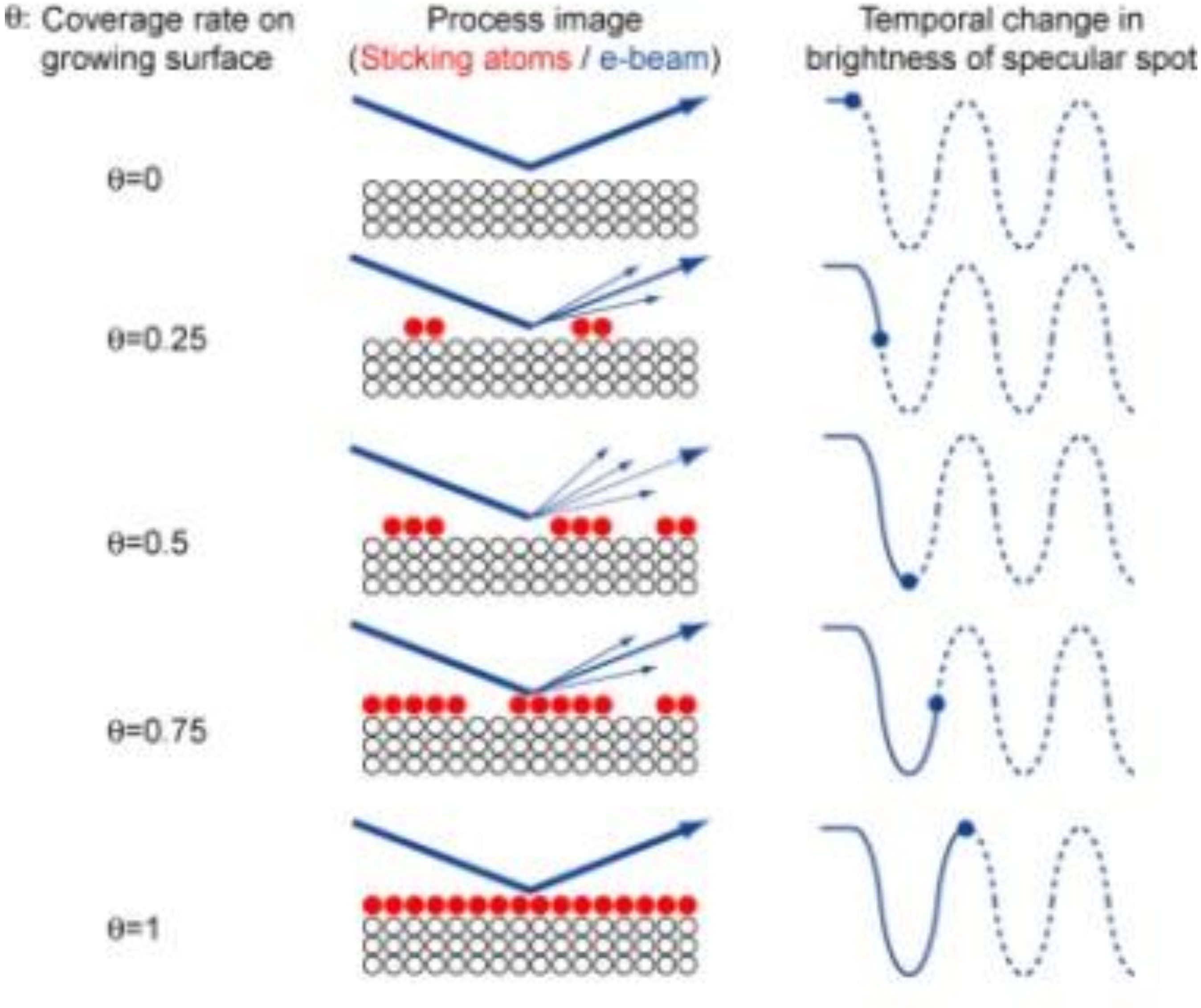
A powerful tool for monitoring epitaxial layer growth in real time

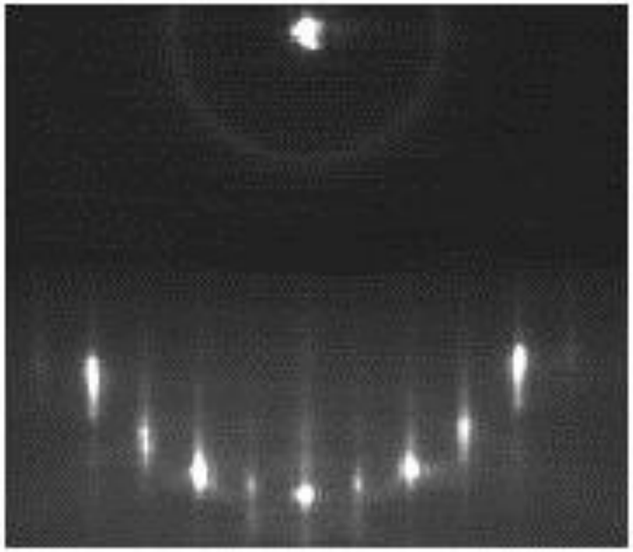


See Woodruff, Section 2.8

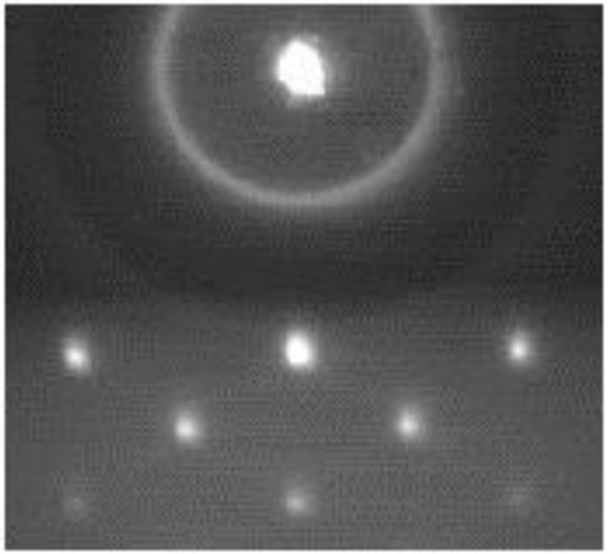
Reflection High-Energy Electron Diffraction (RHEED)



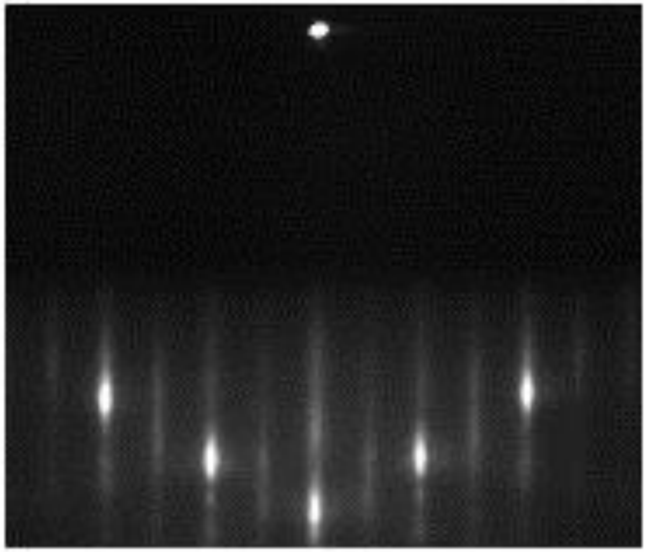

θ: Coverage rate on growing surface
Process image (Sticking atoms / e-beam)
Temporal change in brightness of specular spot
θ=0
θ=0.25
θ=0.5
θ=0.75
θ=1



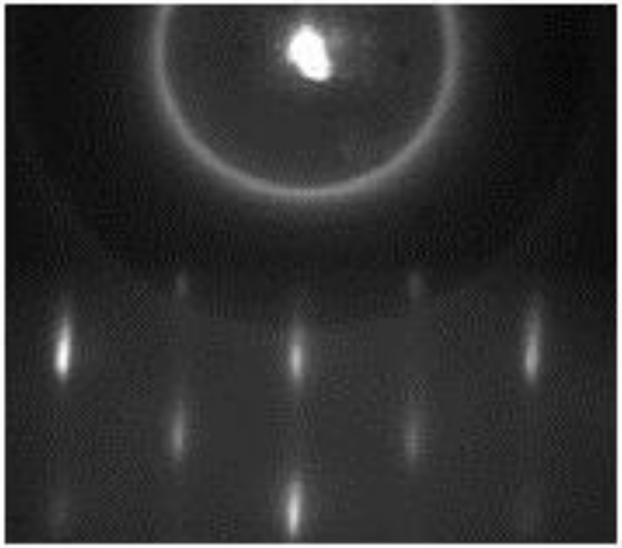
(a) 2D



(b) 3D



(c) quasi-2D



(d) quasi-3D

Atomically Resolved Surface Structure of SrTiO3(001) Thin Films Grown in Step-Flow Mode by Pulsed Laser Deposition

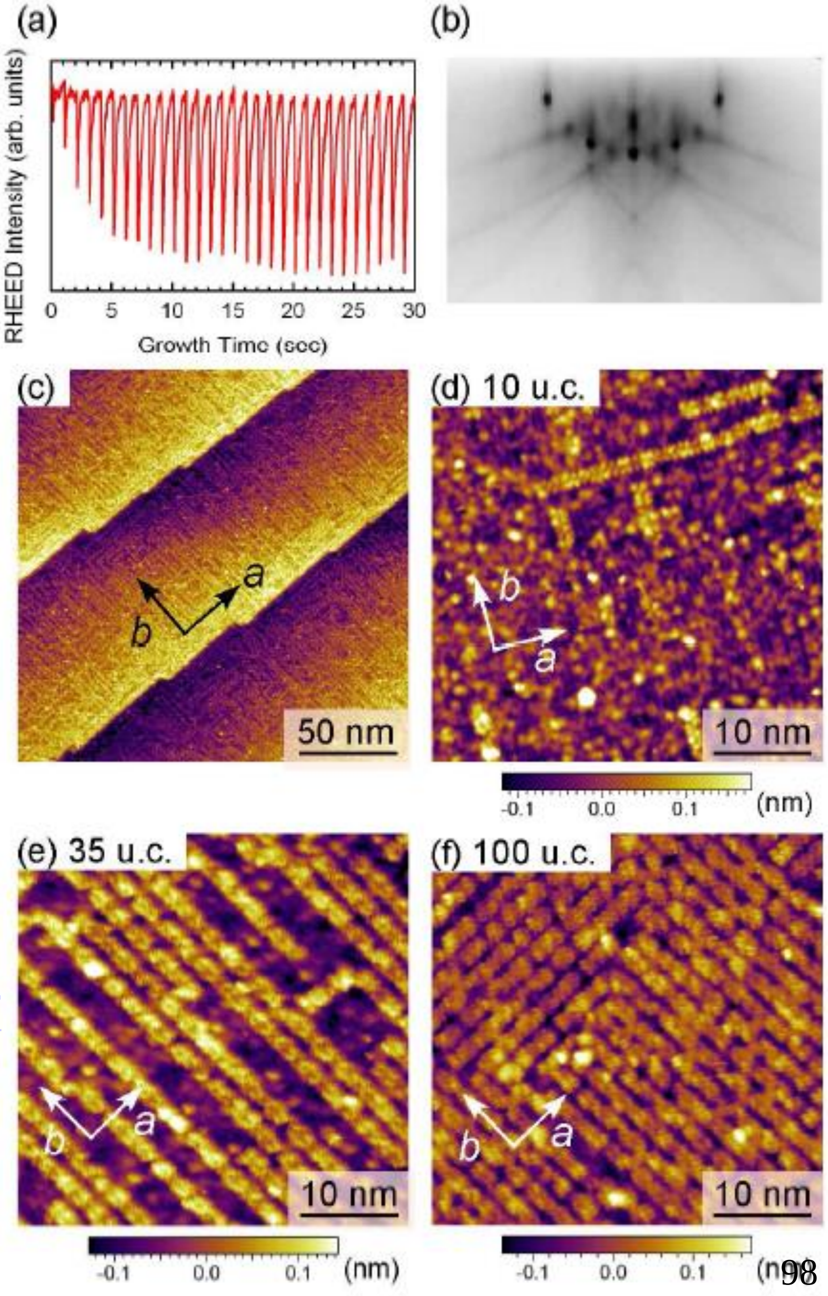


Figure 1

(a) RHEED intensity oscillations during $SrTiO_3(001)$ homoepitaxial growth at 1100˚C in an oxygen partial pressure of 1×10^{-6} Torr.

(b) RHEED pattern of 10 u.c. $SrTiO_3(001)$ thin film after growth.

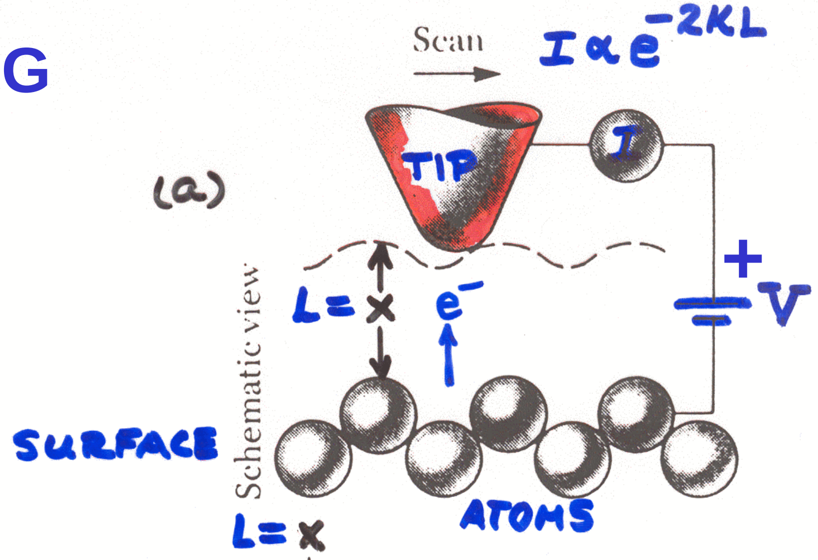
(c) Wide-area constant-current STM image of homoepitaxially-grown $SrTiO_3(001)$ thin film (thickness: 35 u.c.) showing a clear step and terrace structure with a single unit cell height (200 nm × 200 nm. Sample-bias-voltage $V_s = +2$ V, and the set-point tunneling current $I_t =$ 40 pA).

