Defects in Semiconductors

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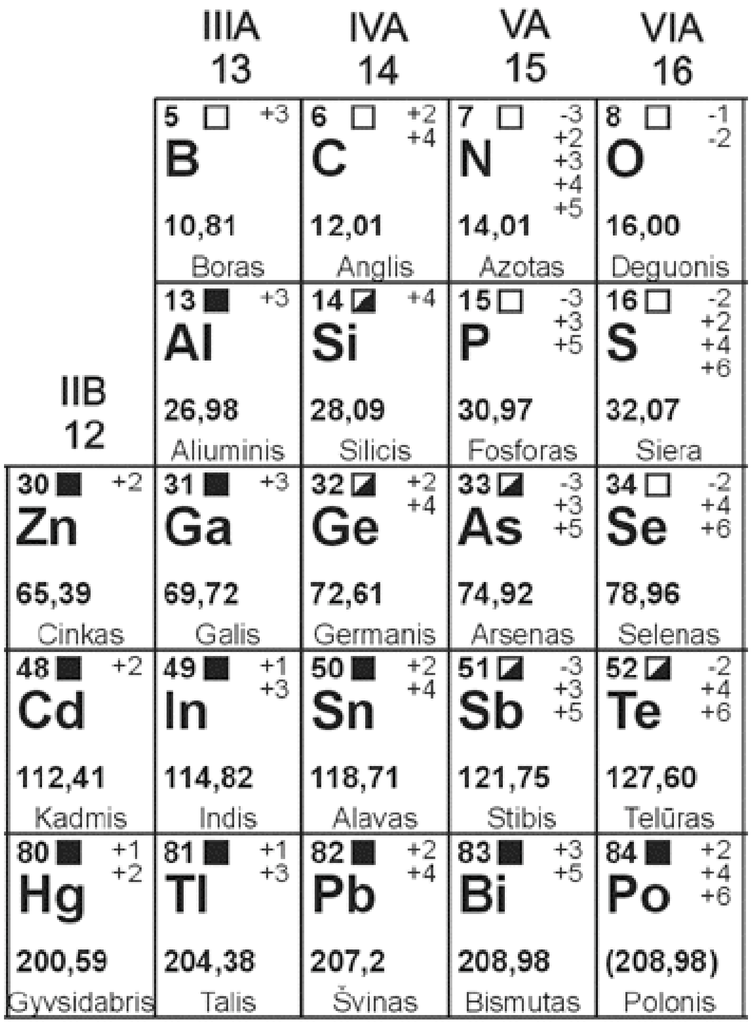
High purity silicon

- High purity materials can be processed
  - Czochralski growth method
    - Single crystals 30cm diameter and meters length
    - High purity, some C, O, B impurities (sufficient for most device applications)
  - Chemical synthesis can produce Si that is “eleven nines” pure (99.999999999%)
- Production of devices requires controlled introduction of impurities

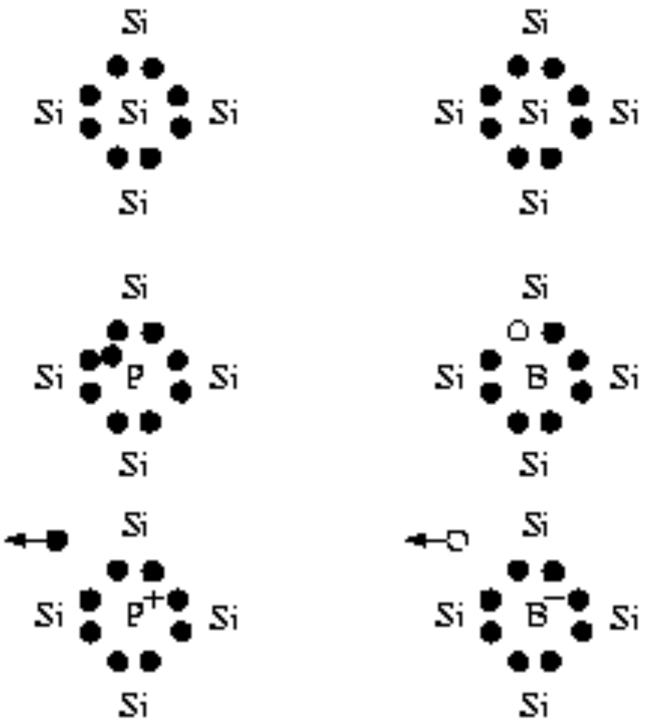
Picture from Dr. Michael L. Turner Chemistry 337 website
http://www.shef.ac.uk/~ch1mlt/teaching/chm337/

