Artificially atomically engineered materials for storage and cognitive computing applications

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→ Complex, multi-functional materials for emerging devices

1. Beyond silicon: cognitive devices for low power computing
2. Spintronic devices: novel phenomena involving electron spin currents
3. 3D devices: e.g. Racetrack Memory – a current controlled shift register

→ Requires combination of deep understanding, advanced theoretical models, computational exploration & analytics and experimental verification

→ Useful devices require materials optimized for many distinct properties

Evolution in World's Compute Capacity

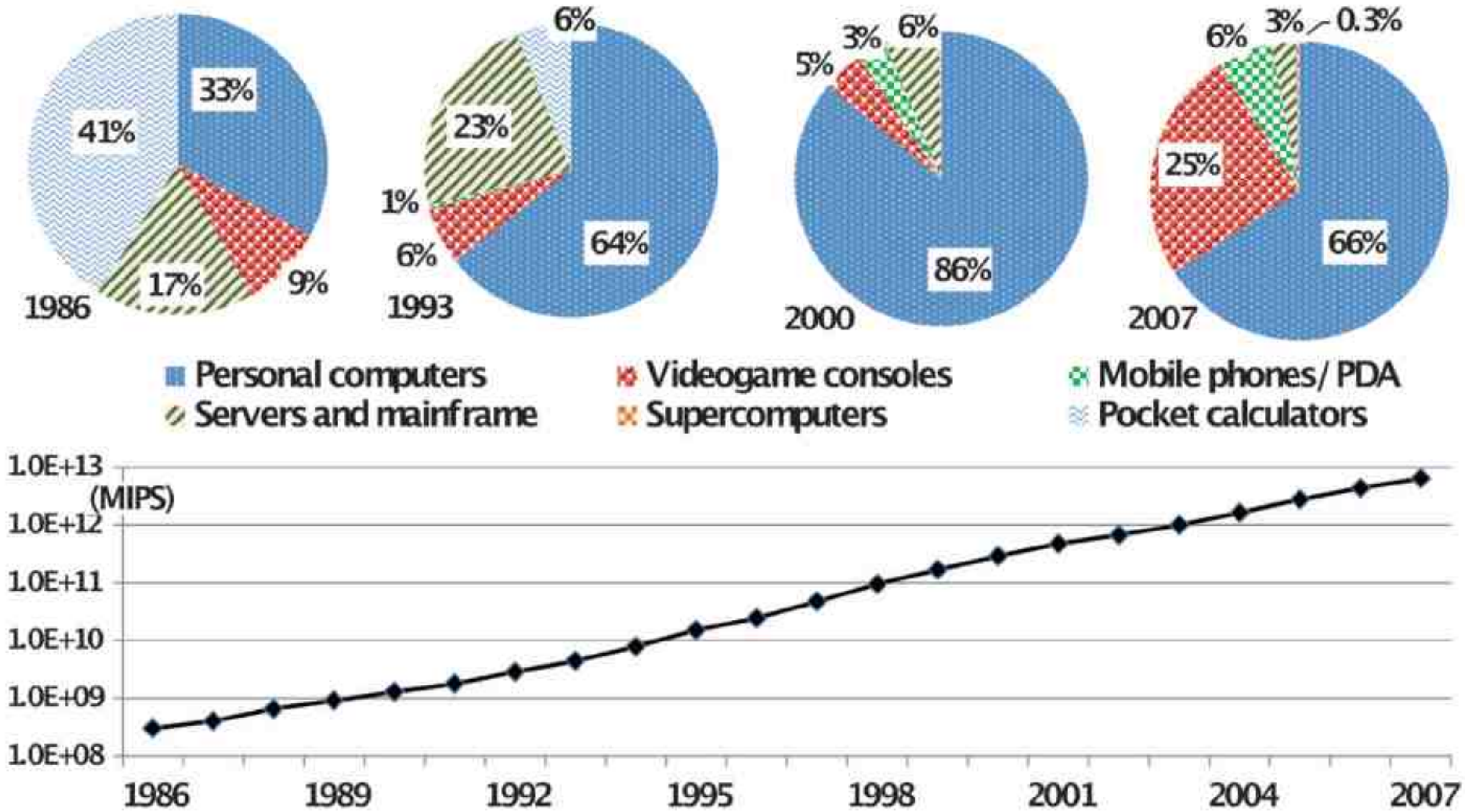


Fig. 5. World's technological installed capacity to compute information on general-purpose computers, in MIPS (table SA3) (*16*).

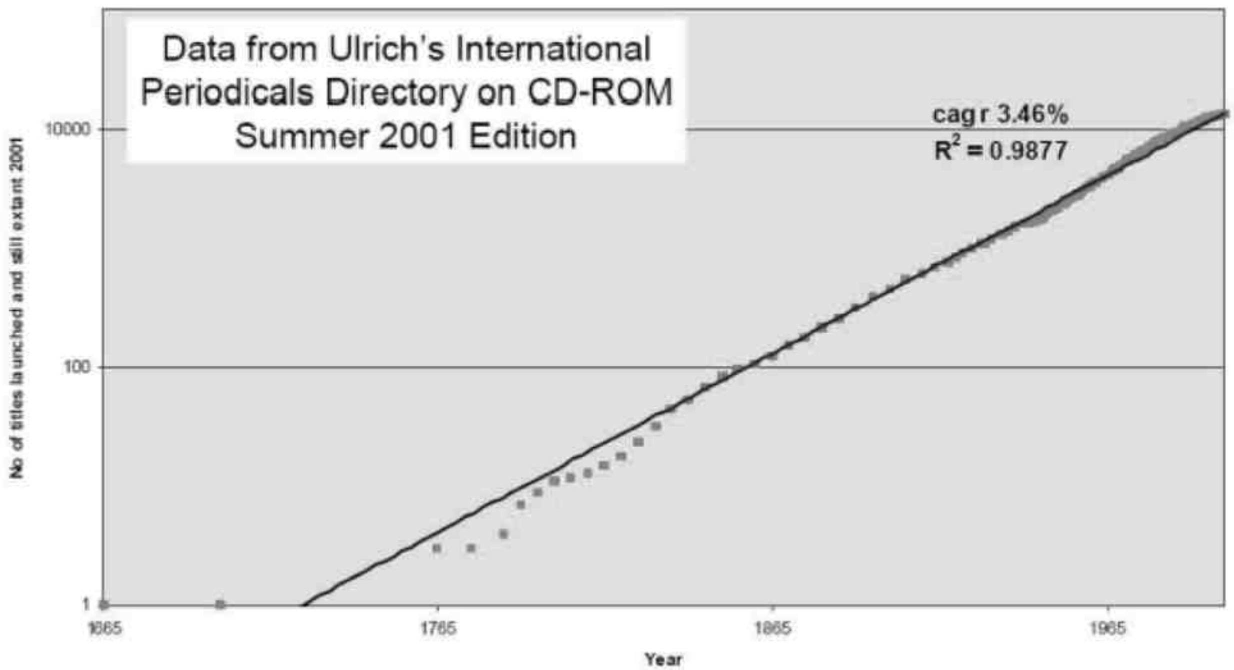
Hilbert et al. Science (2011)

Big Data

"Volume. As of 2012, about 2.5 exabytes of data are created each day, and that number is doubling every 40 months or so. More data cross the internet every second than were stored in the entire internet just 20 years ago. This gives companies an opportunity to work with many petabyes of data in a single data set—and not just from the internet. For instance, it is estimated that Walmart collects more than 2.5 petabytes of data every hour from its customer transactions. A petabyte is one quadrillion bytes, or the equivalent of about 20 million filing cabinets' worth of text. An exabyte is 1,000 times that amount, or one billion gigabytes."

"Big Data: The Management Revolution", McAfee and Brynjolfsson, Harvard Business Review, October 2012

Accessible Scientific Data



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articles
end of

Figure 1. Number of journals launched per year
Source: *Ulrich's International Periodicals Directory*, reproduced with permission from Mabe.[3]

Year

Jinha, A. E. *Learned Publishing* **2010,** 23, 258-263.

Figure 2. Estimated annual global research article output at 3% annual growth
*Year 1985 (2009 – 25 years): the doubling time for annual output for articles of just under 24 years; **1999: corresponds to estimates by Tenopir and King,[6] for research output in the late 1990s – 1 million articles per year; ***2006: corresponds very closely to Björk *et al.*'s,[2] estimate for 2006 – 1.35 million articles; ****2007: corresponds closely to Ware's,[4] estimate for the same period – 1.4 million articles per year.

Accessible Scientific Data

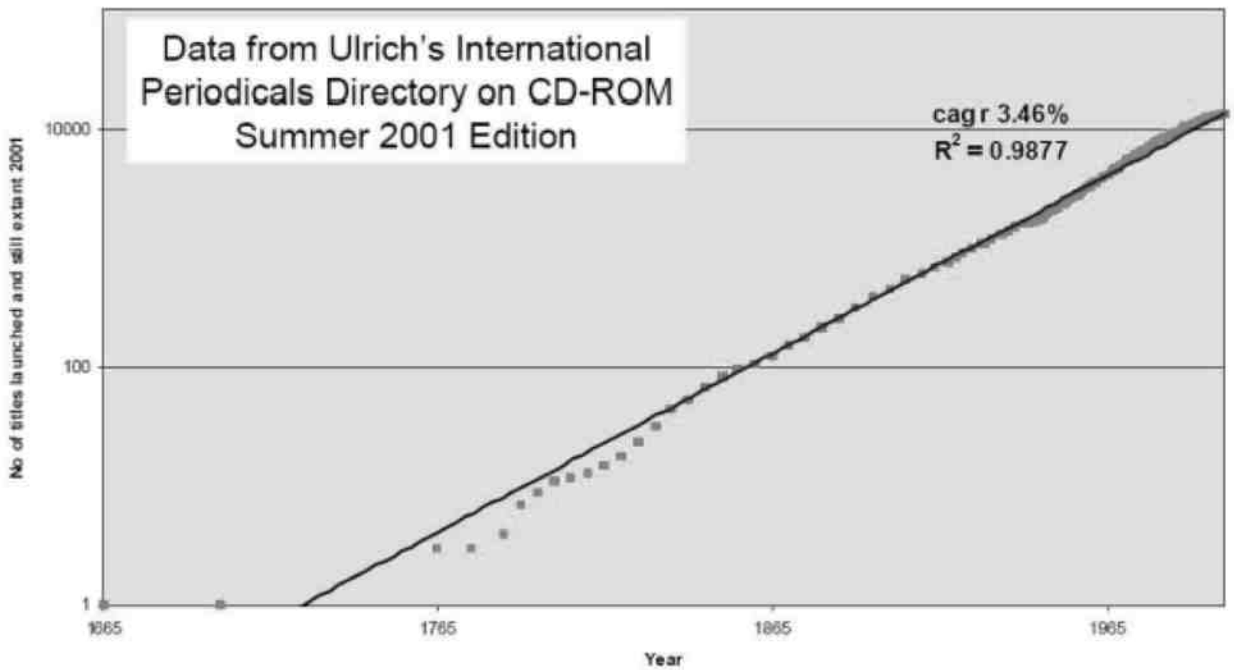


Figure 1. Number of journals launched per year
Source: *Ulrich's International Periodicals Directory*, reproduced with permission from Mabe.[3]

Jinha, A. E. *Learned Publishing* **2010,** 23, 258-263.