(d) –(f) Thickness dependence of surface structure of $SrTiO_3(001)$ thin films (40 nm × 40 nm, $V_s = +2$ V, $I_t = 40$ pA). (d) 10 u.c. (e) 35 u.c. (f) 100 u.c.

http://arxiv.org/ftp/arxiv/papers/1004/1004.0040.pdf

SCANNING TUNNELING MICROSCOPY

See Ibach, pp. 55-56, and Dejonqueres and Spanjaard, p. 575 (website Download)



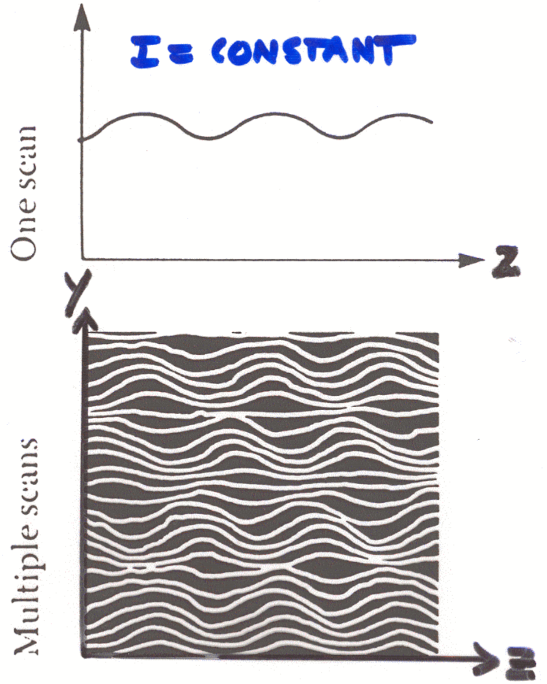
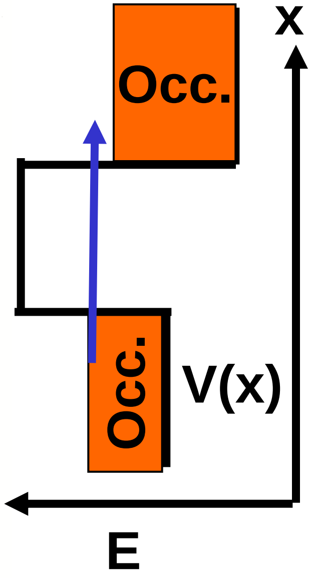


Figure 4 Scanning tunneling microscopes can be operated in either (a) the constant current mode or (b) the constant height mode. The images of the surface of graphite were made by Richard Sonnenfeld at the University of California at Santa Barbara. The constant height mode was first used by A. Bryant, D. P. E. Smith, and C. F. Quate, *Applied Physics Letters* 48: 832, 1986.

$\Delta x = \Delta L \approx 0.01 \mathring{A}$!

$\Delta y = \Delta z \approx 0.3\text{-}0.4 \mathring{A}$



More accurate model: Tersoff & Hamann, PRL 50, 1998 (1983)

THE SCANNING TUNNELING MICROSCOPE:

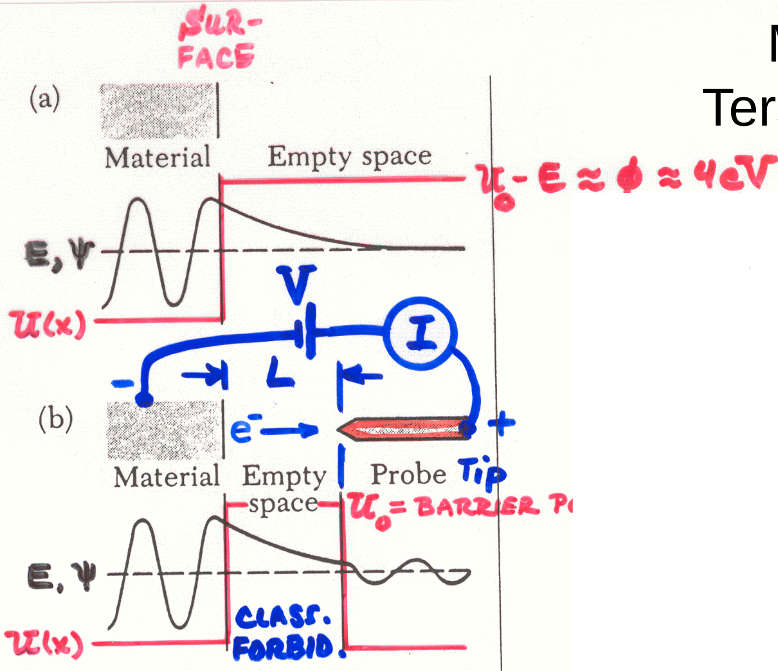


Figure 3 (a) The wavefunction of an electron in the surface of the material to be studied. The wavefunction extends beyond the surface into the empty region. (b) The sharp tip of a conducting probe is brought close to the surface. The wavefunction of a surface electron penetrates into the tip, so that the electron can "tunnel" from surface to tip. Compare this figure to Figure 6.7b.

j = CURRENT/UNIT AREA

$$\approx \frac{e^2 V}{4\pi^2 L \delta \hbar} e^{-2L/\delta} \propto e^{-2\ldots}$$

$$\delta = \frac{1}{\kappa} = \sqrt{\frac{\hbar^2}{2m(U_0 - E)}} \approx 1.0 \text{ Å}$$

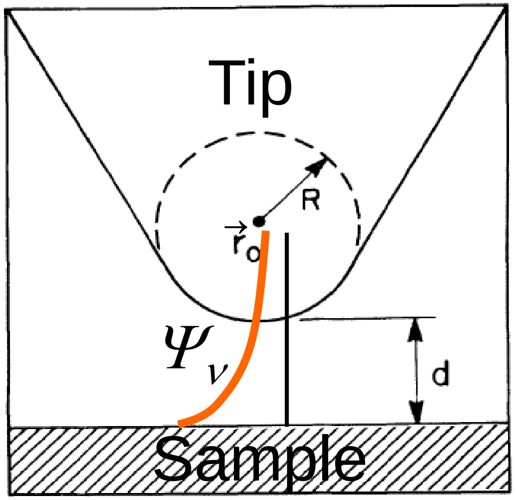


FIG. 1. Schematic picture of tunneling geometry. Probe tip has arbitrary shape but is assumed locally spherical with radius of curvature R, where it approaches nearest the surface (shaded). Distance of nearest approach is d. Center of curvature of tip is labeled $\vec{r}_0$.

$$I = 32\pi^3\hbar^{-1}e^2V\varphi^2D_t(E_F)R^2\kappa^{-4}e^{2\kappa R}$$

$$\times\sum_\nu |\psi_\nu(\vec{r}_0)|^2\delta(E_\nu - E_F),$$

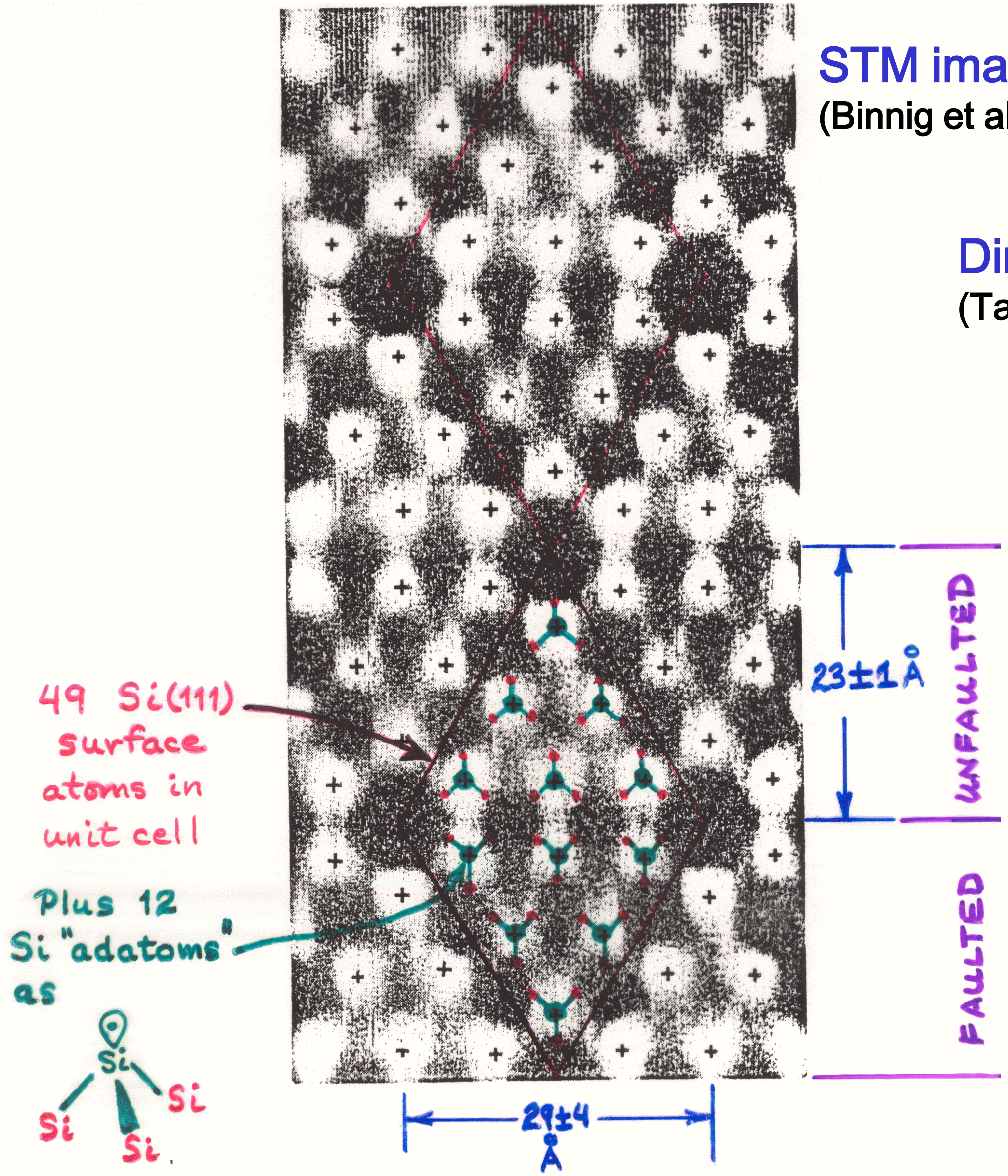
$D_t(E_F)$ = tip density of states at E_F

φ = work function = $U_0 - E_F$

See also Dejonqueres and Spanjaard, website download, Eqs. G.18 & G.24

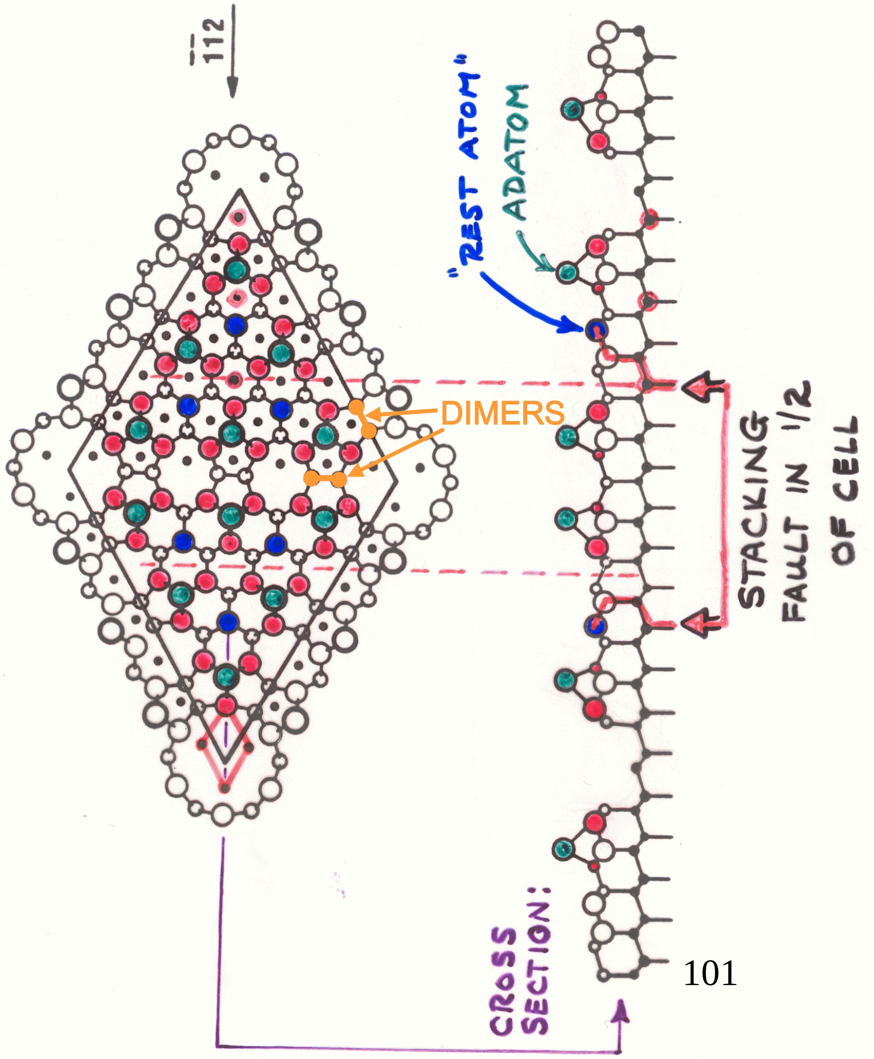
STM image of (7x7) reconstruction of Si(111)

(Binnig et al., Phys. Rev. Lett. 50, 120 ('83))