Doping of silicon



IIB 12	IIIA 13	IVA 14	VA 15	VIA 16
	5 □ +3 B 10,81 Boras	6 □ +2 +4 C 12,01 Anglis	7 □ -3 +2 +3 +4 +5 N 14,01 Azotas	8 □ -1 -2 O 16,00 Deguonis
	13 ■ +3 Al 26,98 Aliuminis	14 ◪ +4 Si 28,09 Silicis	15 □ -3 +3 +5 P 30,97 Fosforas	16 □ -2 +2 +4 +6 S 32,07 Siera
30 ■ +2 Zn 65,39 Cinkas	31 ■ +3 Ga 69,72 Galis	32 ◪ +2 +4 Ge 72,61 Germanis	33 ◪ -3 +3 +5 As 74,92 Arsenas	34 □ -2 +4 +6 Se 78,96 Selenas
48 ■ +2 Cd 112,41 Kadmis	49 ■ +1 +3 In 114,82 Indis	50 ■ +2 +4 Sn 118,71 Alavas	51 ◪ -3 +3 +5 Sb 121,75 Stibis	52 ◪ -2 +4 +6 Te 127,60 Telūras
80 ■ +1 +2 Hg 200,59 Gyvsidabris	81 ■ +1 +3 Tl 204,38 Talis	82 ■ +2 +4 Pb 207,2 Švinas	83 ■ +3 +5 Bi 208,98 Bismutas	84 ■ +2 +4 +6 Po (208,98) Polonis

Periodic table from Michael Canov’s website
http://www.jergym.hiedu.cz/~canovm/vyhledav/varianty/



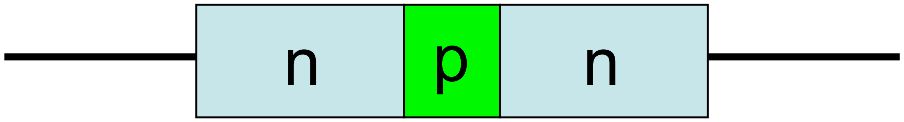
n-type semiconductor

p-type semiconductor

- Impurities modify electrical properties of silicon

Devices on silicon wafers

- The interaction between regions with different electronic properties enable devices
  - Simplest transistor npn bipolar transistor



  - Modern devices use field effect transistors (FET) which are much more complicated
- Devices possible due to precise control of doping

Photo from National Taiwan Normal University
http://www.phy.ntnu.edu.tw/

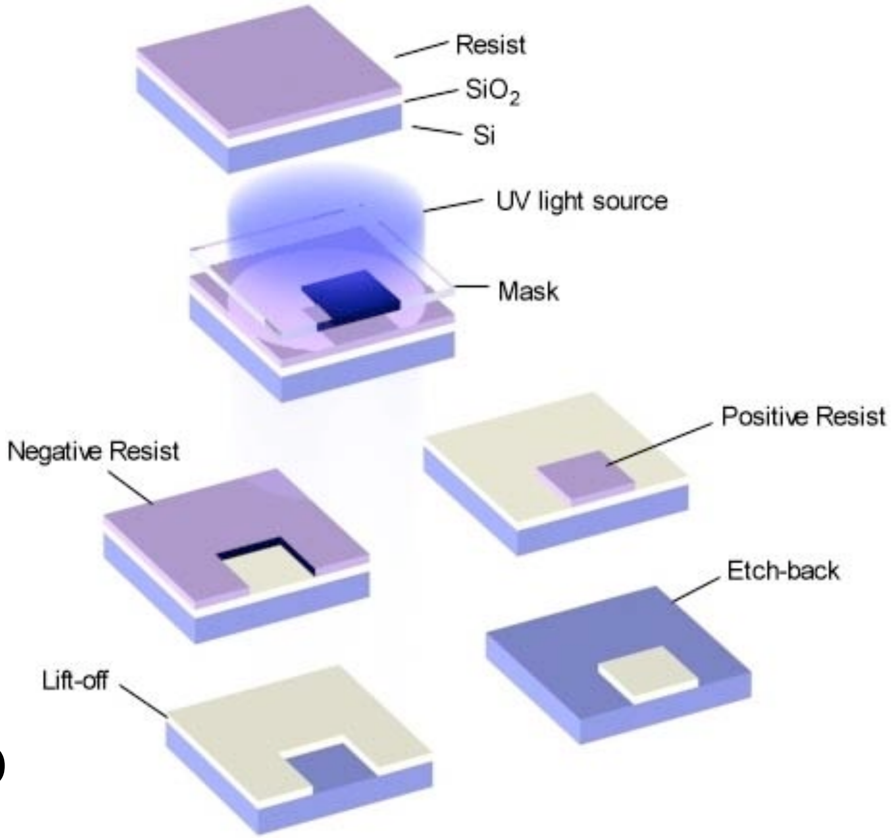
Chip Name	Date	Transistors	Feature size
8080	1979	29k	6 μm
80486	1989	1.2M	1 μm
Pentium IV	2000	42M	0.18 μm