Most data is “locked”
→ In thousands of distinct journals
→ Not in open source journals
→ Not in searchable formats e.g. figures and tables
→ Similarly, difficult to extract useful data from patent literature

Accessible Scientific Data

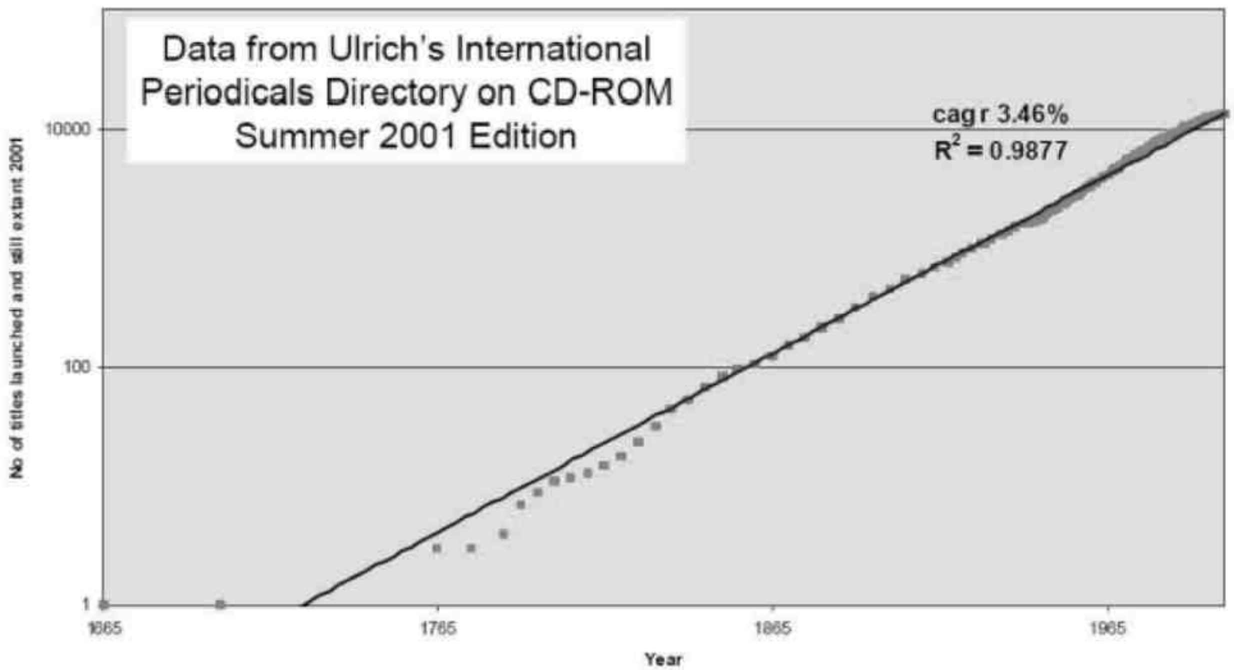
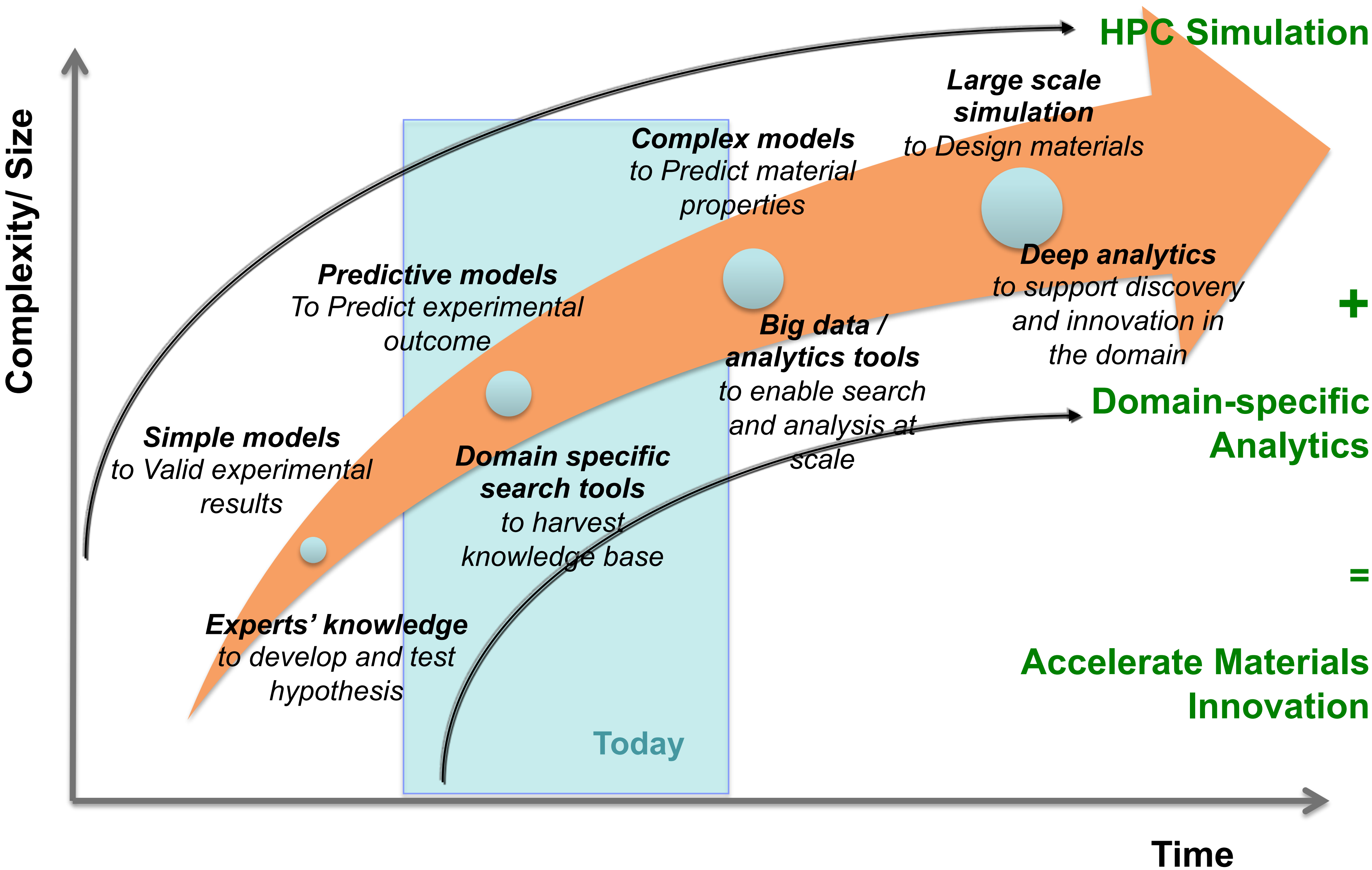


Figure 1. Number of journals launched per year
Source: *Ulrich's International Periodicals Directory*, reproduced with permission from Mabe.[3]

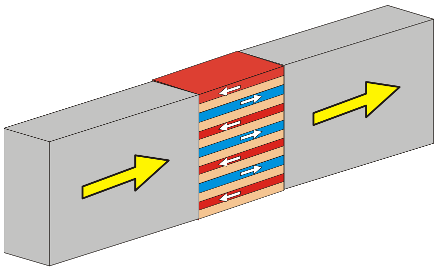
Jinha, A. E. *Learned Publishing* **2010,** 23, 258-263.

MGI: provide access to materials data
→ via a "MGI" social network
→ Need to "map" the Materials Genome with the help of all scientists
→ Need access to failures as well as successes!
→ experiments that failed are just as important as those that worked

Analytics for accelerated materials discovery



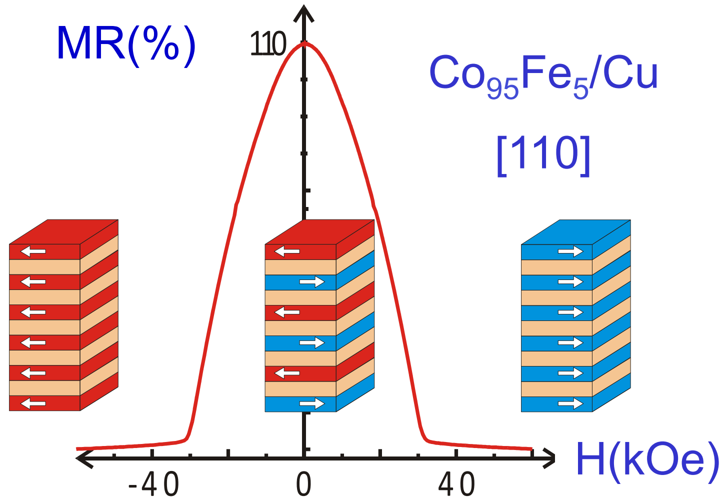
Giant Magnetoresistance (GMR)