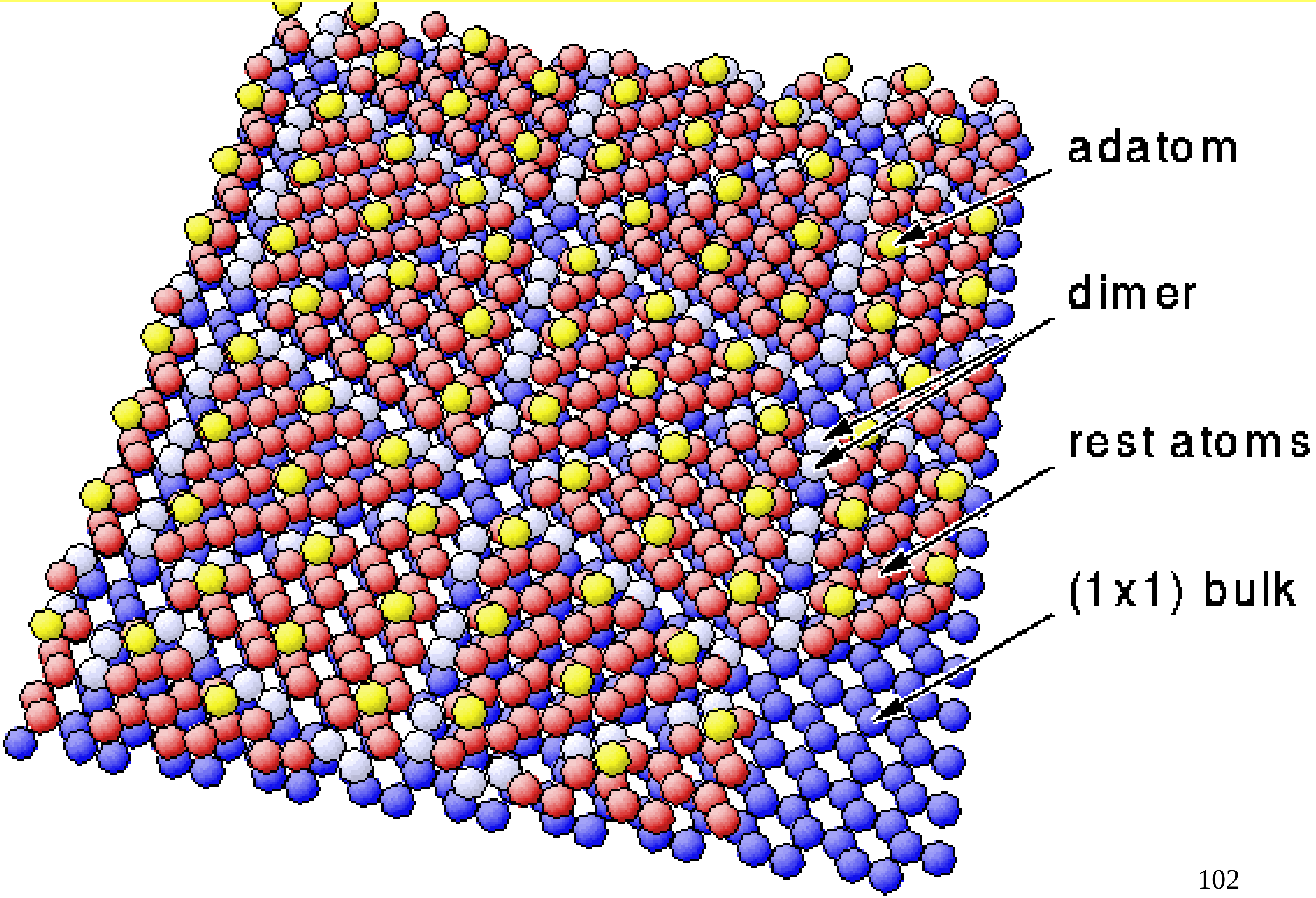


Dimer-Adatom-Stacking Fault Model

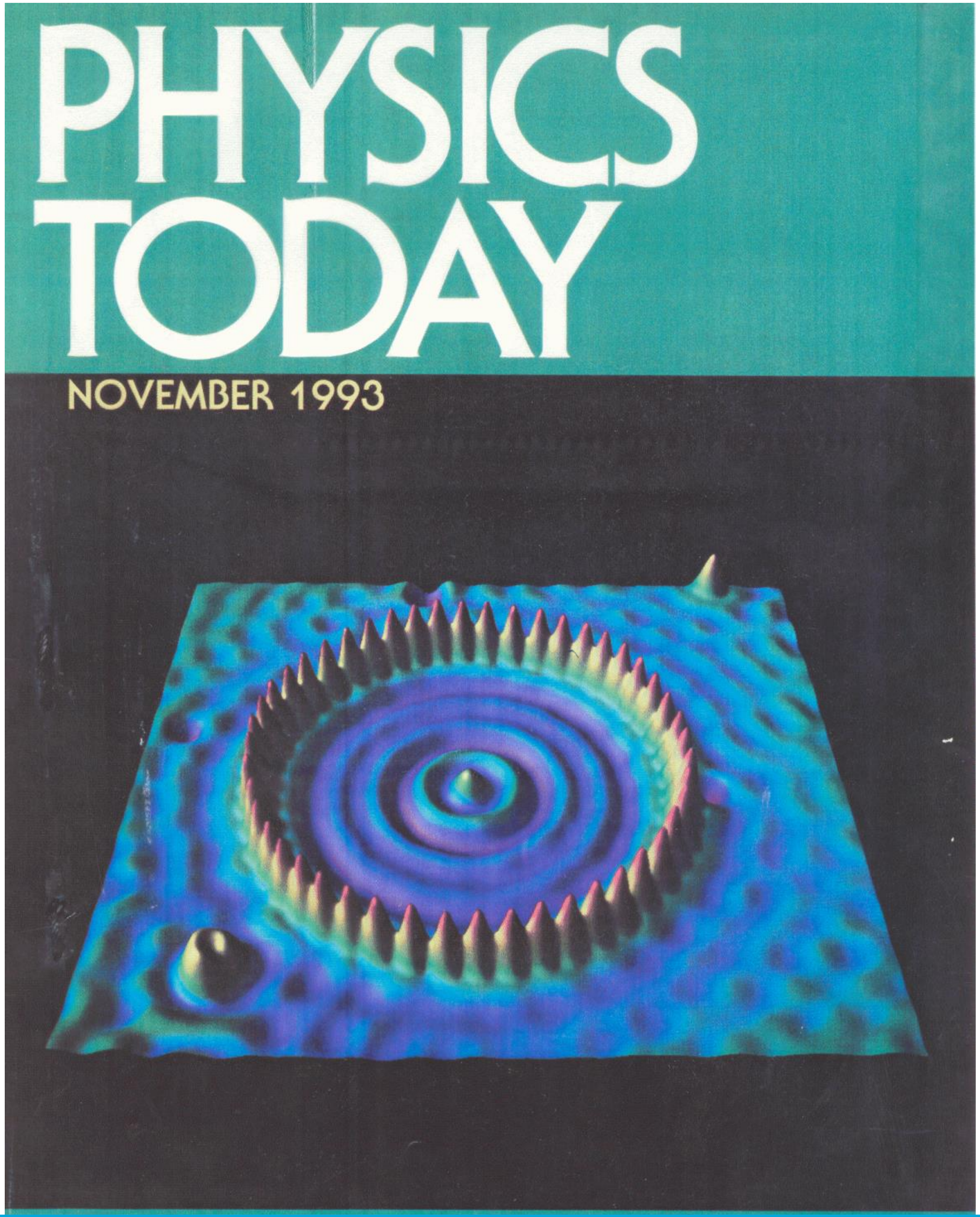
(Takayanagi et al., J. Vac. Sci. Tech. A3, 1502 ('85))



Si(111)-(7x7)—Dimer-adatom-stacking fault model

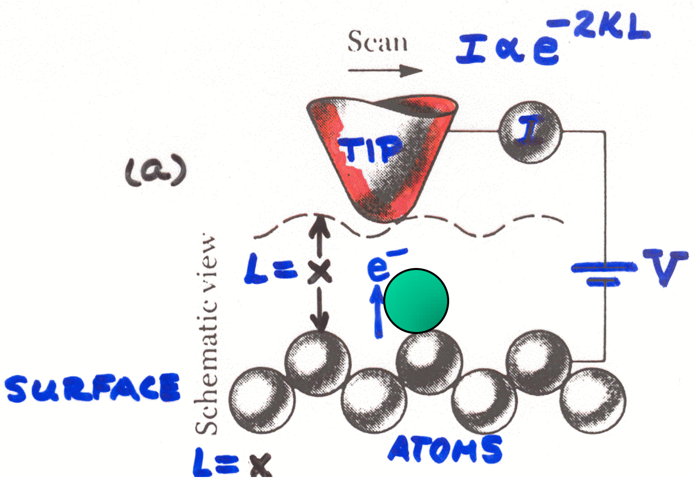


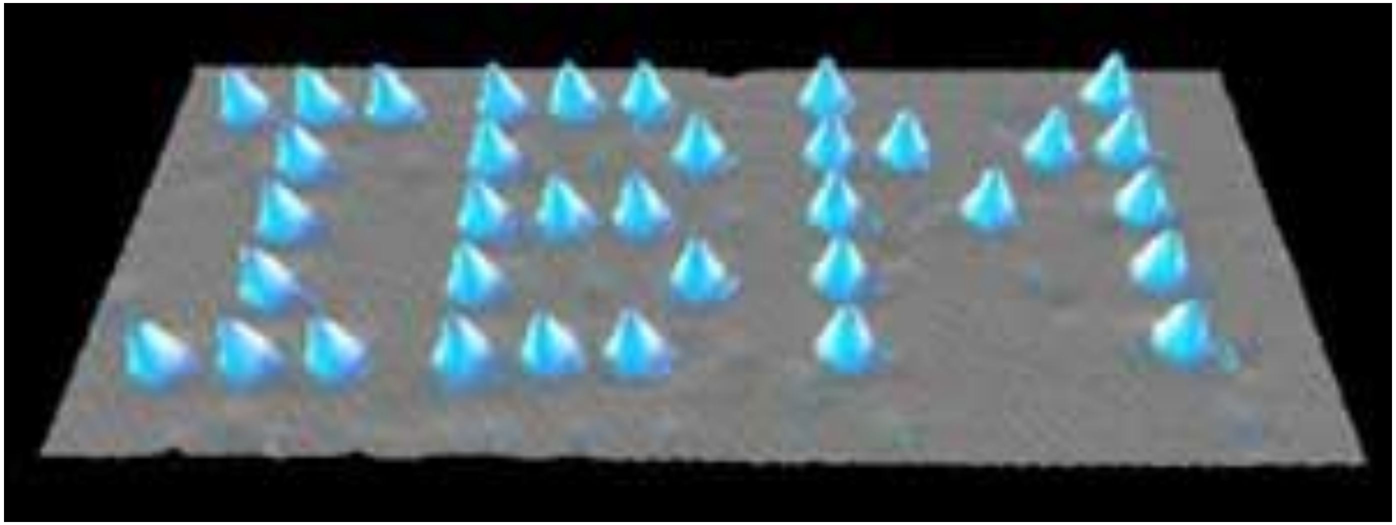
IMAGING, AND MANIPULATING, ATOMS AT SURFACES WITH THE STM



48 iron atoms on a Cu(111) surface—a “quantum corral”

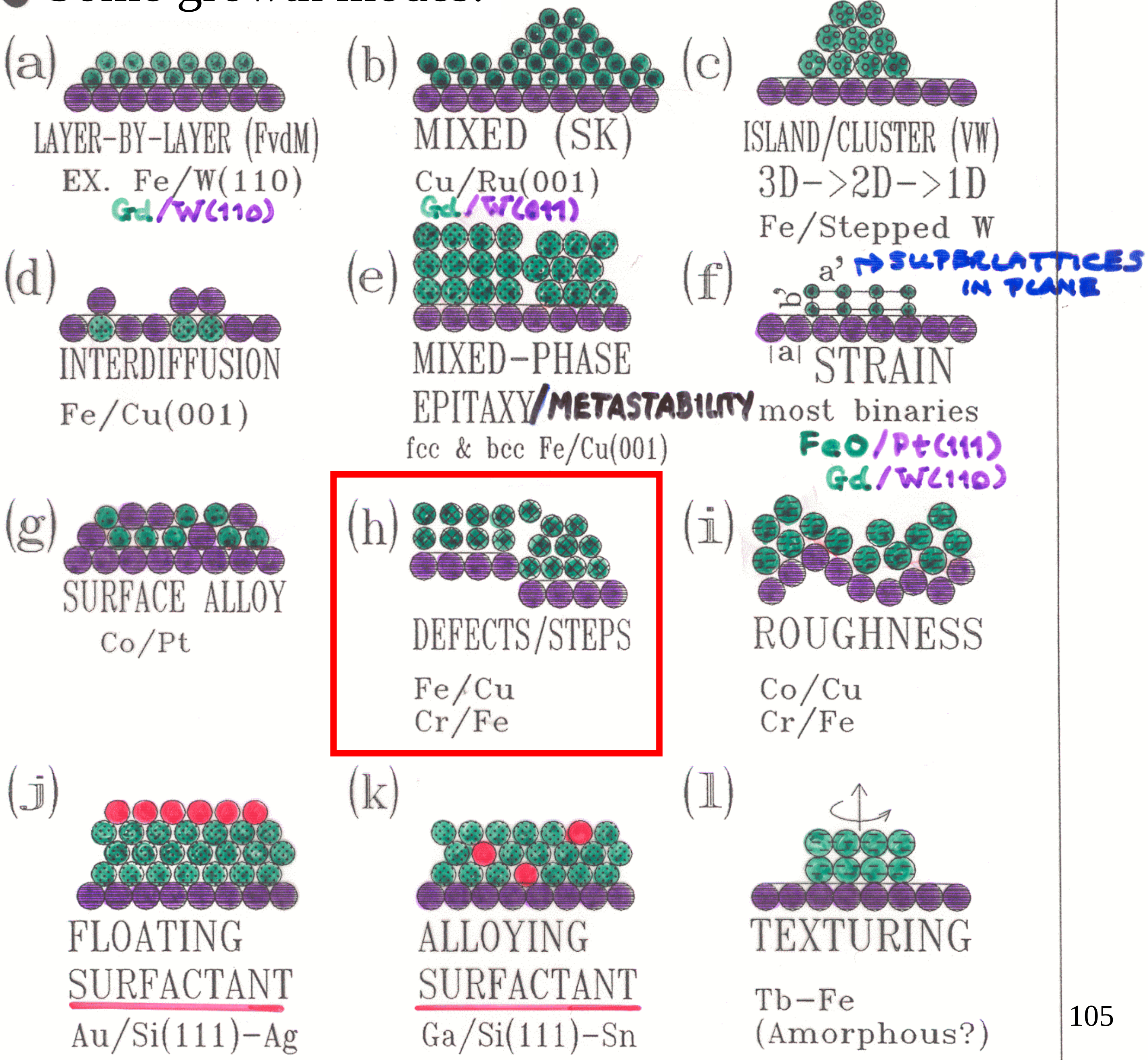
Writing with single atoms—30 years later





1989--IBM, written with single xenon atoms, using a scanning tunneling microscope

- Some growth modes:



(a) LAYER-BY-LAYER (FvdM)
EX. Fe/W(110)
Gd/W(110)

(b) MIXED (SK)
Cu/Ru(001)
Gd/W(011)

(c) ISLAND/CLUSTER (VW)
3D->2D->1D
Fe/Stepped W

(d) INTERDIFFUSION
Fe/Cu(001)

(e) MIXED-PHASE
EPITAXY/METASTABILITY
fcc & bcc Fe/Cu(001)

(f) → SUPERLATTICES IN PLANE
STRAIN
most binaries
FeO/Pt(111)
Gd/W(110)

(g) SURFACE ALLOY
Co/Pt

(h) DEFECTS/STEPS
Fe/Cu
Cr/Fe

(i) ROUGHNESS
Co/Cu
Cr/Fe

(j) FLOATING
SURFACTANT
Au/Si(111)-Ag

(k) ALLOYING
SURFACTANT
Ga/Si(111)-Sn

(l) TEXTURING
Tb-Fe
(Amorphous?)