Human hair is 100 microns

Data from Dwayne H. Moore
http://webinstituteforteachers.org/~dmoore/IntroBasicWebDesign/cpu.htm

Patterning silicon

- Lithographic masks are used to introduce pattern of SiO_2 on surface
- Dopants introduced through oxide free surface
- Advanced lithoographic techniques allow for sub 0.1 micron features



Picture from Britney's Guide to Semiconductor Physics
http://britneyspears.ac/lasers.htm

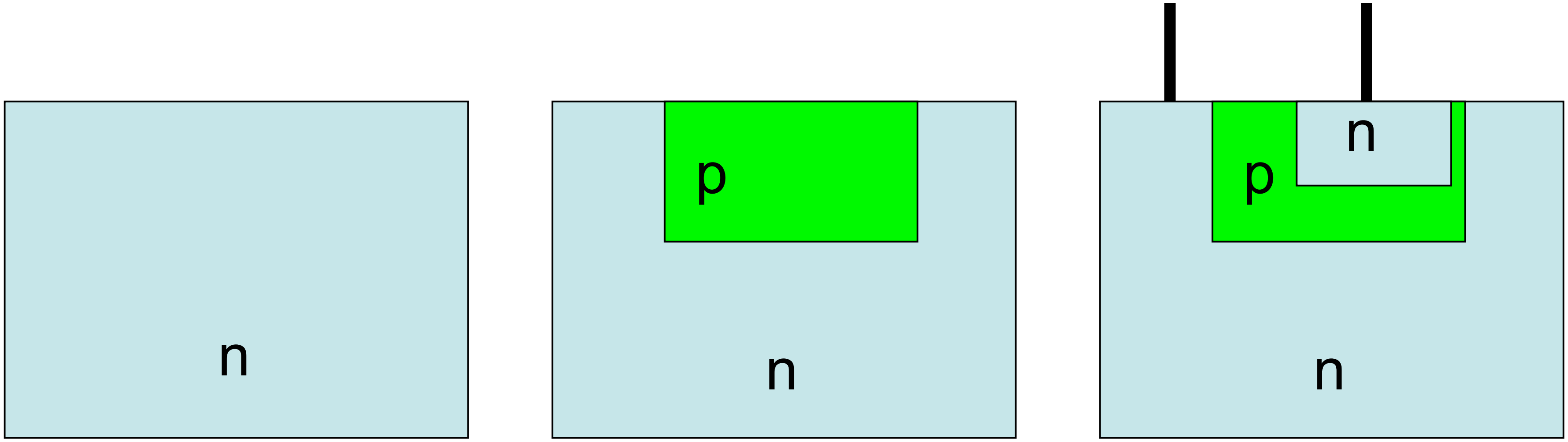
Defects

- The properties of pure material can't be controlled
- Properties of materials can be tailored by adding defects to materials
- Semiconductor devices possible because:
  - understanding of defects
  - technology to control them
- Material science is the science of understanding and controlling defects

Experiment and Computation

- Experimental and computational studies compliment each other
- Experimental:
  - An exact measurement of an unknown structure
- Computation:
  - An approximate calculation of an exact structure