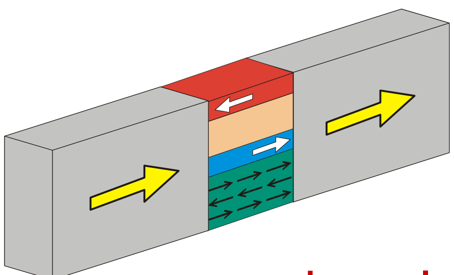


multi-layer

ΔR/R~110% at RT

Field ~10,000 Oe

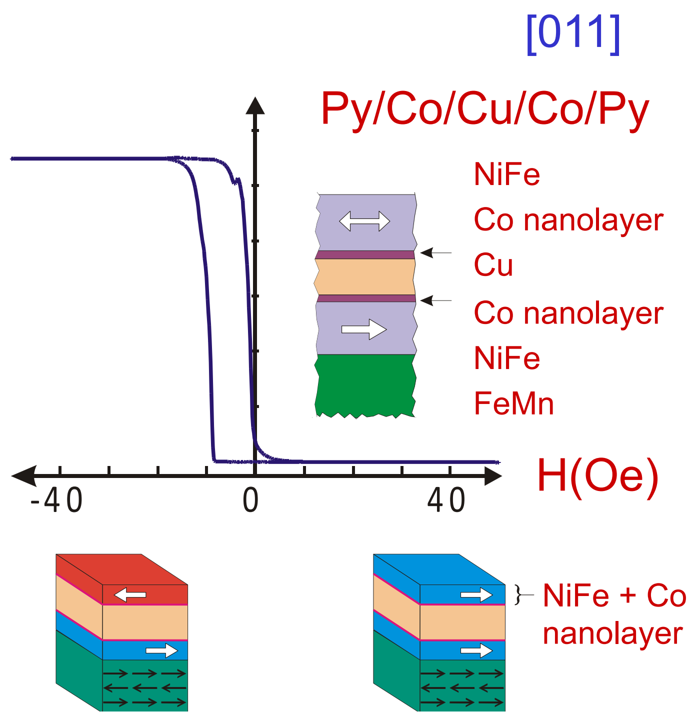




spin-valve

ΔR/R~8-17% at RT

Field ~1 Oe



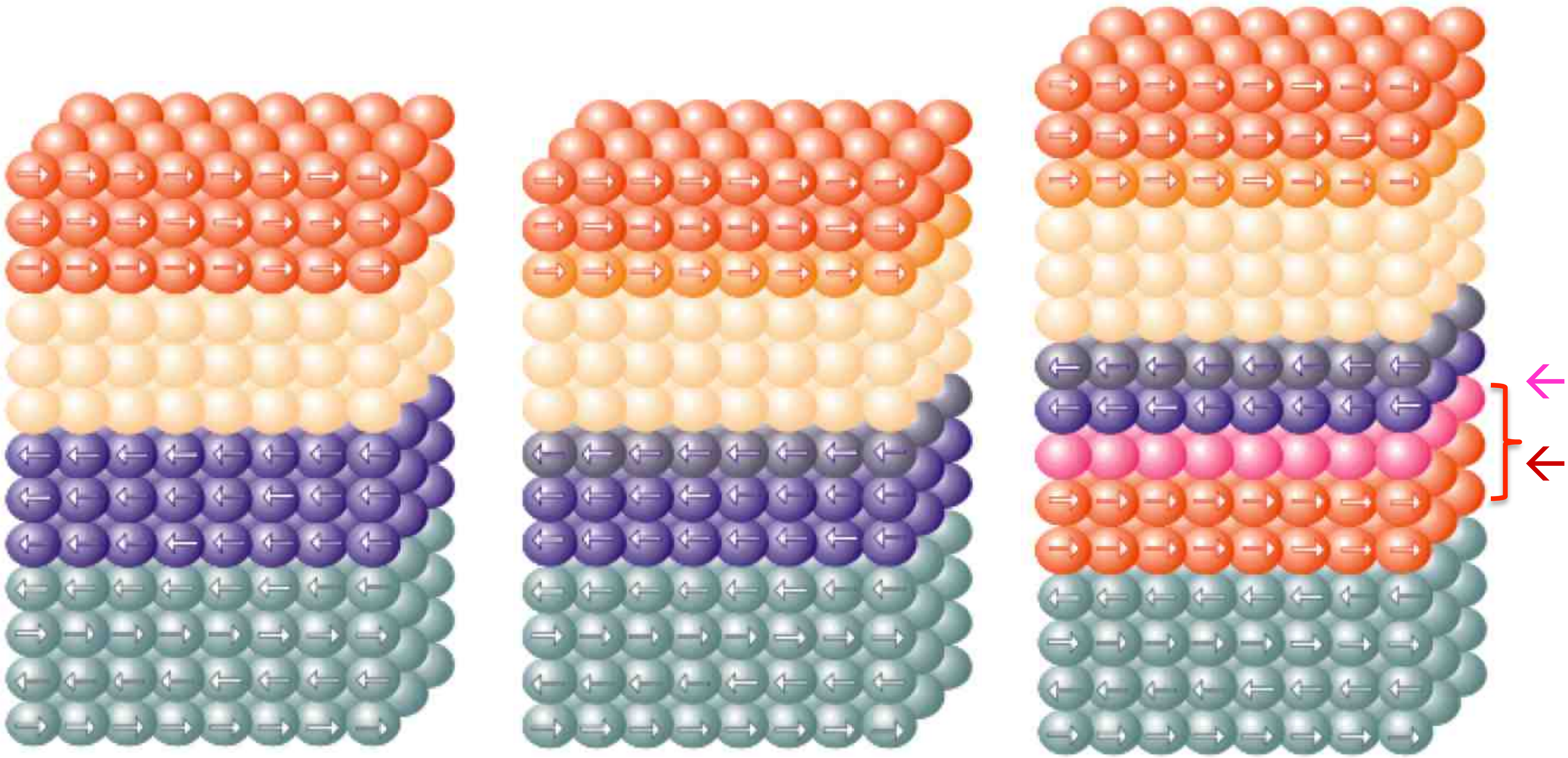
GMR

- metallic spacer between magnetic layers
- current flows in-plane of layers

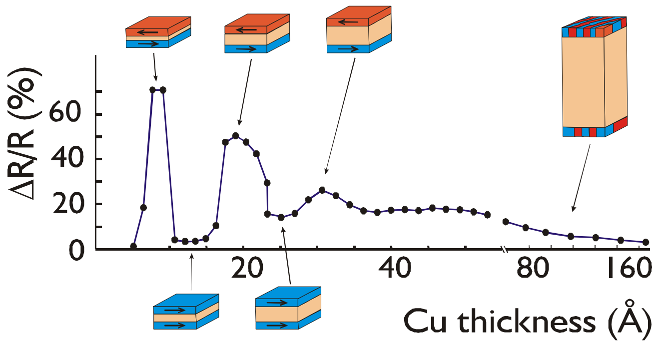
S.S.P. Parkin, in *Ultrathin Magnetic Structures*, edited by B. Heinrich and J.A.C. Bland (Spinger-Verlag, Berlin, 1994), Vol. II, pp. 148.

Magnetic engineering at the atomic scale

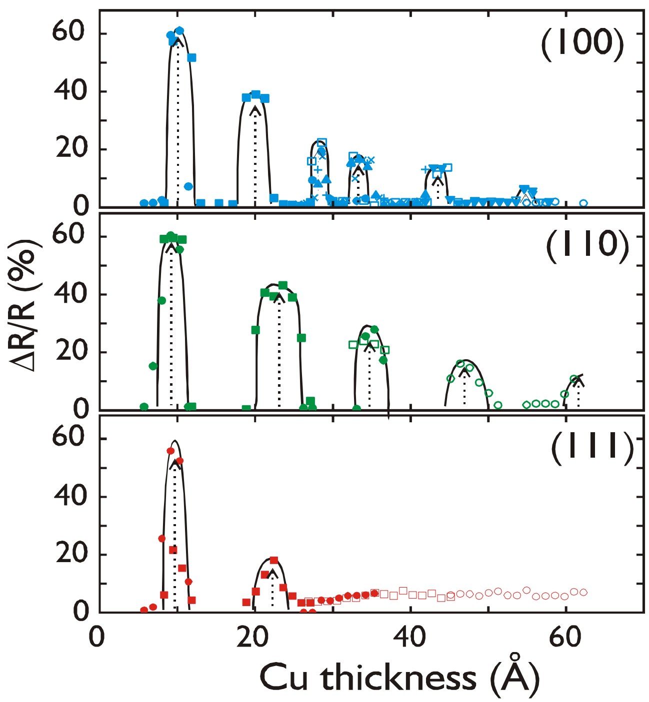
Spin-valve GMR sensor → + interface engineering to optimize transport → + Artificial Antiferromagnet to engineer magnetics

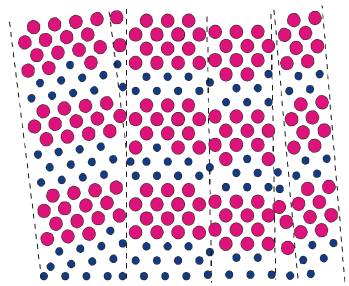


Oscillatory Giant Magnetoresistance (GMR)

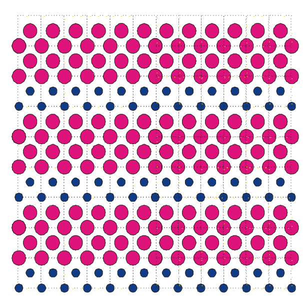


→ Peaks in GMR when AF coupling via Cu layer





Polycrystalline



Single crystalline

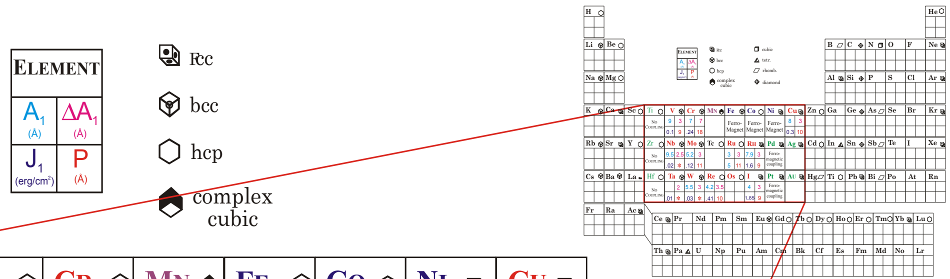
→ oscillatory interlayer coupling mediated by atomically thin Cu layers

→ oscillation periods ranging from 5 to 12 Å

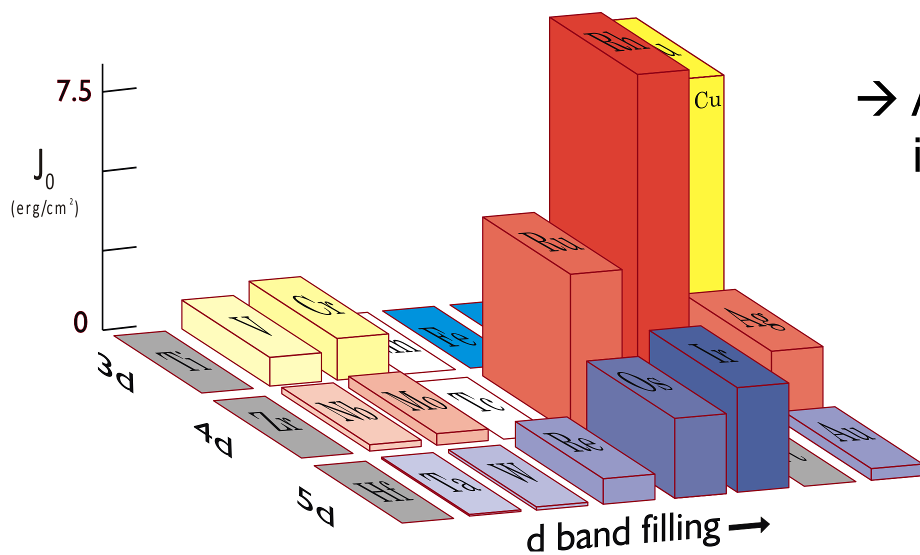
→ oscillation periods could be foreseen from Fermi surface topology

Parkin et al, Phys. Rev. Lett. 66, 2152 (1991)

Periodic Table of Oscillatory Exchange Coupling Strengths



Element	Structure	A_1 (Å)	ΔA_1 (Å)	J_1 (erg/cm²)	P (Å)
Ti	hcp	No coupling			
V	bcc	9	3	0.1	9
Cr	bcc	7	7	.24	18
Mn	complex cubic				
Fe	bcc	Ferro-magnet			
Co	hcp	Ferro-magnet			
Ni	fcc	Ferro-magnet			
Cu	fcc	8	3	0.3	10
Zr	hcp	No coupling			
Nb	bcc	9.5	2.5	.02	*
Mo	bcc	5.2	3	.12	11
Tc	hcp				
Ru	hcp	3	3	5	11
Rh	fcc	7.9	3	1.6	9
Pd	fcc	Ferro-magnetic coupling			
Ag	fcc				
Hf	hcp	No coupling			
Ta	bcc		2	.01	*
W	bcc	5.5	3	.03	*
Re	hcp	4.2	3.5	.41	10
Os	hcp				
Ir	fcc	4	3	1.85	9
Pt	fcc	Ferro-magnetic coupling			
Au	fcc				

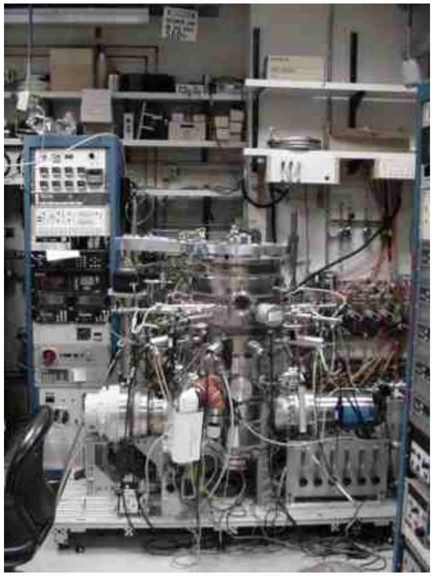


- Strength of interlayer coupling could not be predicted without a detailed understanding of underlying physics
- Interfacial property

→ Analytical models are very important!