Scanning tunneling microscopy: stepped Si(111) surface

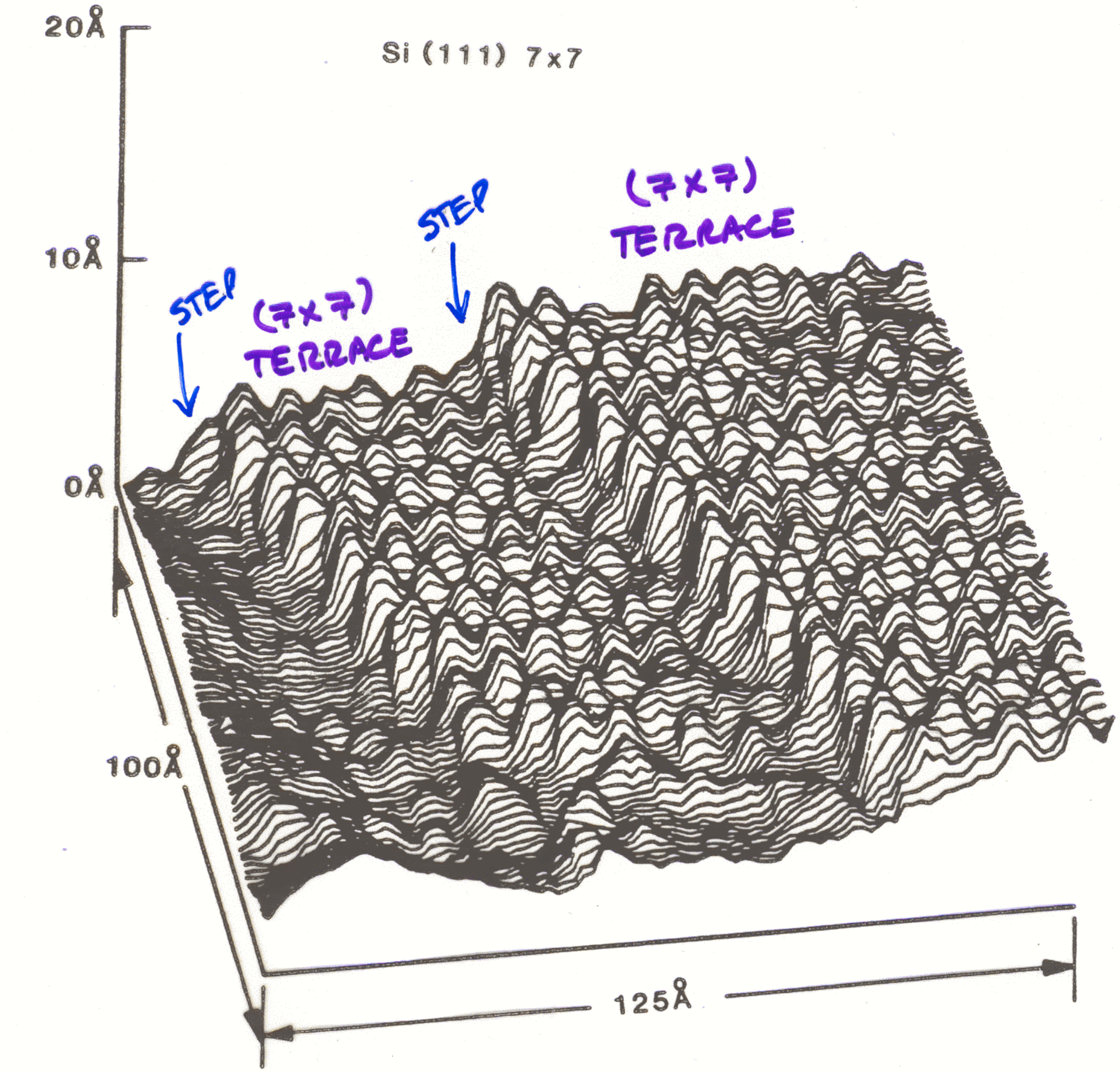
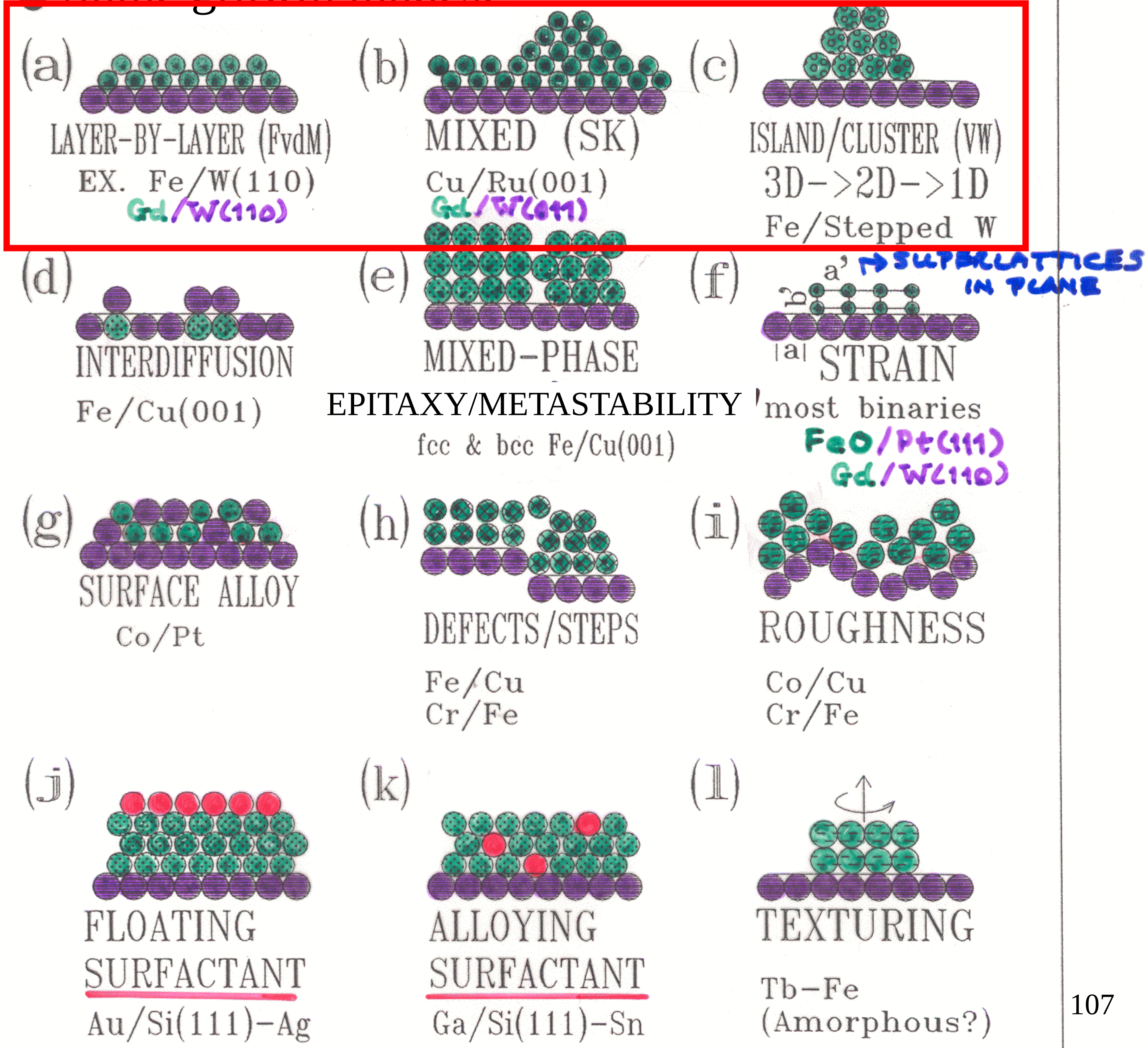


Fig. 2. Tunneling image of silicon (111) surface that shows the 7×7 atomic reconstruction on terraces separated by atomic steps.

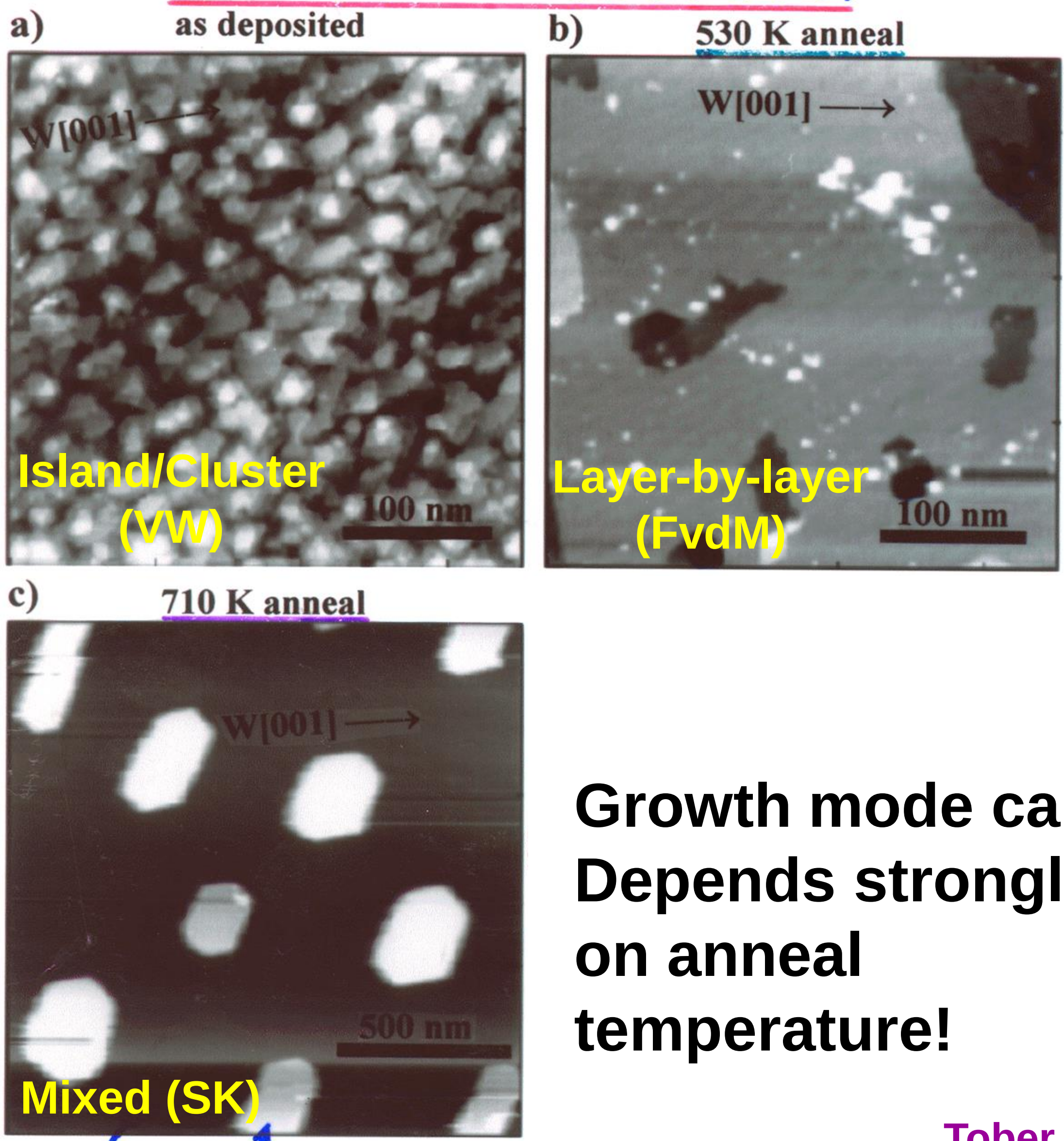
- **Frank-van der Merwe (FvdM) = layer-by-layer growth (2D).**
- **Stranski-Krastanow (SK) = layer-by-layer + island ...**
- **Volmer-Weber (VW) = island growth (3D).**

- Some growth modes:



Scanning tunneling microscopy: metal-on-metal epitaxial growth

GROWTH OF 11 ML Gd ON W(110)