Parkin, Phys. Rev. Lett. 67, 3598 (1991)

Thin-film materials exploration



1992-1995: S-System

6 magnetron sources

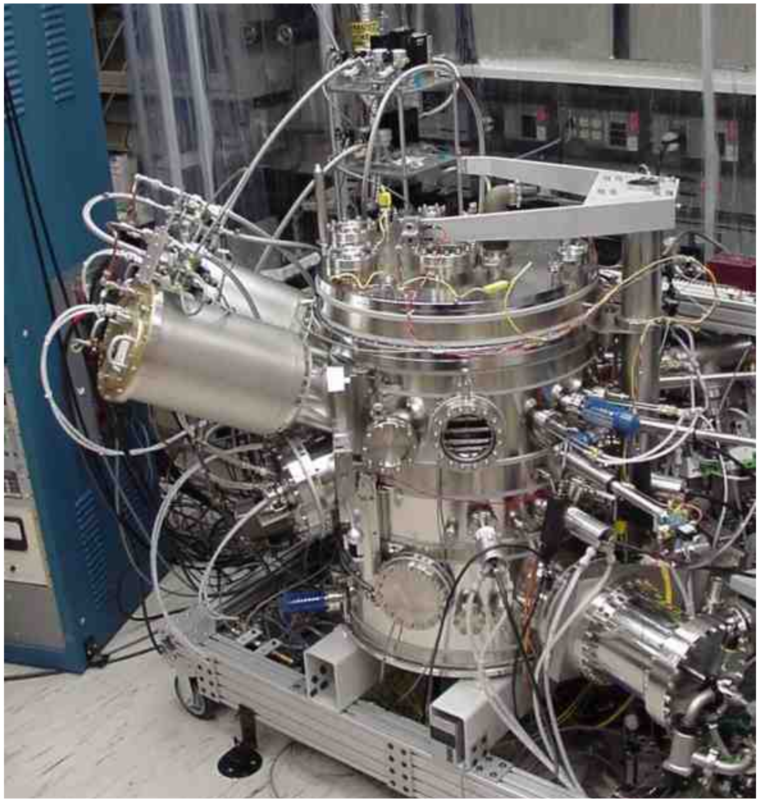
1 oxidation source

max deposition temp: 550 C

~82,000 films

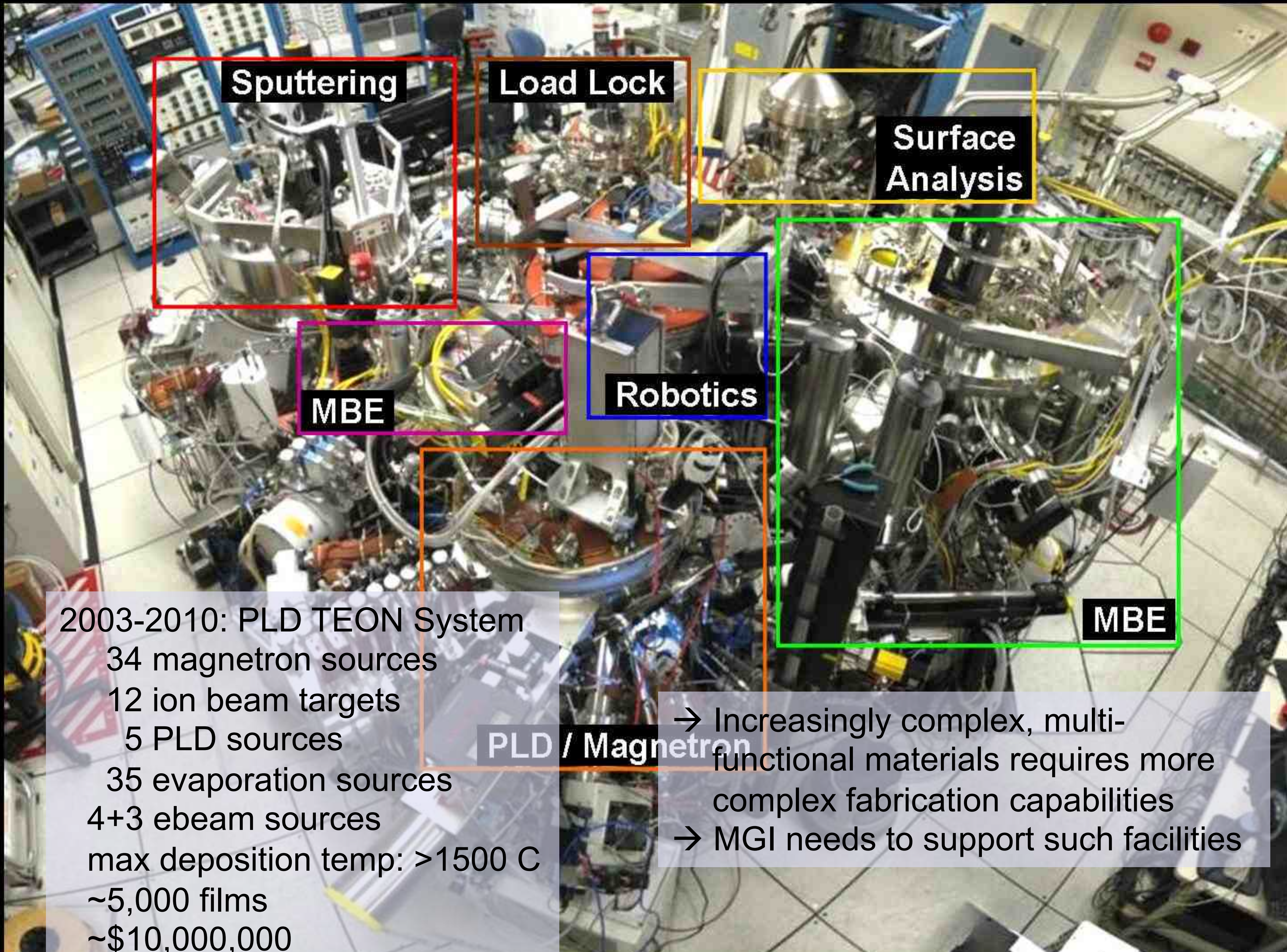
~$100,000

Thin-film materials exploration



1997-1999: A system

- 9 magnetron sources
- 5 ion beam sputter targets
- max deposition temperature: 550 C
- ~52,000 films
- ~$400,000



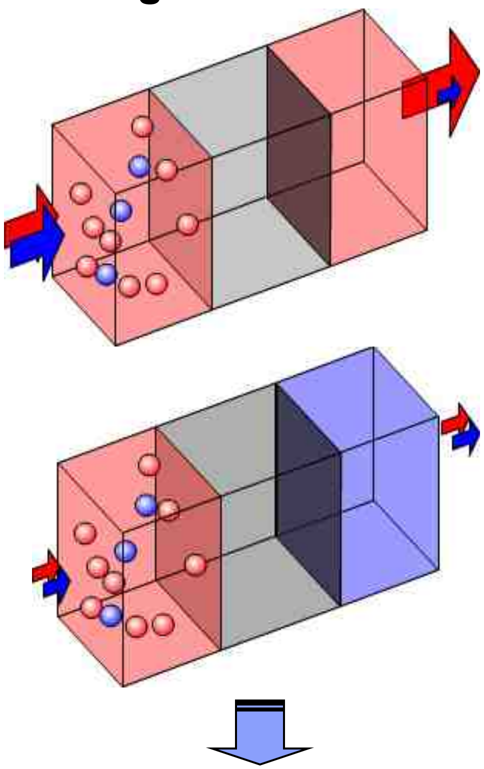
2003-2010: PLD TEON System
- 34 magnetron sources
- 12 ion beam targets
- 5 PLD sources
- 35 evaporation sources
- 4+3 ebeam sources
- max deposition temp: >1500 C
- ~5,000 films
- ~$10,000,000

→ Increasingly complex, multi-functional materials requires more complex fabrication capabilities

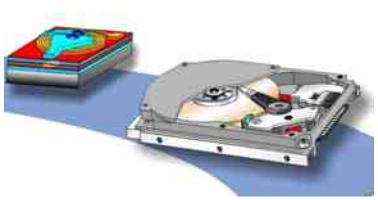
→ MGI needs to support such facilities

Magnetic Memory & Storage

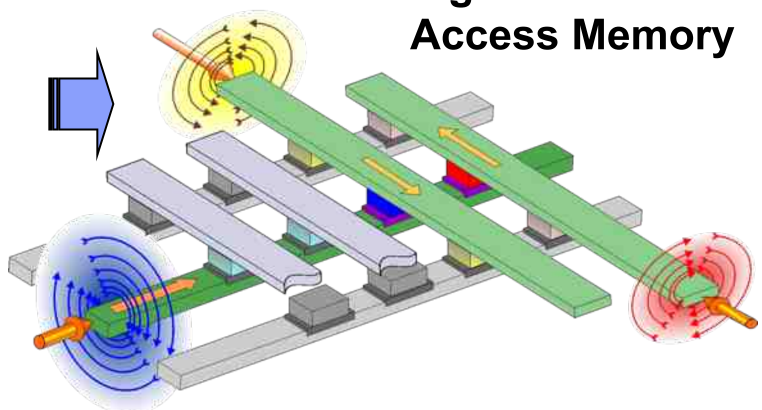
Magnetic Tunnel

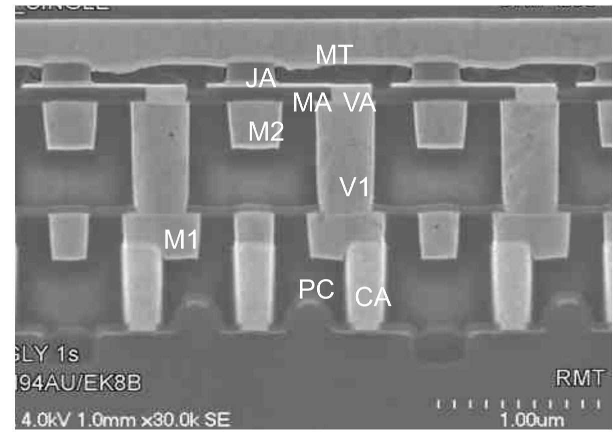


Read Heads – Disk Drives



Magnetic Random Access Memory





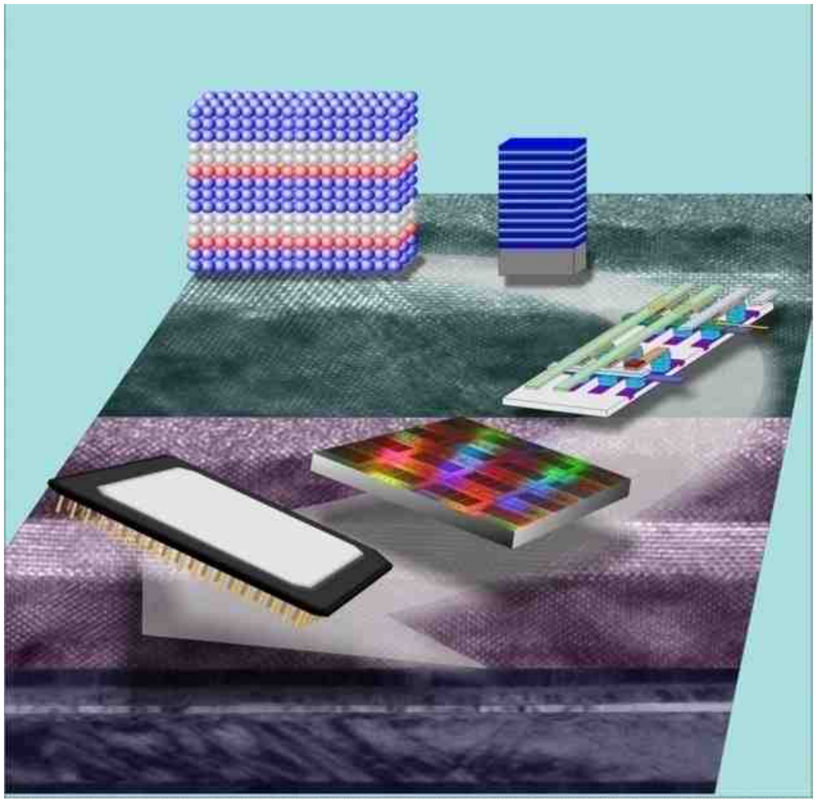
IBM-IFX 16Mbit MRAM

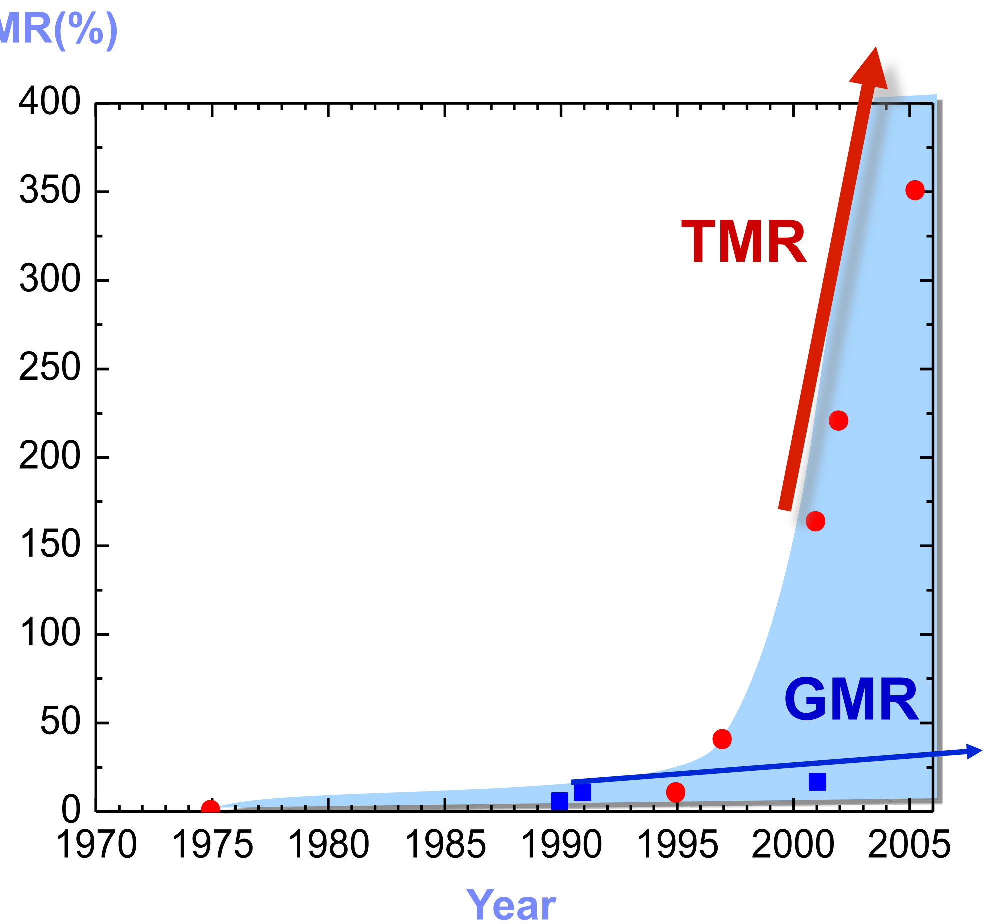
Fast reading and writing
→ High performance
→ Good endurance
→ High cost

New materials for MTJ needed
→ Extant materials (CoFeB/MgO) suitable to ~30 nm node
→ Need materials with higher magnetic anisotropy for 10 nm node

Massive storage capacity
→ Very cheap
→ But slow and unreliable!

Giant Magnetoresistance – materials evolution

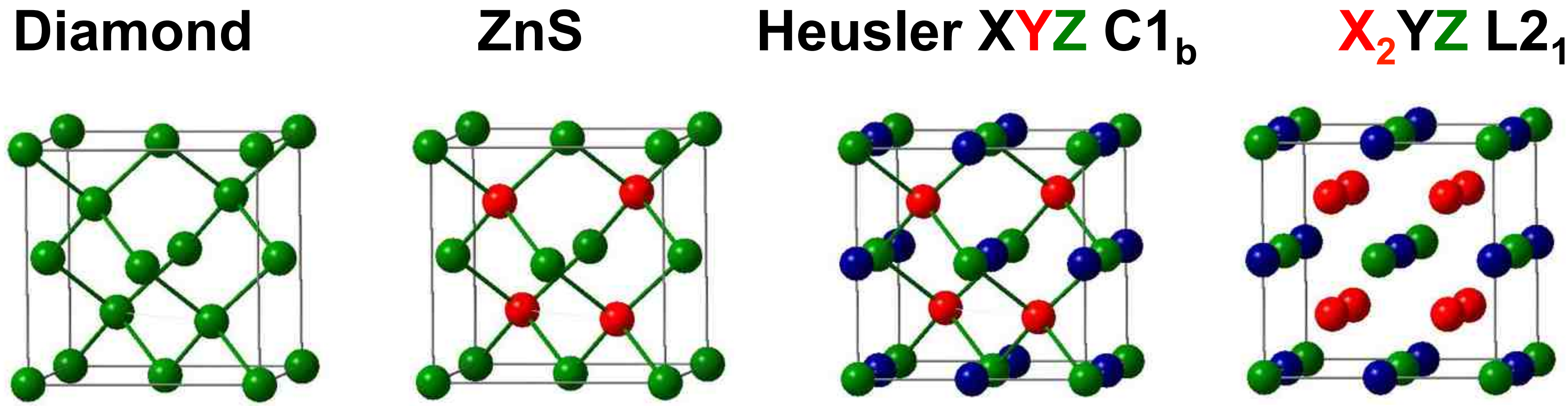




→Huge room temperature TMR values in MTJs useful for memory and sensing applications using CoFe(B) / MgO ~220% in 2001-2002: → 400-600% today!

[*Parkin et al. Nature Mater. (2004); Yuasa et al. Nature Mater. (2004)*]

Heusler Compounds

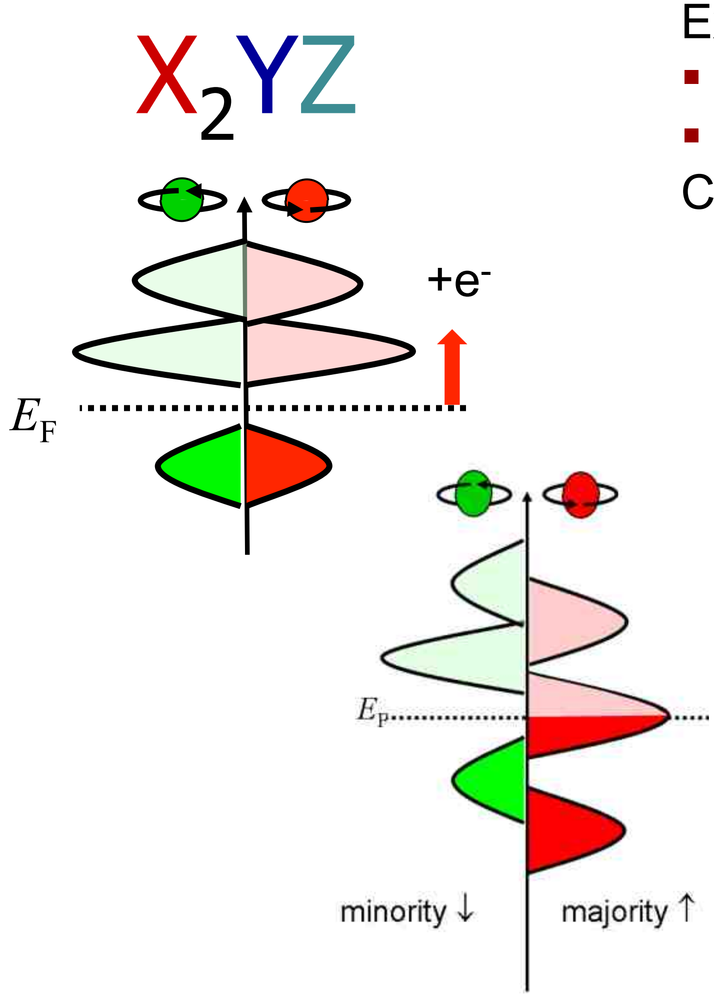


C 2.55	N 3.04
Si 1.90	P 2.19
Ge 2.01	As 2.18
Sn 1.96	Sb 2.05

H 2.20																	He
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60
Cs 0.79	Ba 0.89		Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn
Fr 0.70	Ra 0.90																
			La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27
			Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30

Graf, Felser, and Parkin, IEEE Trans. Magn. **47**, 367 (2011)
Graf, Felser, and Parkin, Prog. Solid State Chem. **39**, 1 (2011)

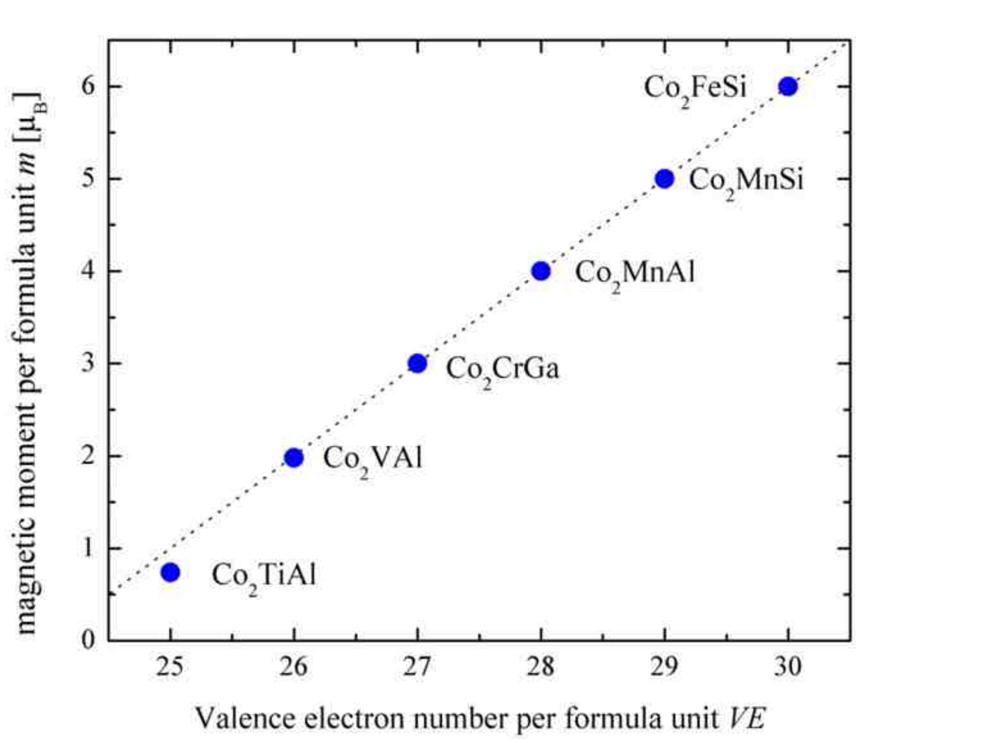
Heusler compounds → Half-metallic ferromagnets



Example: Co_2MnSi

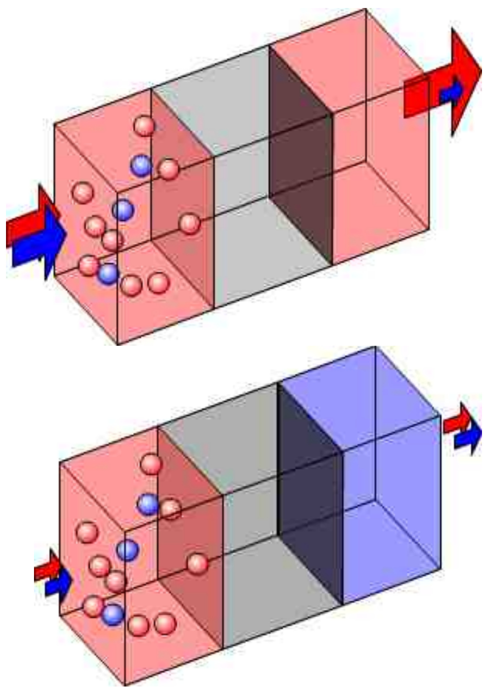
- magic valence electron number: 24
- valence electrons = 24 + magnetic moments

Co_2MnSi: 2x9 + 7 + 4 = 29 $M_s = 5\mu_B$



Kübler *et al*., PRB **28**, 1745 (1983)
Galanakis *et al*., PRB **66**, 012406 (2002)