WETTING SINGLE LAYER

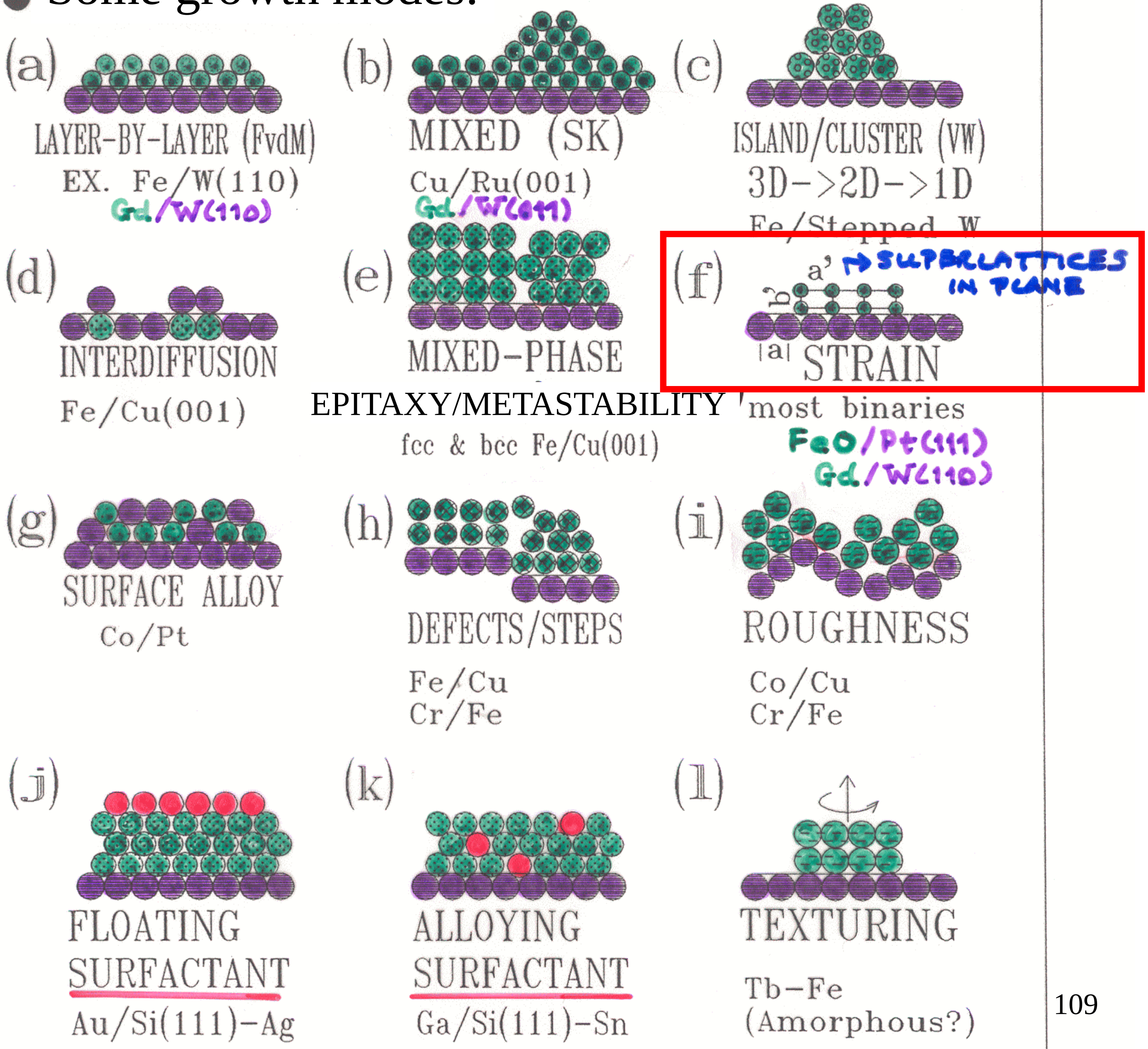
ISLANDS: ~ 10 nm (~35 ML) THICK (= t)
x ~ 310 nm IN DIAMETER (≡ d)

Growth mode can Depends strongly on anneal temperature!

Tober et al. Phys. Rev. B 53, 5444 (1996).

- **Frank-van der Merwe (FvdM) = layer-by-layer growth (2D).**
- **Stranski-Krastanow (SK) = layer-by-layer + island ...**
- **Volmer-Weber (VW) = island growth (3D).**

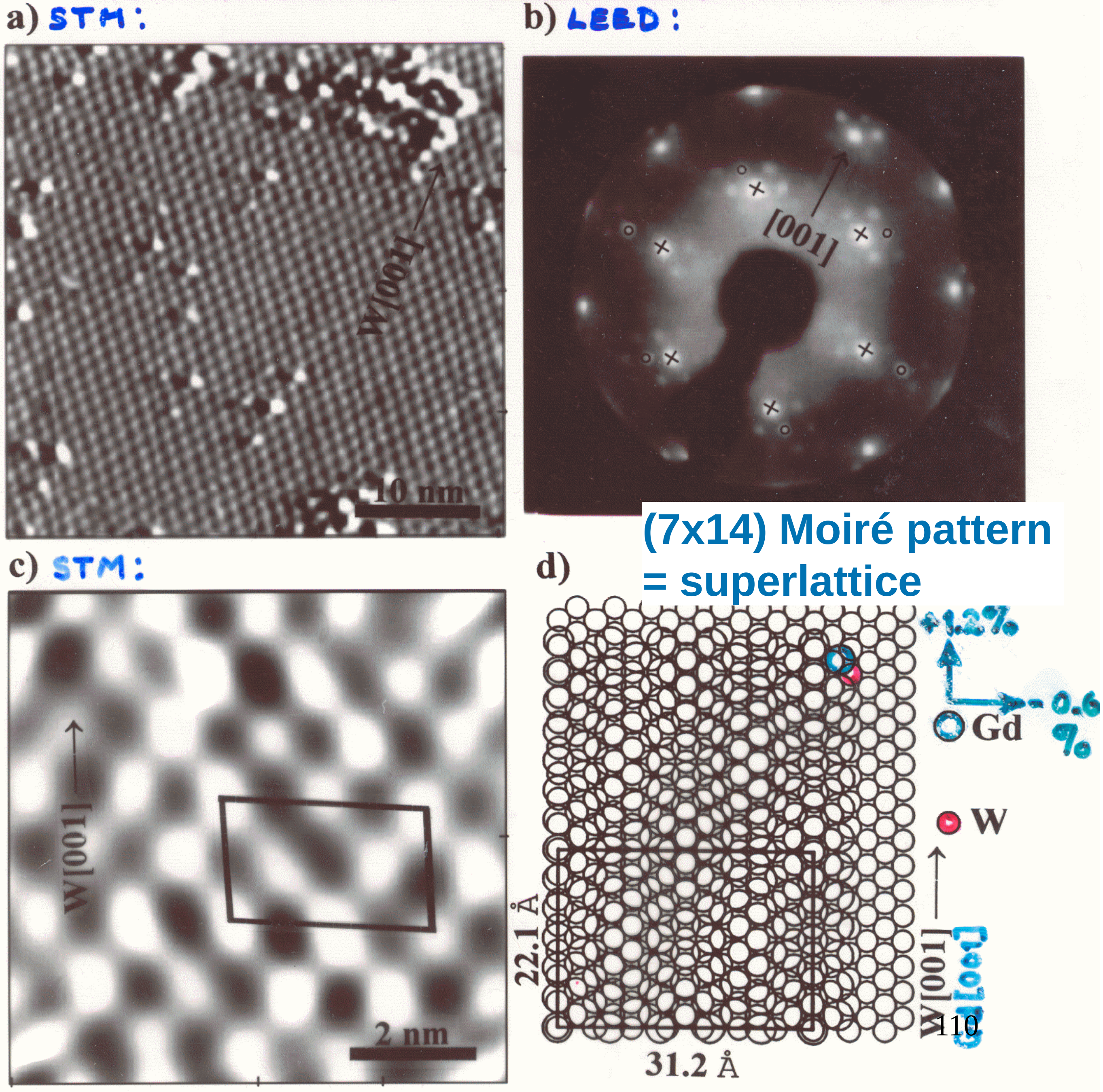
Some growth modes:



EPITAXY/METASTABILITY

Superlattice = Moiré structure in metal-on-metal epitaxial growth

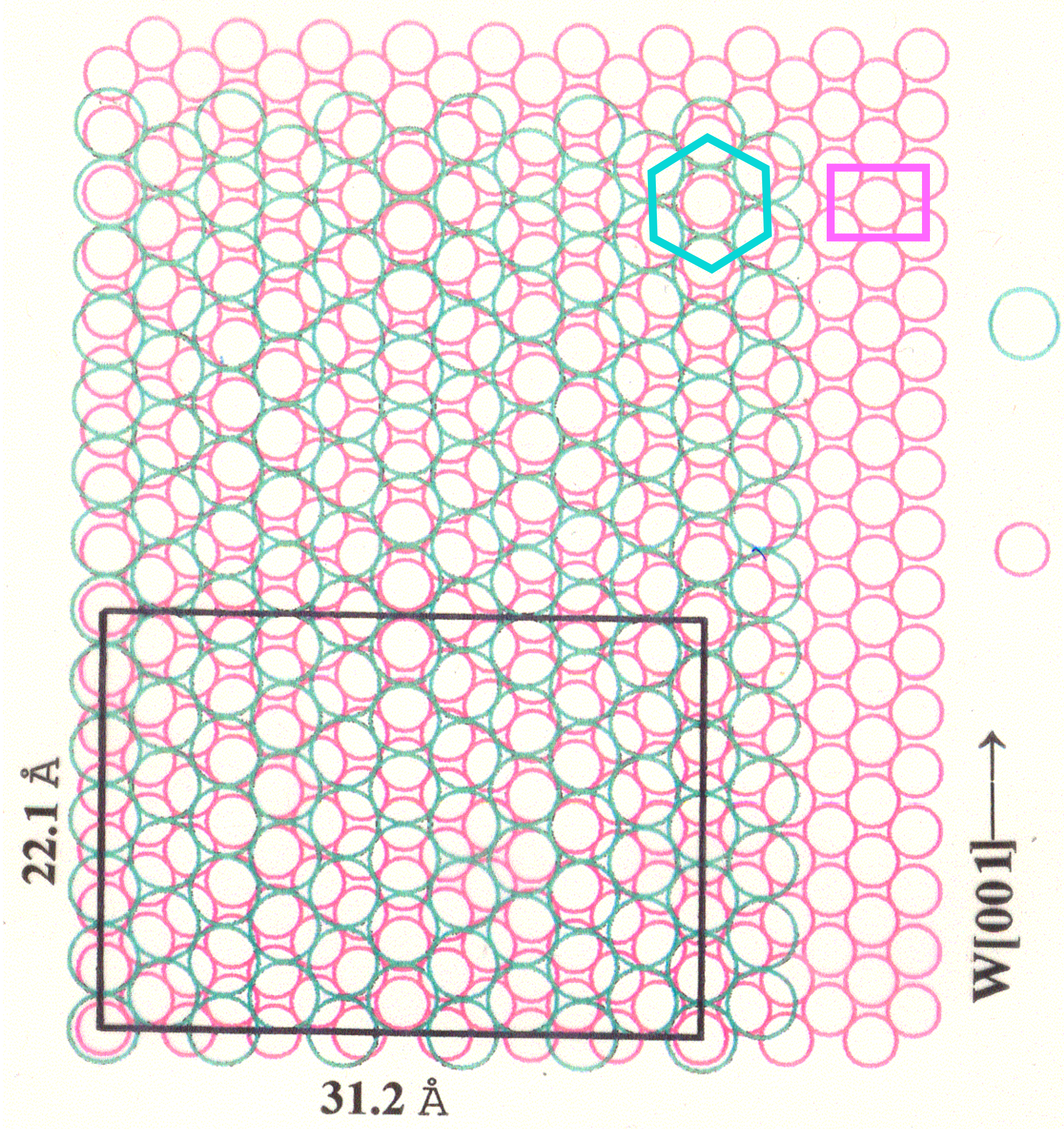
"WETTING" SINGLE MONOLAYER OF Gd ON W(110)



(7x14) Moiré pattern = superlattice

E. Tober et al.
Phys. Rev. B
53, 544 ('96)

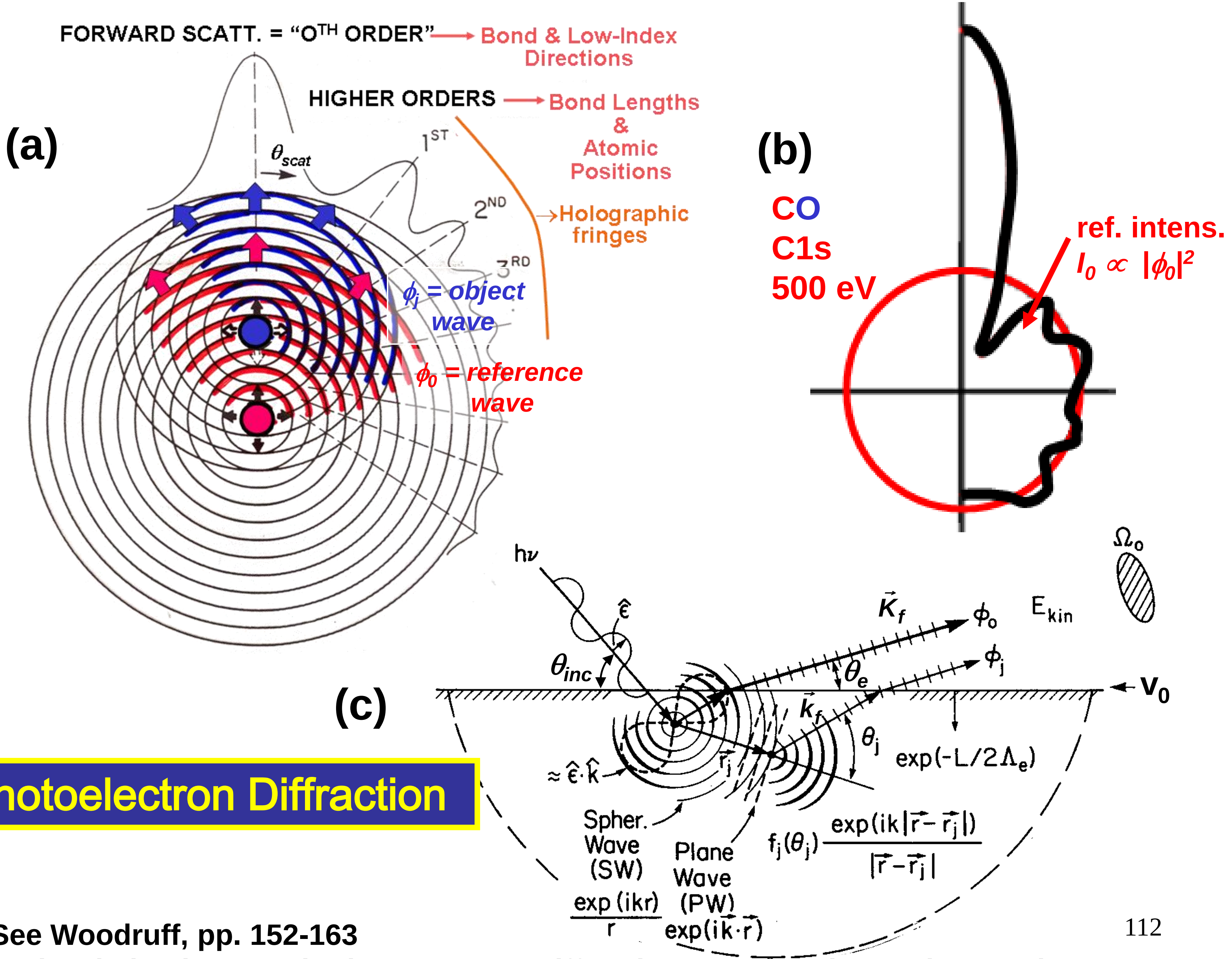
A Moiré pattern—Monolayer Gd on W(110)



Gd(0001)—
hexagonal

W(110)—
rectangular

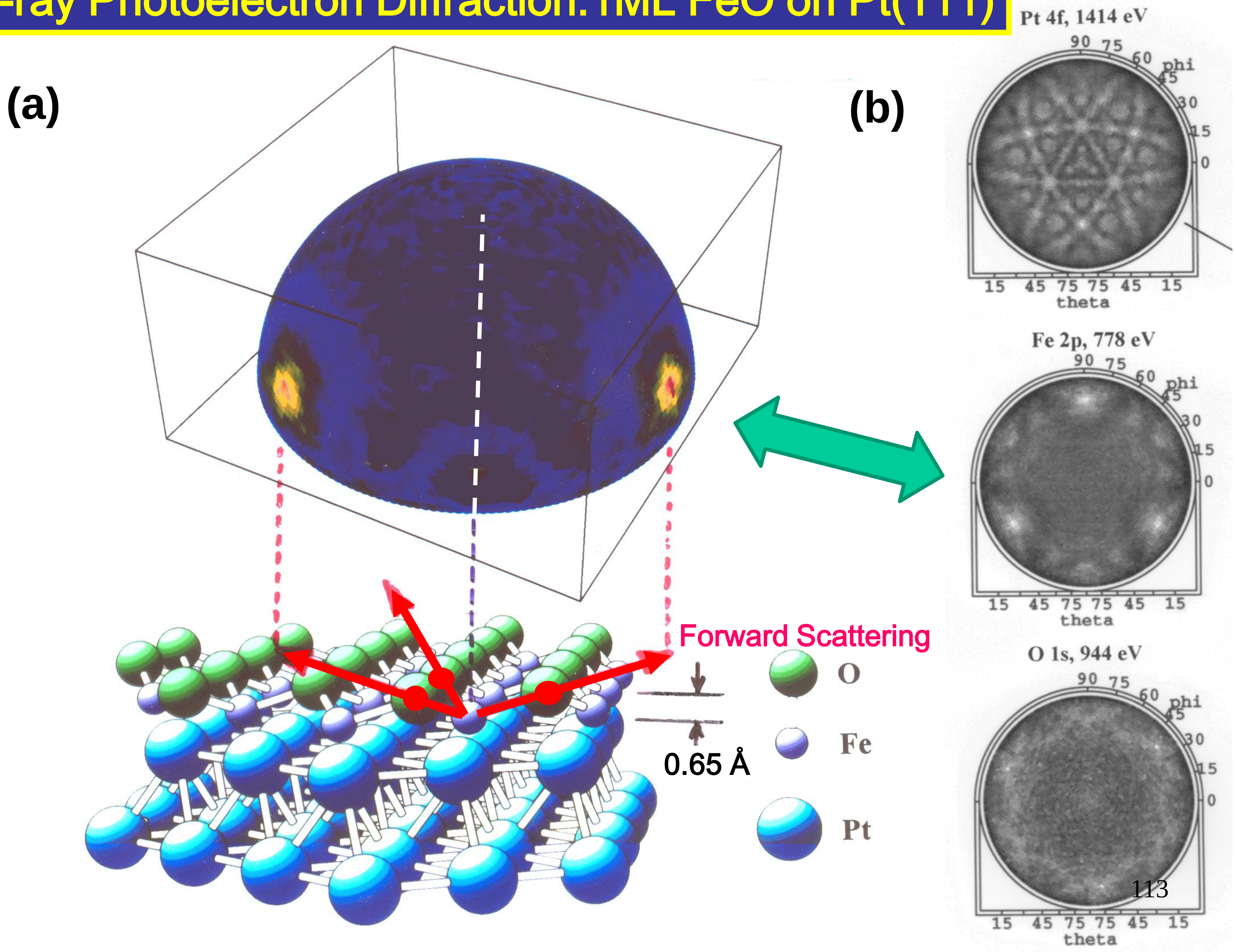
Photoelectron Diffraction

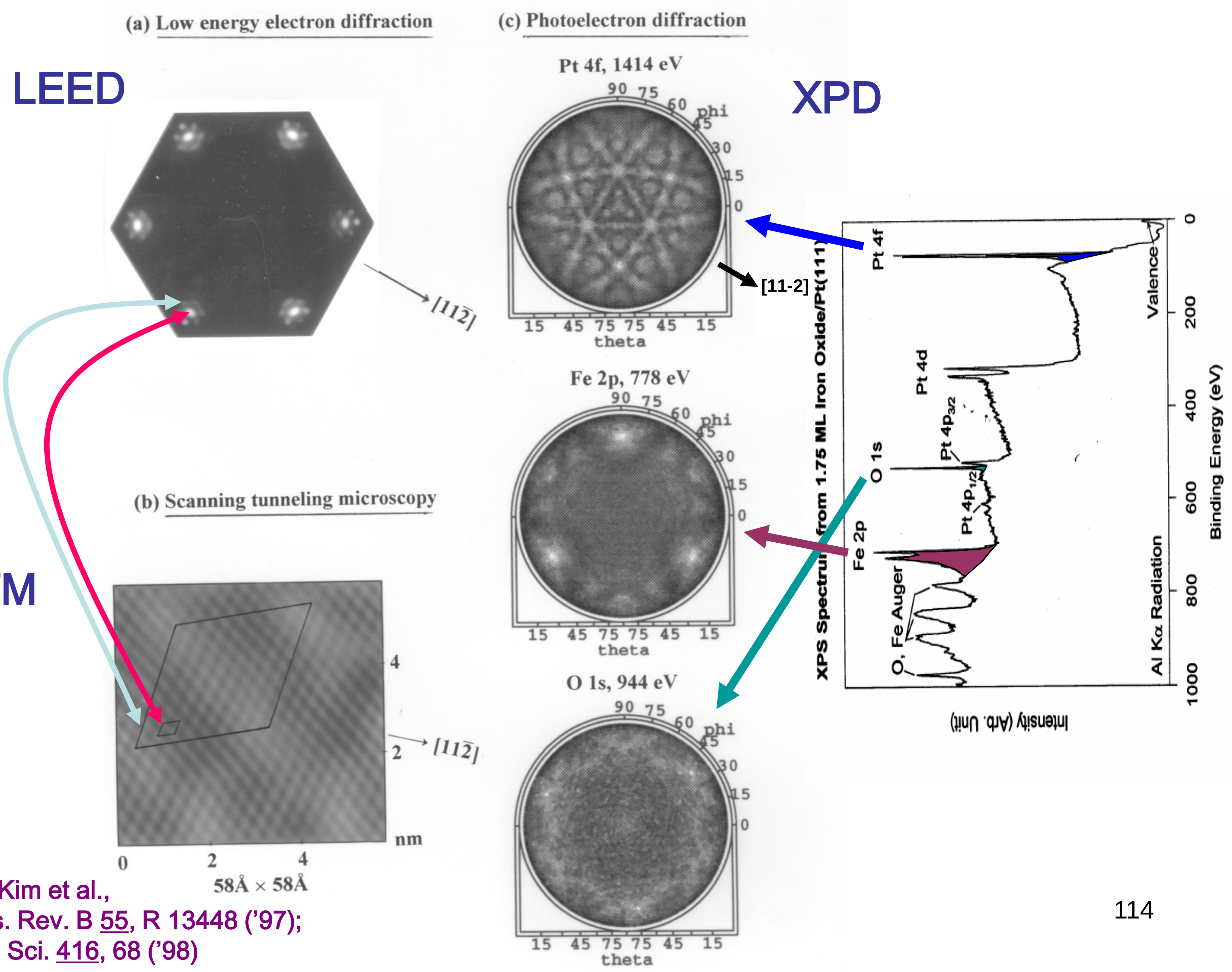


See Woodruff, pp. 152-163

And website download: Photoelectron Diffraction: An Overview Article, Fadley

X-ray Photoelectron Diffraction:1ML FeO on Pt(111)