MRAM→ ferromagnet electrode materials



$J \approx 1 - 100\ \text{MA/cm}^2$

$$J \approx \frac{e}{\hbar g} \alpha M_s H_U d$$

Shopping list for STT devices

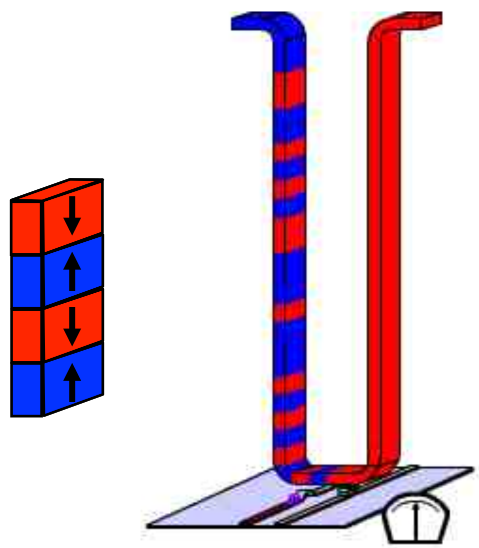
Switching by current

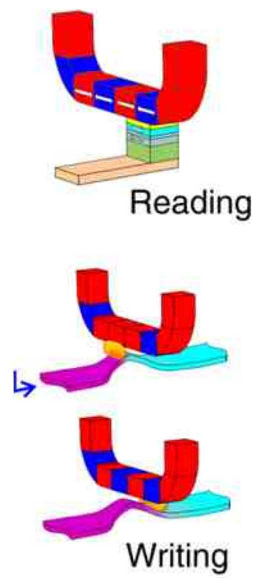
- High spin polarization
- High Curie temperature, T_C
- low magnetic damping
- low saturation magnetization
- high perpendicular anisotropy

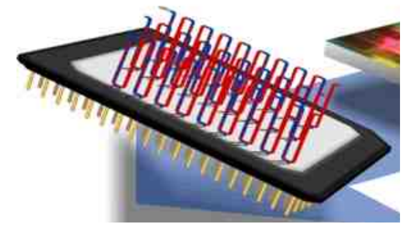
Magnetic Racetrack Memory

IBM

Vertical Racetrack

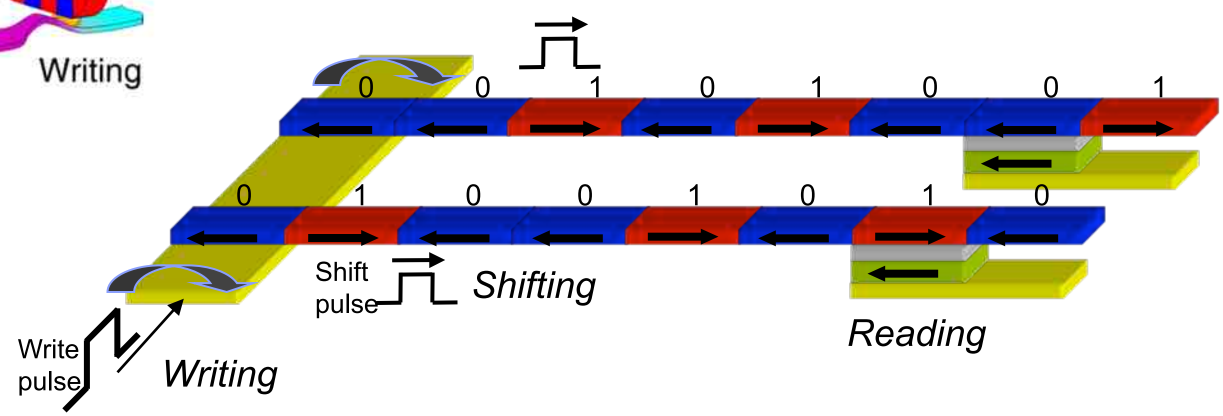






- Bits = Domains in the tracks

Horizontal Racetrack



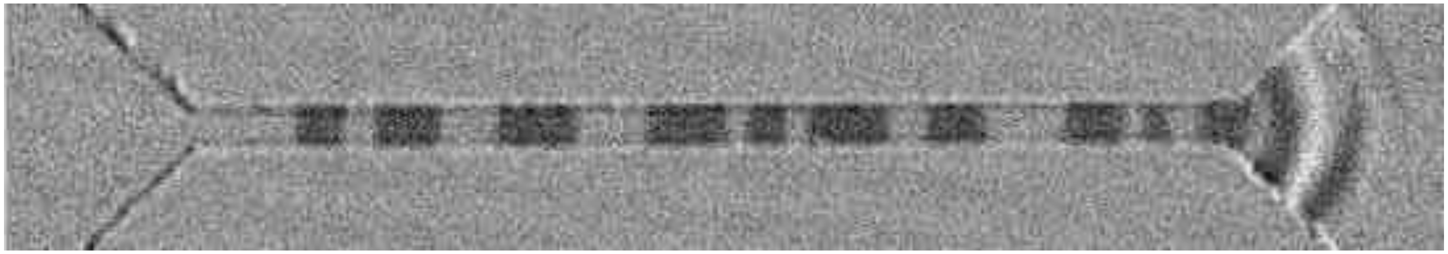
- A novel three-dimensional storage class memory

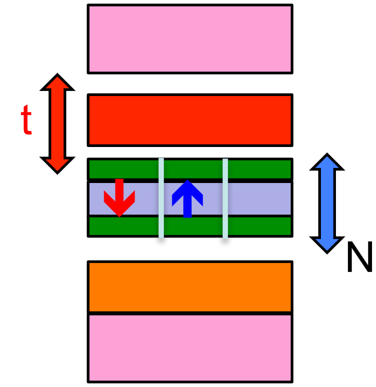
- The capacity of a hard disk drive

- The capacity of a FLASH

Parkin, US patents 6834005, 6898132
Parkin et al., Science 320, 190 (2008)
Parkin, Scientific American (2009)

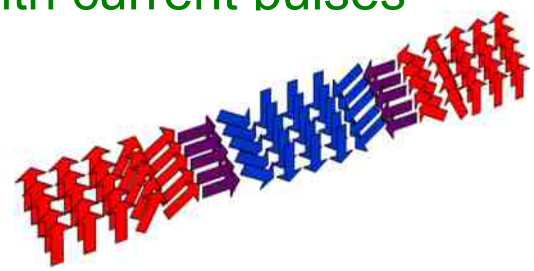
Racetrack Memory 2.0





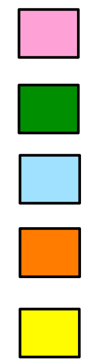
→ 20 domain walls moved in lock step with current pulses

→ High velocity at low current density

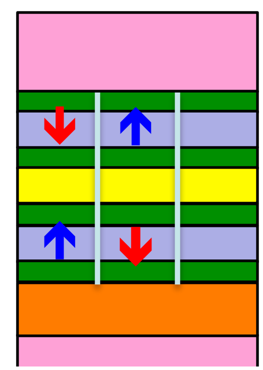


→ Narrow domain walls

→ Very thin racetracks
– writing domain walls possible with SHE, Rashba, STT



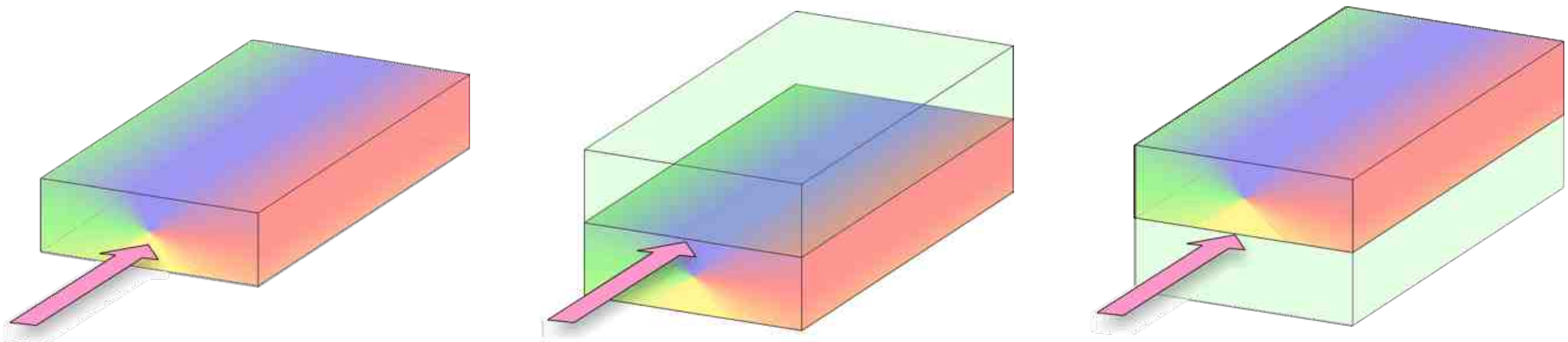
→ Remaining problem: magnetostatic coupling between domain walls solved by using a "synthetic antiferromagnet (SAF)"



Ryu et al. Nature Nano. (6- 2013)

Spin Hall Effect: due to spin orbit coupling from Pt

- Spin orbit coupling effect from current flowing in Pt layer leads to Spin Hall Effect



When current flows, spin accumulates on the edges and surfaces of the Pt layer

Spin polarization in Pt induces torque on adjacent Co layer

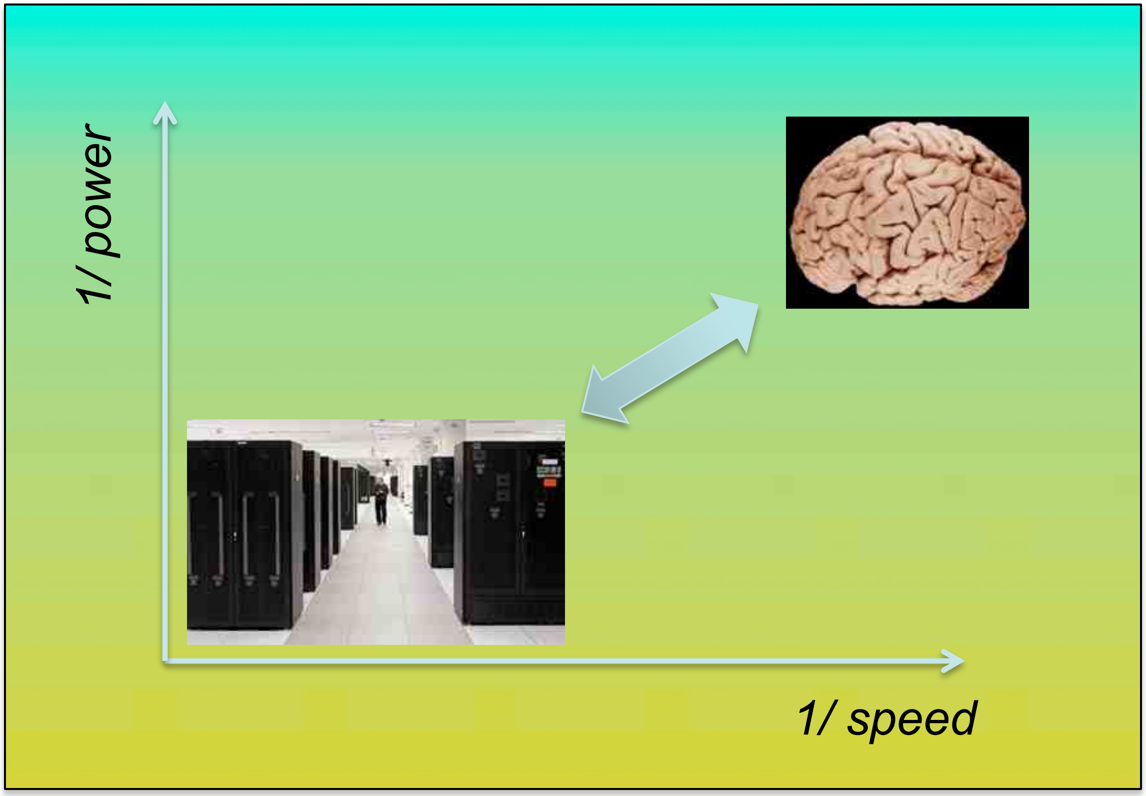
Effect on adjacent layers depends on Pt-Co order

→ Magnitude of SHE has both intrinsic and extrinsic origins

→ MGI very important to quickly identify materials with large SHE

→ Use of Inverse SHE could lead to novel cheap energy harvesting devices (Saitoh/NEC)

Silicon versus biology!



x 10^6 !

→ 10^6 performance/ energy gap between CMOS and biology!