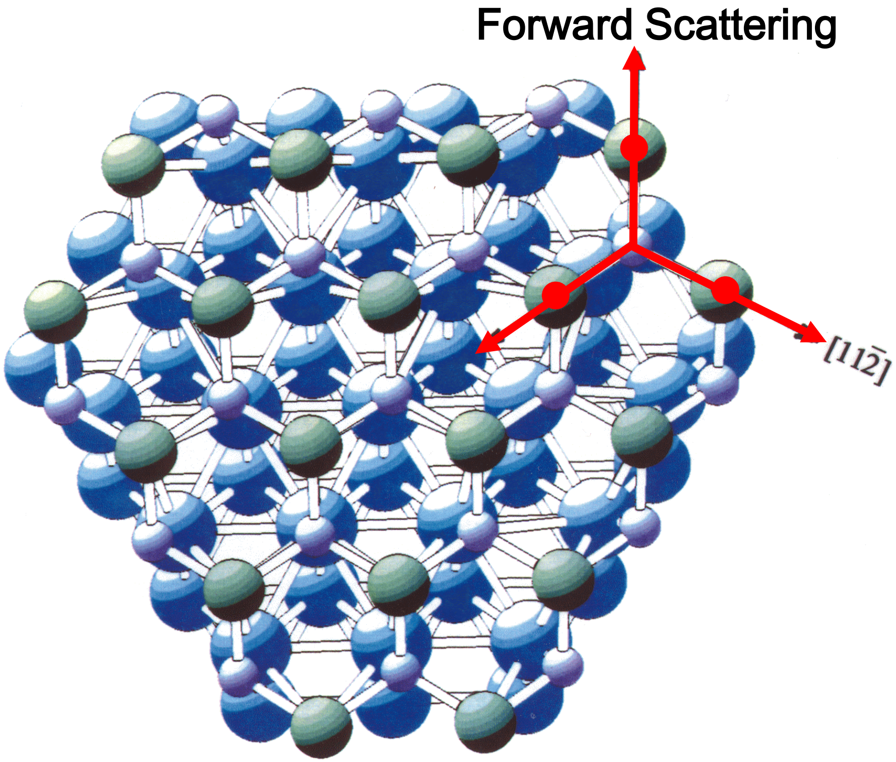
LEED

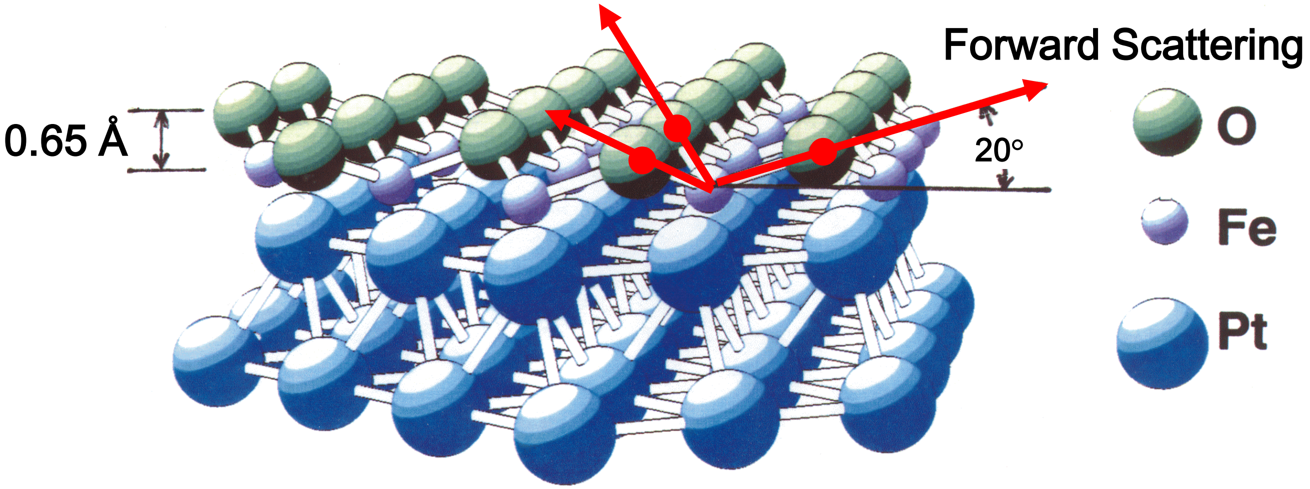
XPD

STM

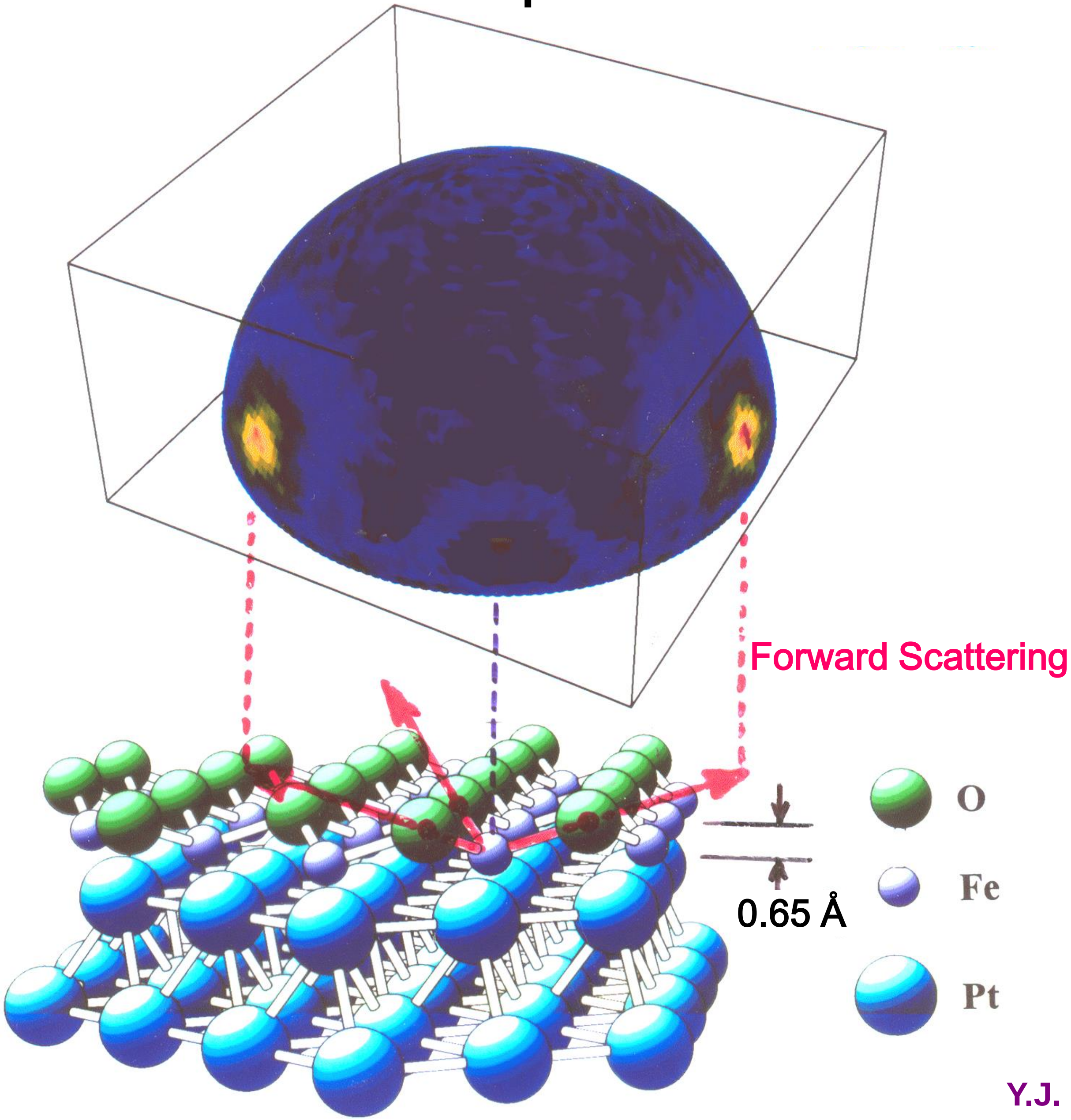
Y.J. Kim et al.,
Phys. Rev. B 55, R 13448 ('97);
Surf. Sci. 416, 68 ('98)

FeO/Pt(111)


Forward Scattering
$[11\bar{2}]$

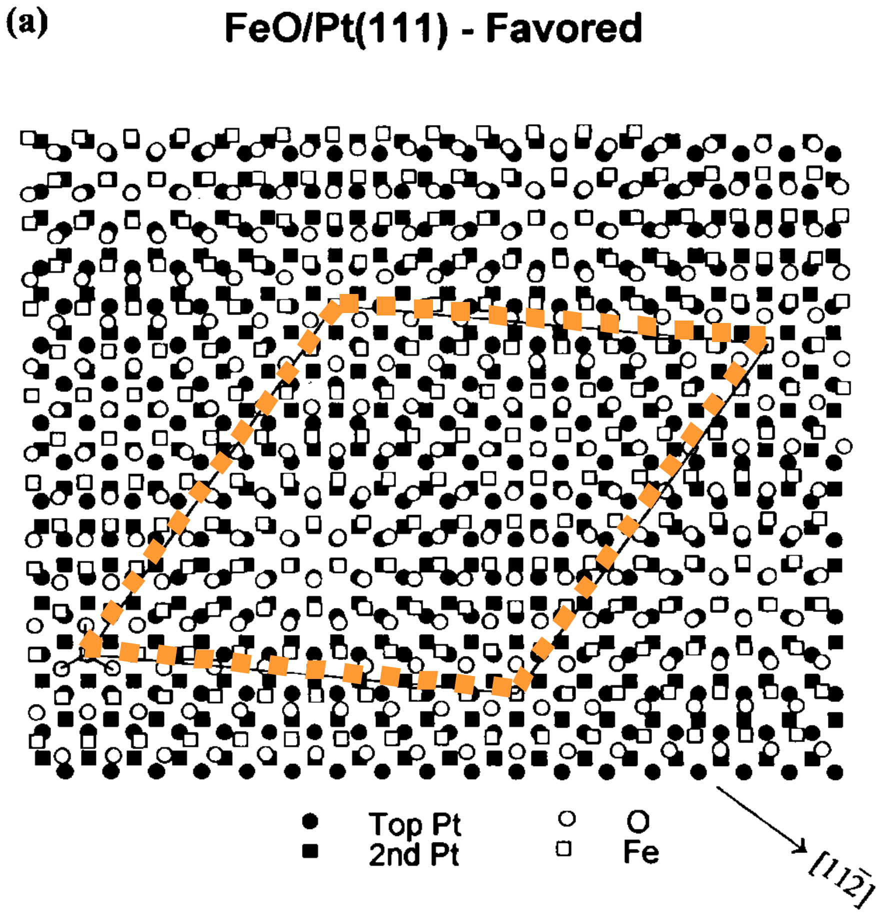

Forward Scattering
0.65 Å
20°
O
Fe
Pt

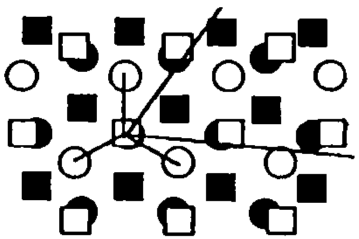
X-ray Photoelectron Diffraction: Fe 2p from 1ML FeO on Pt(111)

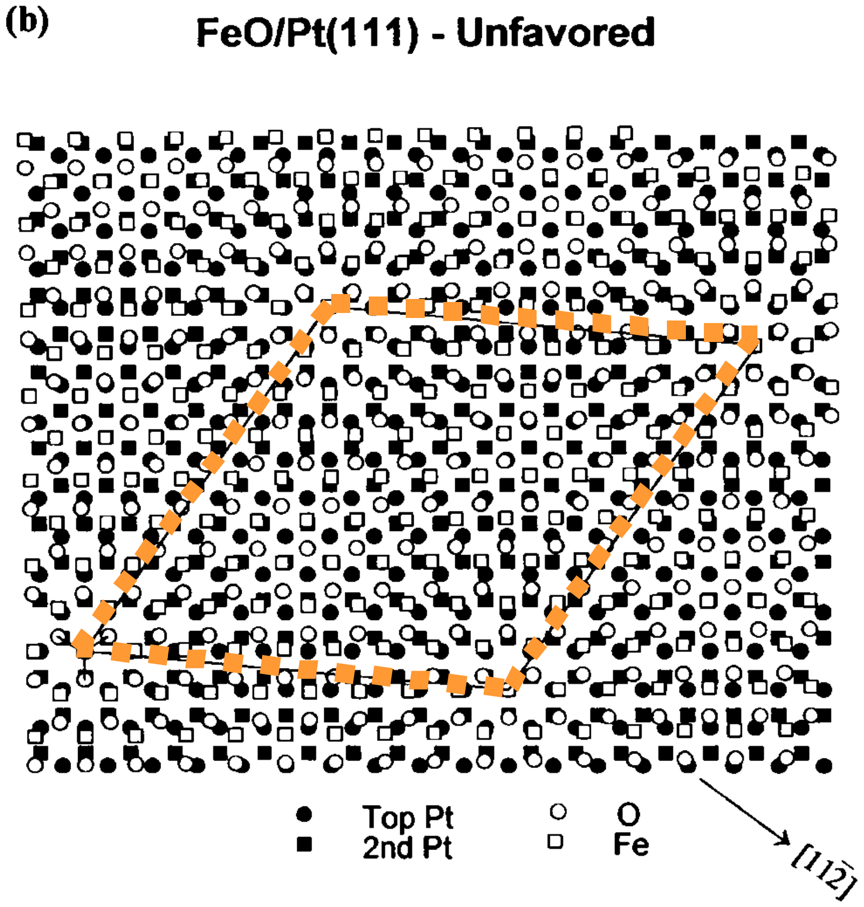


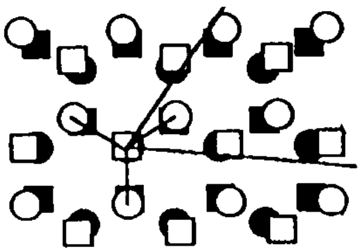
Y.J. Kim et al.
Phys. Rev. B 55, R 13448 ('97)

Permits selecting favored domain of growth—2nd layer Pt effect

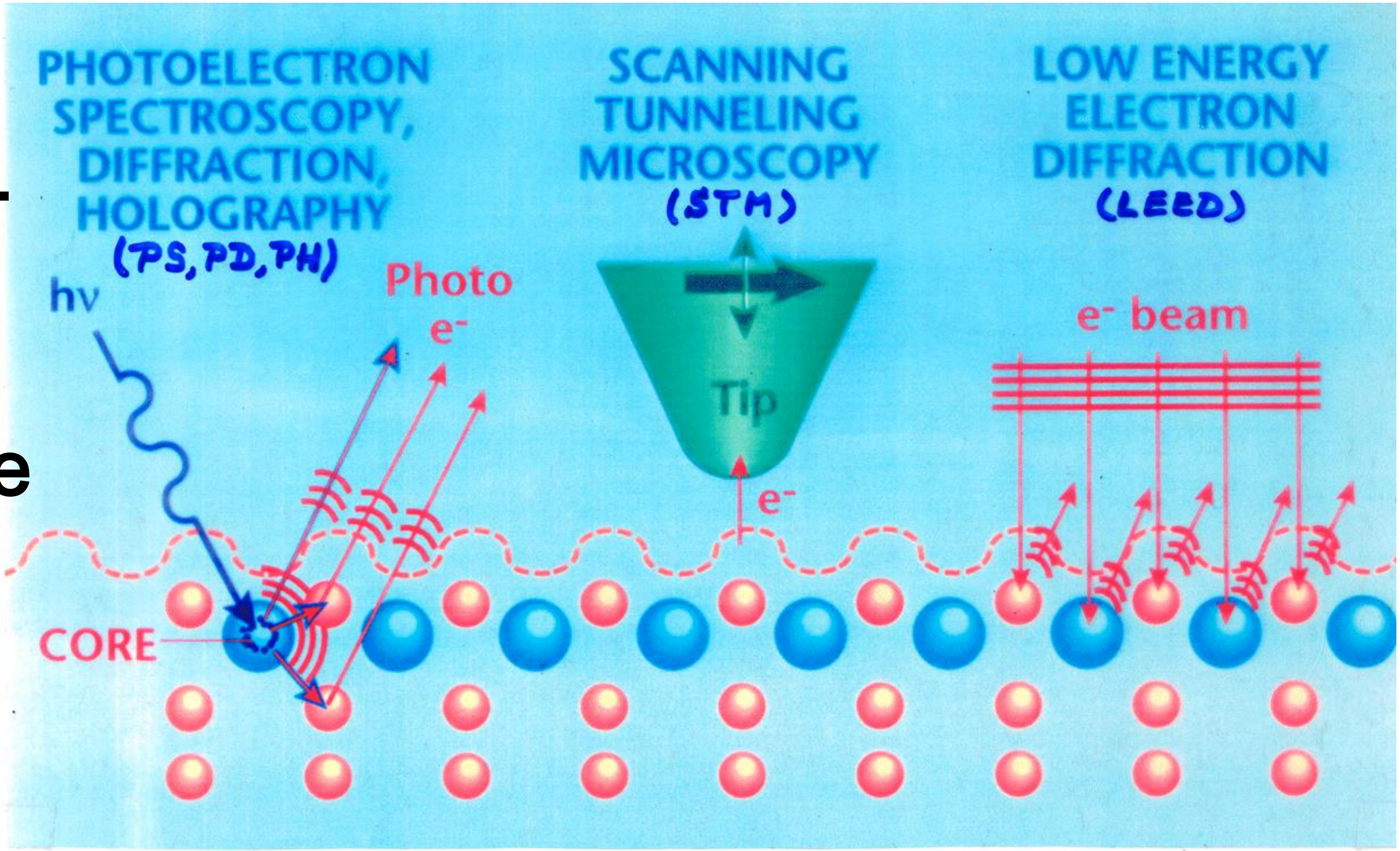








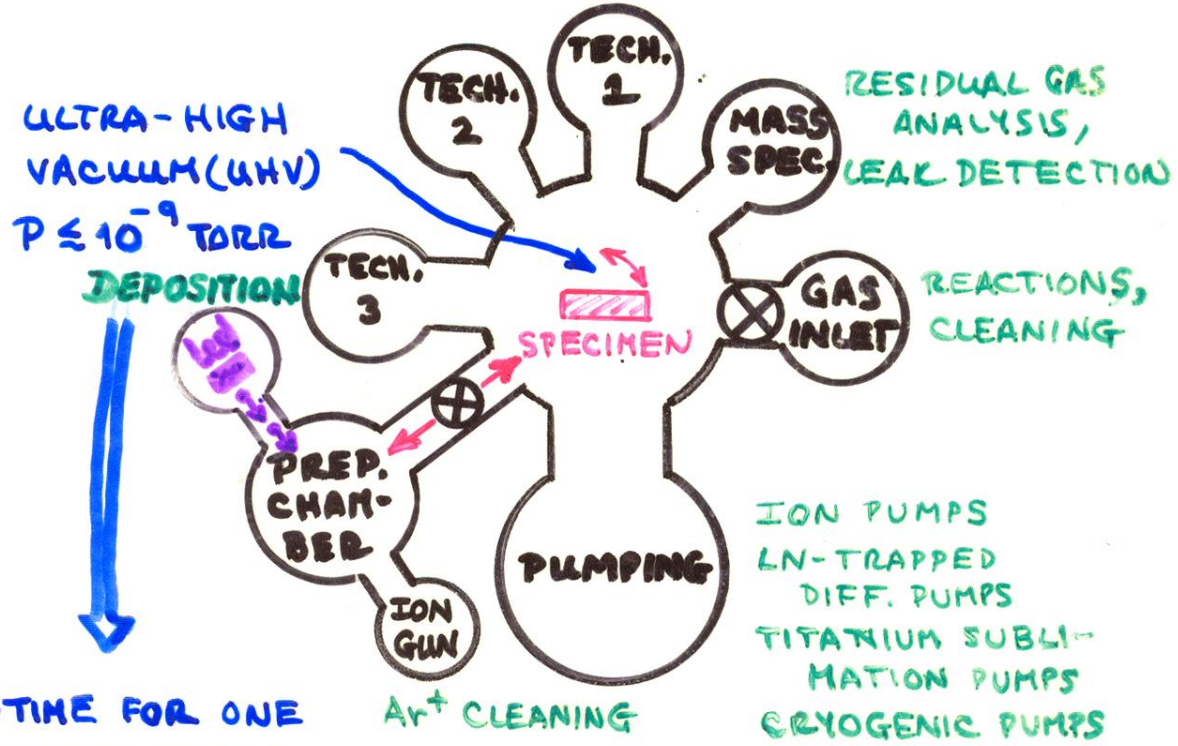
Some Complementary Surface Structure Probes