Computers and the Brain are Dramatically Different

Computers	Brain
Separates memory and processor	Integrates memory and processor
Sequential, centralized processing	Parallel, distributed processing
Ever increasing clock rates, high active power	Event-driven, low active power
Huge passive power	Does "nothing" better, low passive power
Programmed system, hard-wired, fault-prone	Learning system, reconfigurable, fault-tolerant
Algorithms and analytics	Substrate and pattern recognition

Tuning the electronic properties of complex oxides

Charge carrier modulation by electric field effect gating

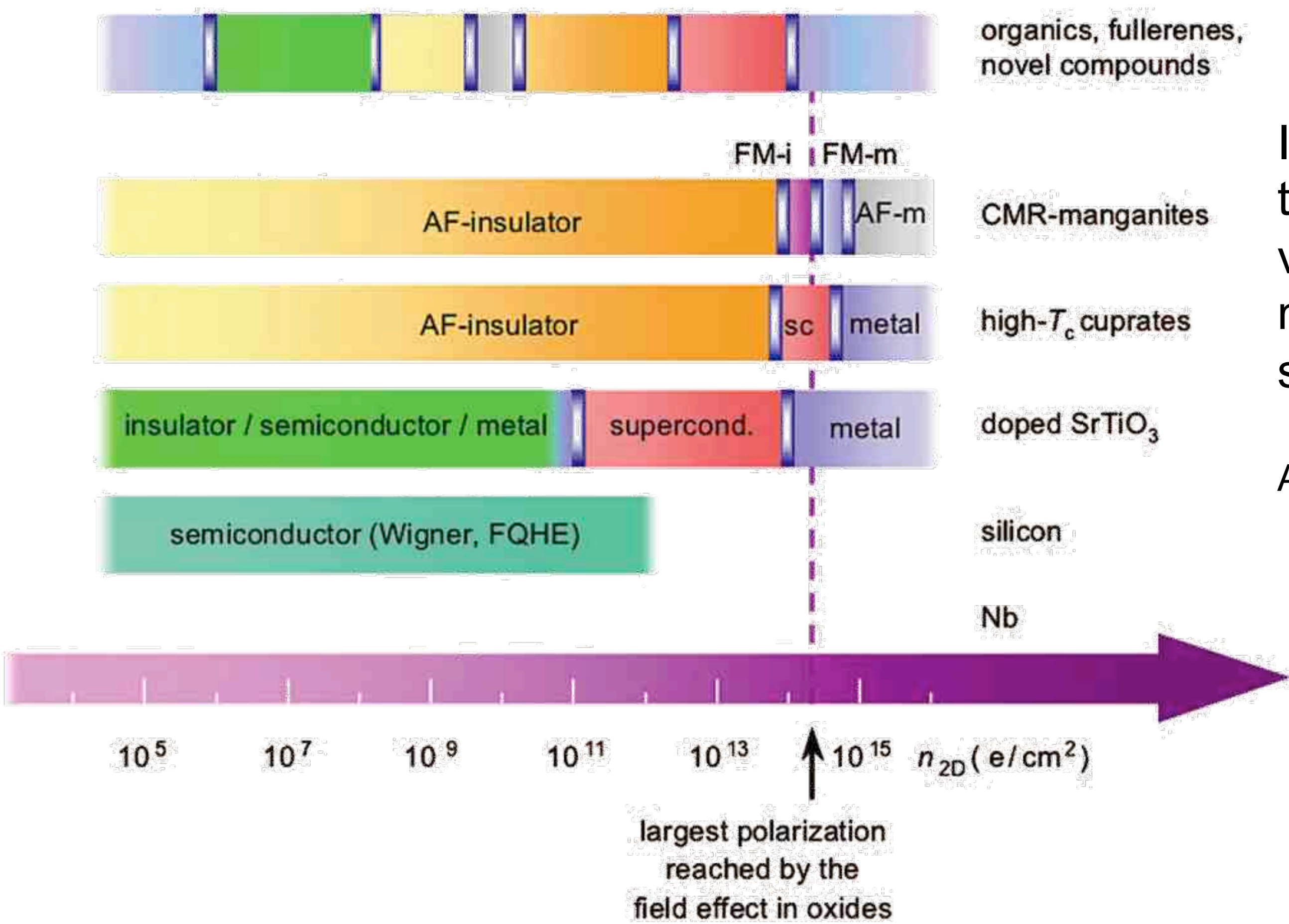
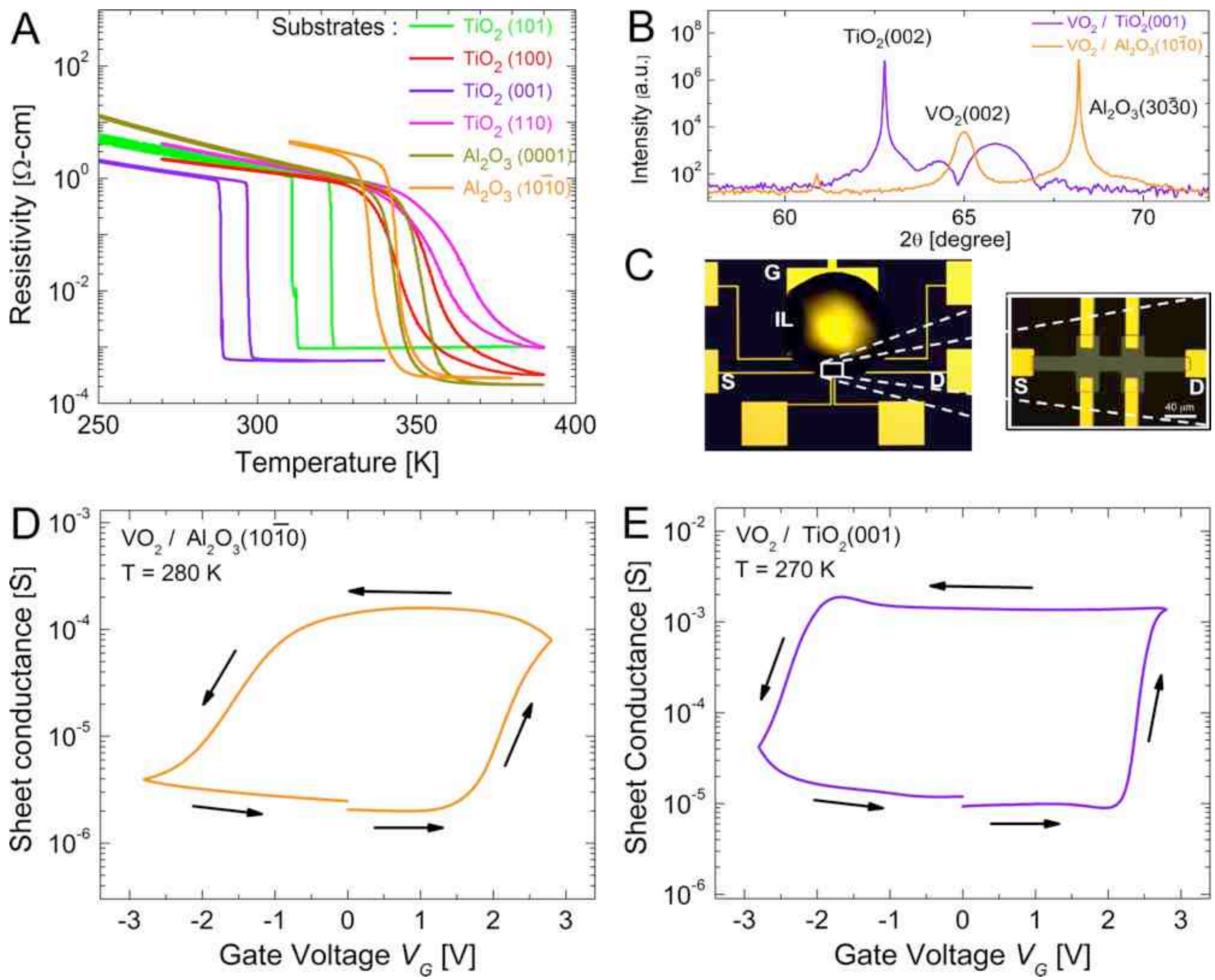
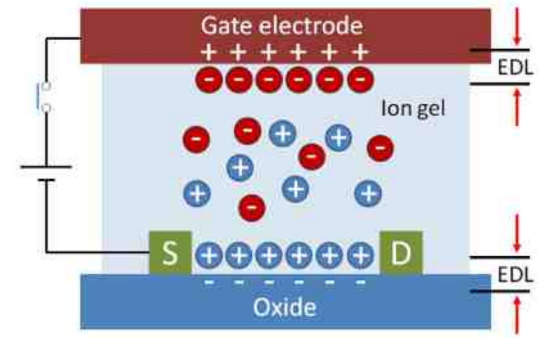


Illustration of the zero temperature behavior of various correlated materials as a function of sheet charge density.

Anh et *al.*, *Rev. Mod. Phys.* (2006)

Ionic liquid gating → electric field migration of oxygen





Ionic liquids provide for very high electric field at insulator interfaces
→ electrostatic?
→ Induces flow of ionic currents associated with migration of oxygen to/fro surface

- IL gating effect similar for VO_2 films grown on Al_2O_3 and TiO_2

Liquid Electronics

REPORTS

Suppression of Metal-Insulator Transition in VO_2 by Electric Field–Induced Oxygen Vacancy Formation

Jaewoo Jeong,[1,2] Nagaphani Aetukuri,[1,3] Tanja Graf,[1] Thomas D. Schladt,[1] Mahesh G. Samant,[1] Stuart S. P. Parkin[1*]

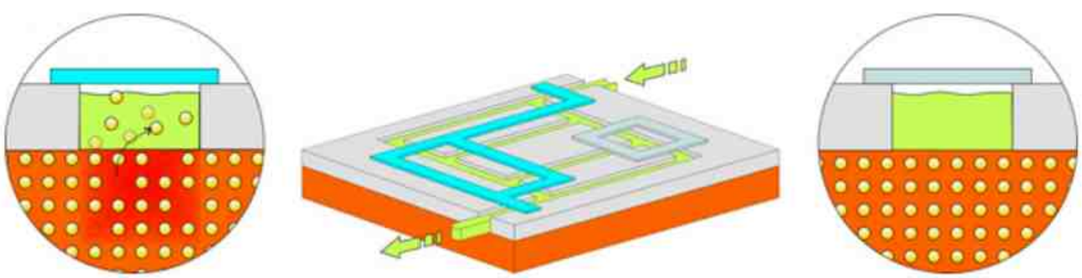
Electrolyte gating with ionic liquids is a powerful tool for inducing novel conducting phases in correlated insulators. An archetypal correlated material is vanadium dioxide (VO_2), which is insulating only at temperatures below a characteristic phase transition temperature. We show that electrolyte gating of epitaxial thin films of VO_2 suppresses the metal-to-insulator transition and stabilizes the metallic phase to temperatures below 5 kelvin, even after the ionic liquid is completely removed. We found that electrolyte gating of VO_2 leads not to electrostatically induced carriers but instead to the electric field–induced creation of oxygen vacancies, with consequent migration of oxygen from the oxide film into the ionic liquid. This mechanism should be taken into account in the interpretation of ionic liquid gating experiments.

Use nanofluidic techniques to deliver ionic liquids
→ “paint” electronic circuits
→ reconfigurable electronics

MARCH 21, 2013, 6:50 PM | 1 Comment

I.B.M. Research Points to Circuits That Mimic the Brain’s Design

By JOHN MARKOFF



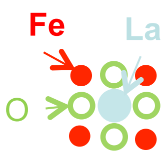
A nanofluidic circuit would operate by passing ionic fluid, shown in green, through conduits fabricated on top of a planar oxide surface, shown in orange.