-Type of order:	Short (< 10Å)	Short, long and disorder	Long (> 100Å)
-Atom & site specific:	Yes	No	No
-Sensing depth:	5-40Å	Mostly surface D.O.S.	5-20Å
-Lateral resolution:	1 mm^2 to (300Å)^2	Single atom	1 mm^2 to 1 micron^2

A typical surface science research system

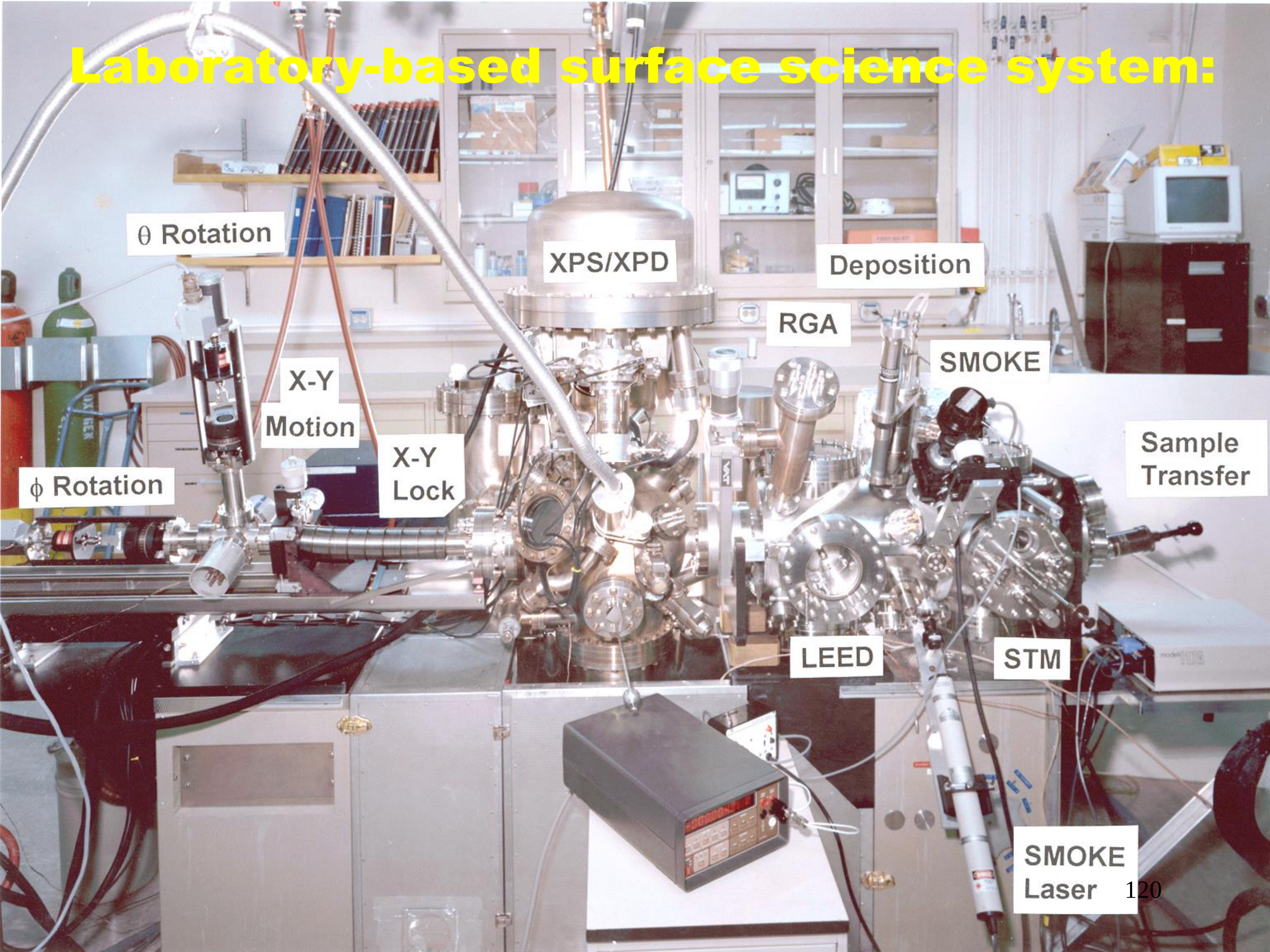
≥ 1 TECHNIQUE: SURFACE SENSITIVE (e^-, IONS,
ATOMS AS PROBES)
NON-DESTRUCTIVE



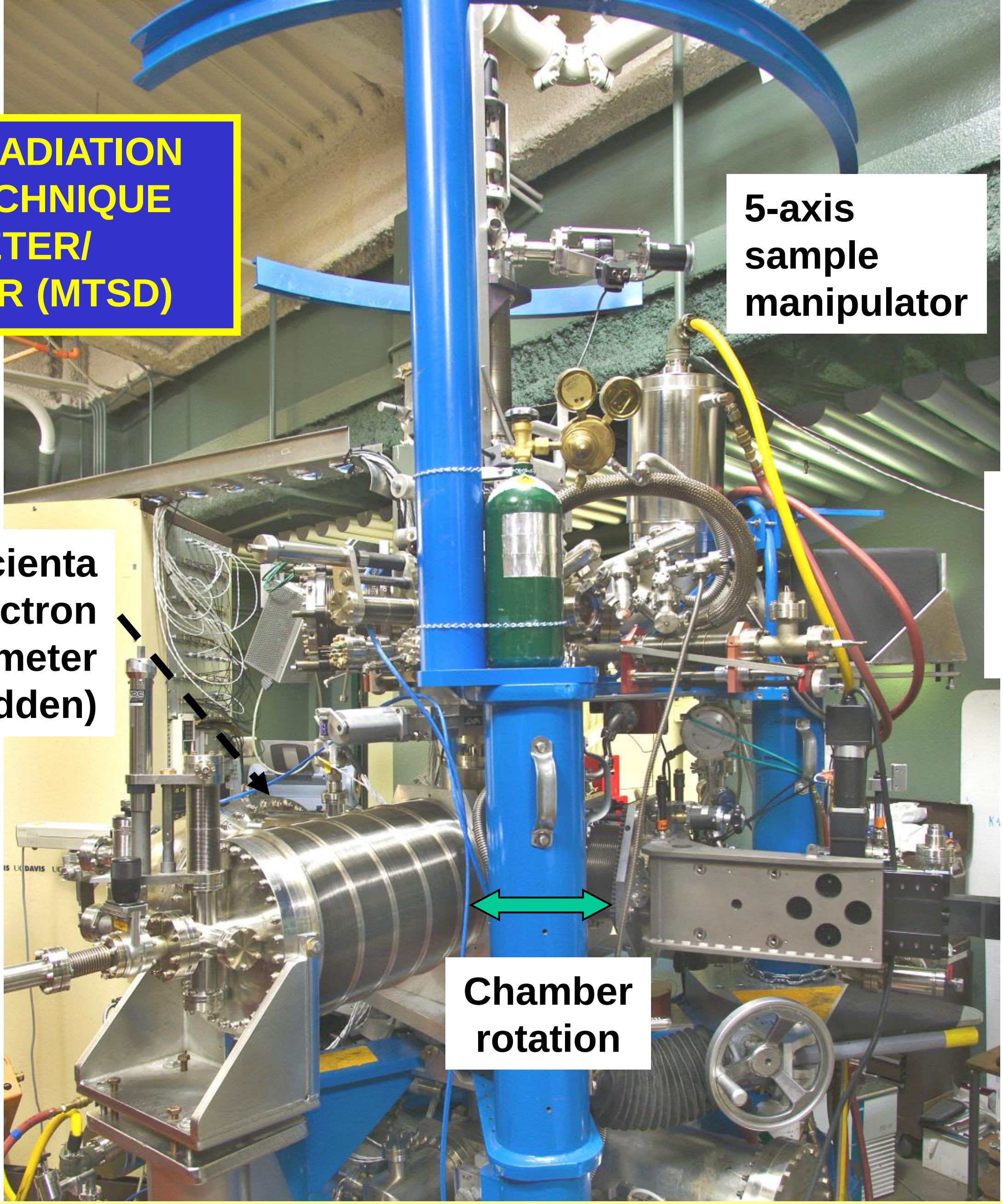
~TIME FOR ONE MONOLAYER:

t	P(torr)
10^{-9} sec	1 atm = 760
25 sec	10^{-7}
40 min	10^{-9}
2.8 days	10^{-11}

Laboratory-based surface science system:



SYNCHROTRON RADIATION BASED MULTI-TECHNIQUE SPECTROMETER/ DIFFRACTOMETER (MTSD)



5-axis
sample
manipulator

Sample prep.
chamber: LEED,
Knudsen cells,
electromagnet,...

Scienta
electron
spectrometer
(hidden)

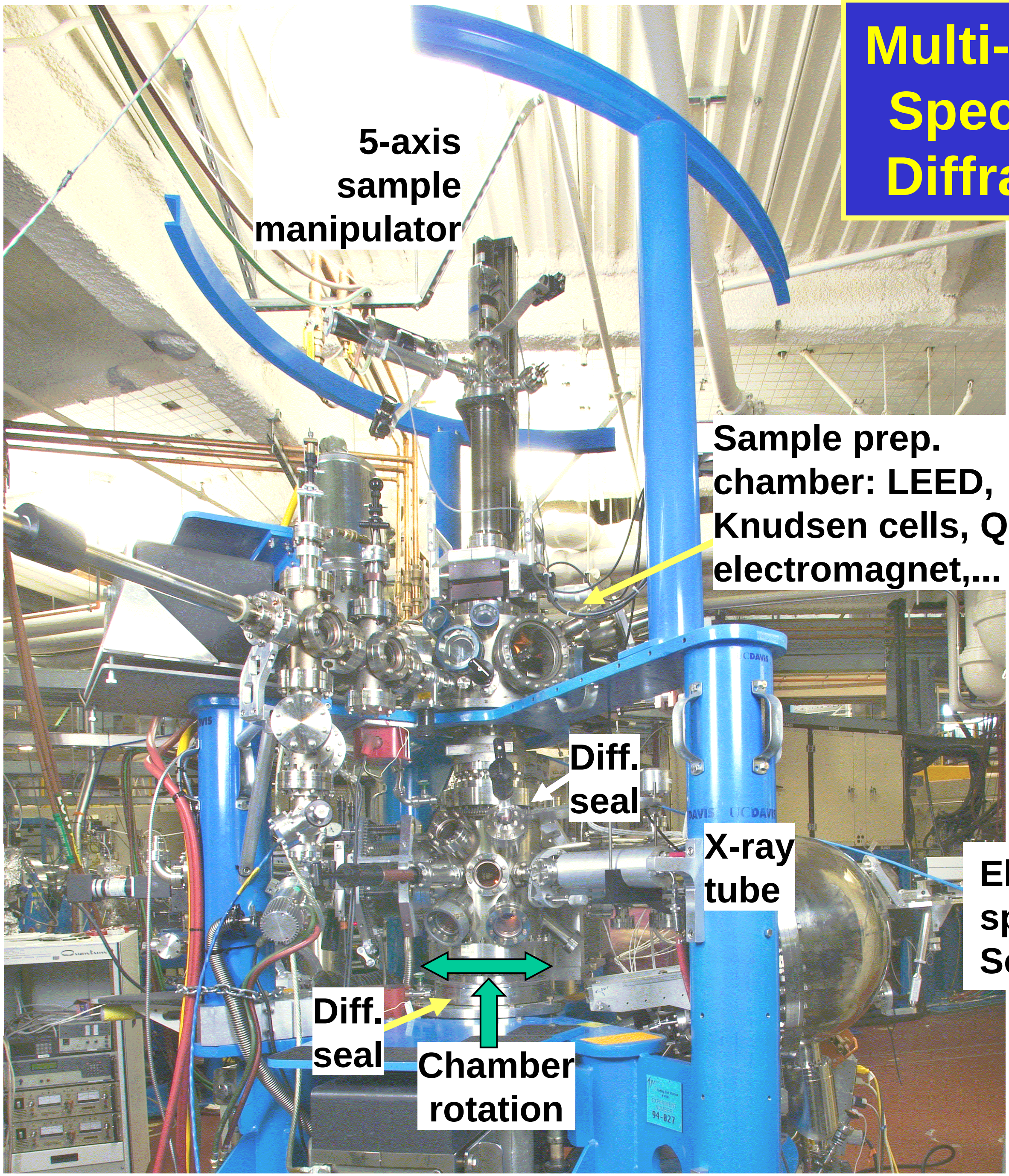
ALS
BL 9.3.1
$h\nu$ = 2-5 keV

Chamber
rotation

Scienta
soft x-ray
spectrometer

Permits using all relevant soft and hard x-ray spectroscopies on a single sample: PS, PD, PH; XAS (e^- or photon detection), XES/RIXS, with MCD, MLD

Multi-Technique Spectrometer/ Diffractometer



5-axis sample manipulator

Loadlock for sample introduction

Sample prep. chamber: LEED, Knudsen cells, QCM, electromagnet,...

Diff. seal

Soft x-ray spectrometer: Scienta XES 300

X-ray tube

Electron spectrometer: Scienta SES 200

Diff. seal

Chamber rotation