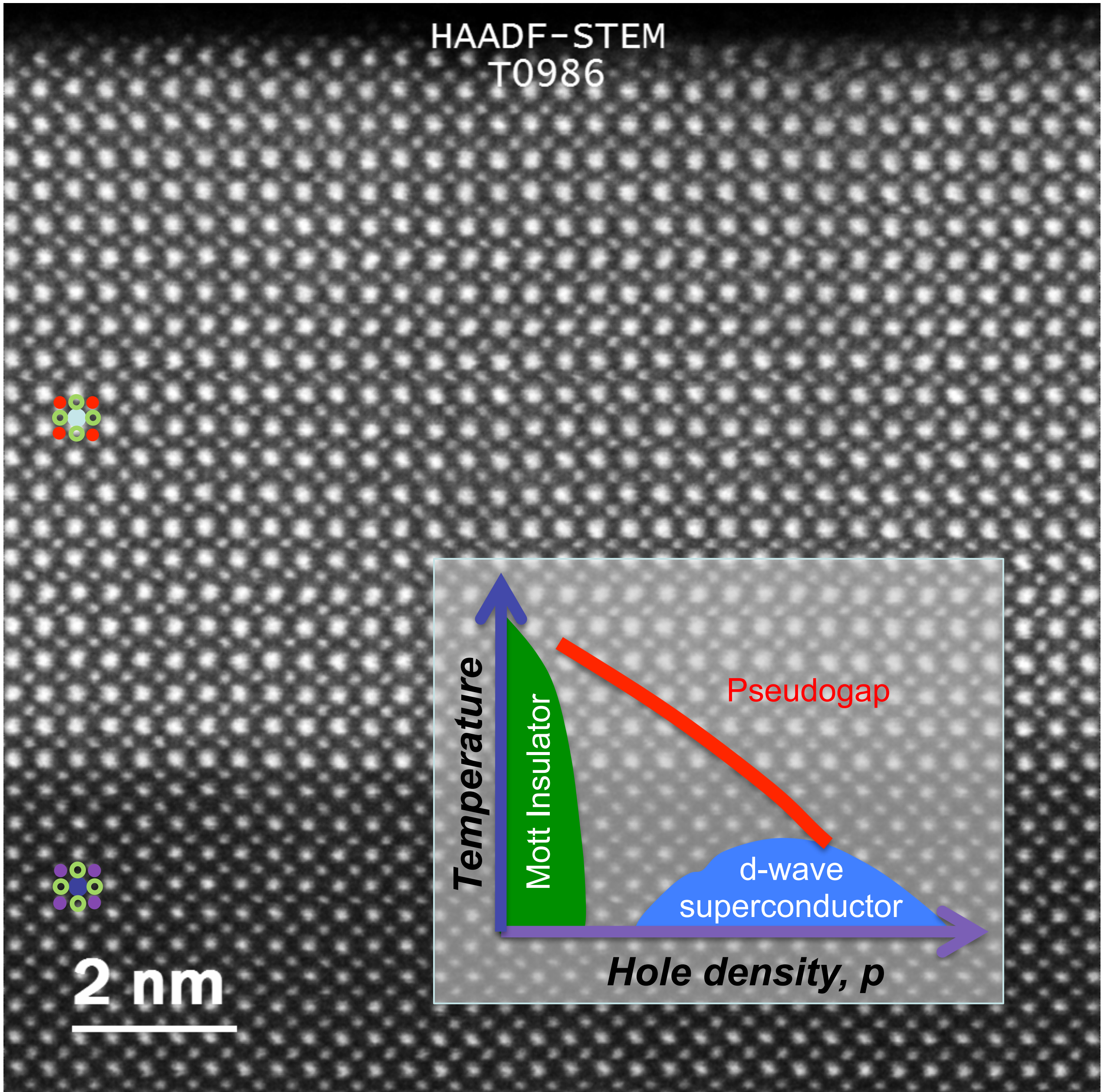

Superconductivity 297K
Synthetic Routes to
Room Temperature Superconductivity
October 17-18, 2012
Summer School: October 15-16, 2012
Chairs: Stuart Parkin, IBM Almaden
Claudia Felser, MPI-Dresden
Invited Speakers Include
(Summer School Speakers are highlighted)
Ganapathy Baskaran
Dmitri Basov
Paul Chu
Piers Coleman
Steve Conradson
John Goodenough
Gernot Guntherodt
Hideo Hosono
Hao Tjeng
Bernhard Keimer
Steve Kivelson
Gabriel Kotliar
Brian Maple
Mike Norman
David Pines
Matt Rosseinsky
George Sawatsky
Darrell Schlom
Kyle Shen
Chandra Varma
Harold Weinstock
Qi-Kun Xue
Space is limited!
For more information:
spinaps@us.ibm.com
www.regonline.com/SC297K
Almaden Institute
IBM
MATERIALS IN SCIENCE MAINZ

High temperature antiferromagnetic oxides

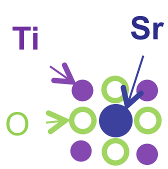
LaFeO_3

22 unit cells thick





SrTiO_3

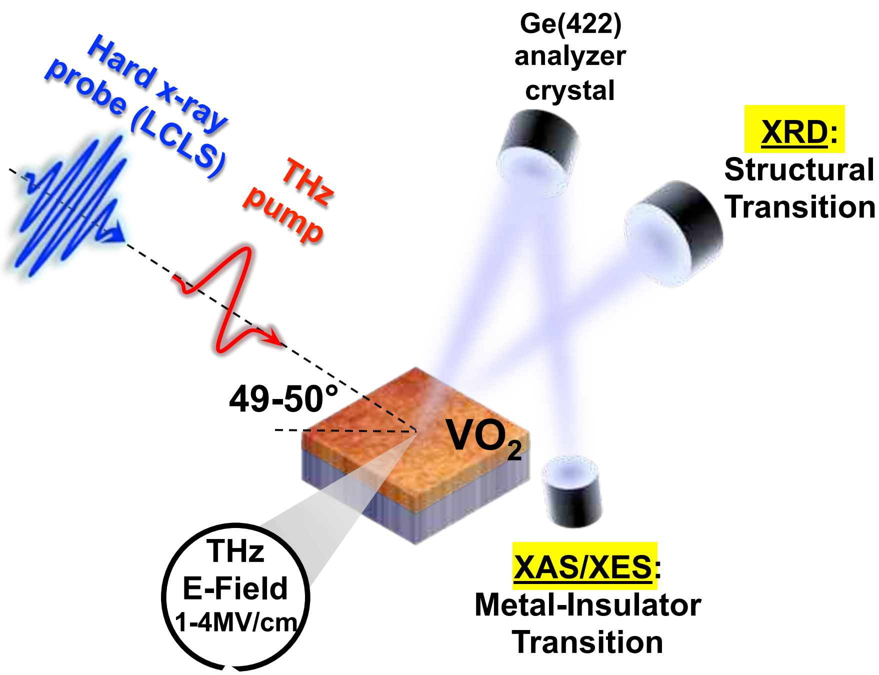


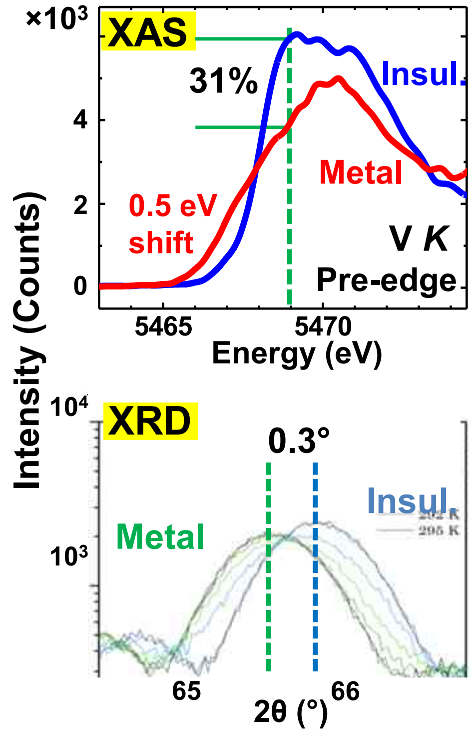
Magnification = $15x10^6$

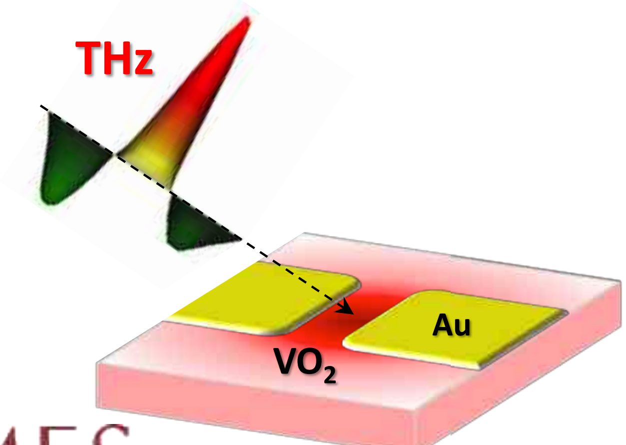
Atomic column intensity is based on the average atomic number of the elements in the column

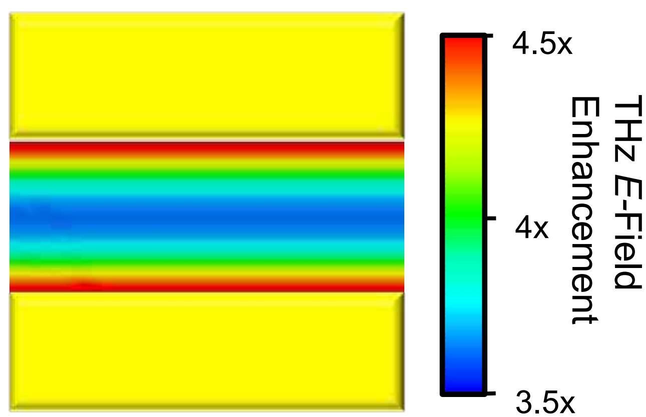
Atomic Number
La = 57
Sr = 38
Fe = 27
Ti = 22
O = 8

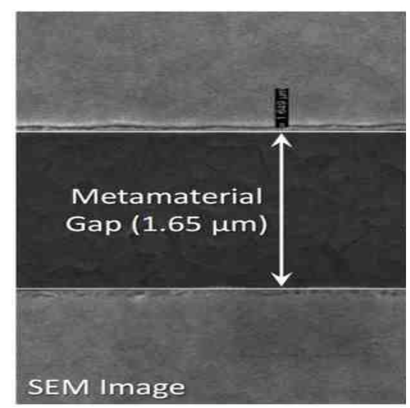
VO_2: Ultrafast Electric Field Induced Switching











Accelerated Materials Discovery - Comments

- ❑ Useful materials are complex with a suite of properties that must be met for a given application
  - → Often promising materials have unforeseen failure mechanisms
- ❑ Interfaces between materials often have very different properties from the constituent materials
  - → Inorganic/organic interfaces have very interesting functionalities
  - → Non-equilibrium materials highly interesting and can be stabilized in thin film form
- ❑ Transport properties highly dependent on defects e.g. structural, morphological..
  - → Generation of spin currents highly useful for sensor, memory, logic and energy harvesting
- ❑ Systems of devices may behave very differently from individual devices
  - → Need systems approach to inverse design/ engineer individual devices
- ❑ Cognitive devices highly important for future low-energy computing
  - → Use of ion currents allows for ultra low energy devices
- ❑ MGI most useful for evolutionary rather than revolutionary materials?
- ❑ Need investments in exploratory thin film deposition systems allowing for multiple deposition techniques

→ Outcome: computing devices that operate at 1,000,000 x less energy and think differently!

Accelerating Materials Discovery: Materials Analytics

- During the past century nearly all disruptive advances in science and technology resulted from the discovery of a new material.
- Major challenges addressing the world today, including sustainability, energy, climate, and health can only be solved by the discovery of new materials or artificially structured nano-materials or composites that address well-defined requirements.
- Advances in analytics and modeling and simulation suggest that we are at a truly disruptive juncture where computing power combined with advanced modeling and materials expertise and data-mining and data-verification could lead to accelerated computational materials discovery with dramatic world-wide impact.
- Data-mining of all extant literature to unearth materials properties and characteristics and advanced computational techniques to verify these properties would lead to an unprecedented encyclopedic database of material properties of tremendous value, which would form the basis for computational materials discovery.
- Challenge encompasses a vast skillset, ranging from the physical to the mathematical and computational sciences.