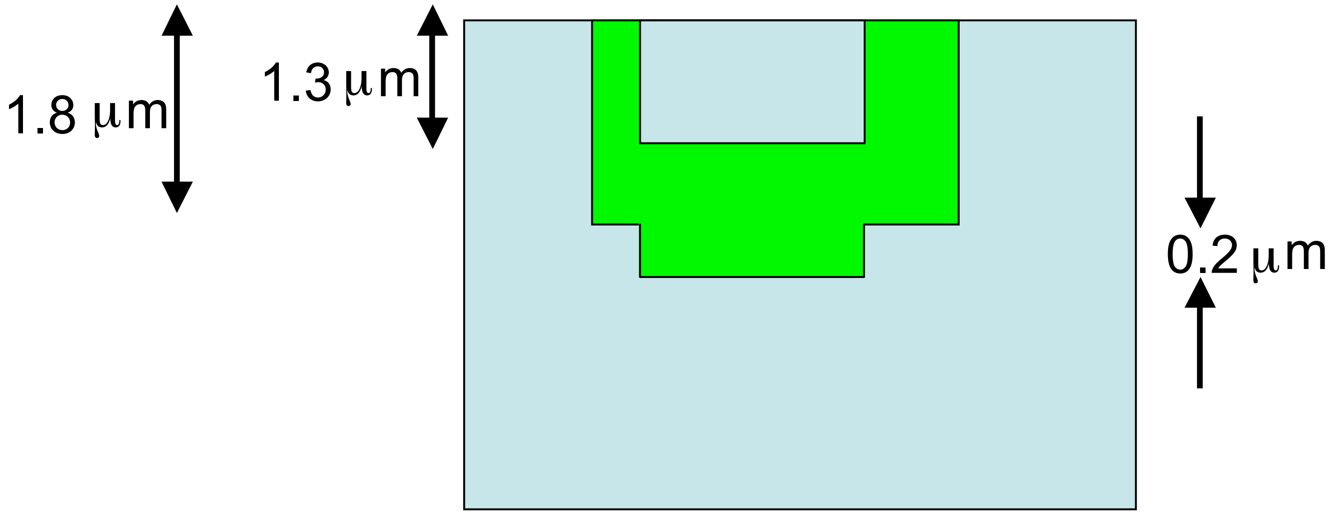
Simple bipolar transistor



- Dope n-type silicon successively with boron and phosphorous

Emitter-Push Effect

- When P is added by ion implantation, B atoms diffuse



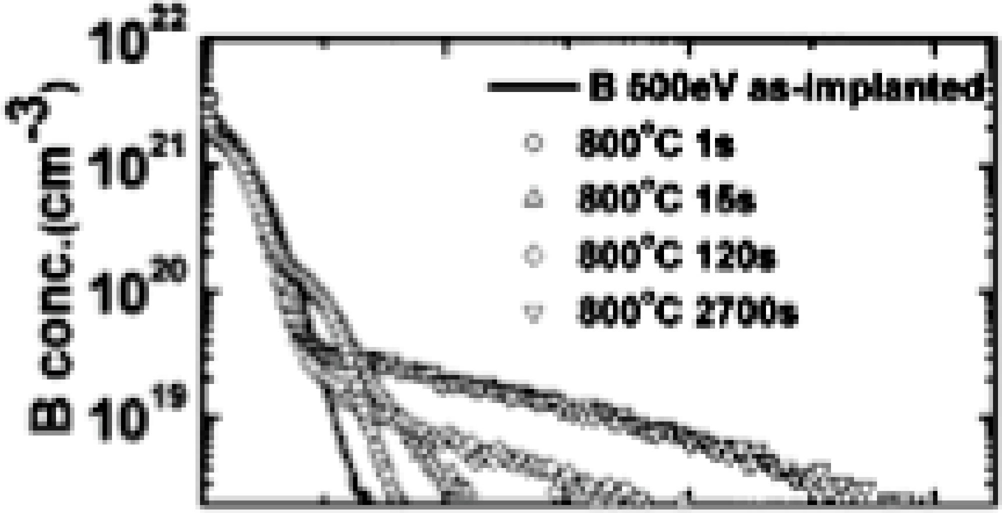
Picture after H. Strunk, U. Gosele, and B. O. Kolbesen, Appl. Phys. Lett. V34 P530 (1979)

Diffusion of B in Si

- Boron will sit on Si site
  - Site to site hopping?
  - Vaccancy assisted diffusion?
- Crystal of Si mostly void
  - Hard sphere packing fraction 0.34 (66% empty!)
  - Long empty channels
- Boron relatively small atom
- Boron will travel by interstitial paths

Experimental study of diffusion

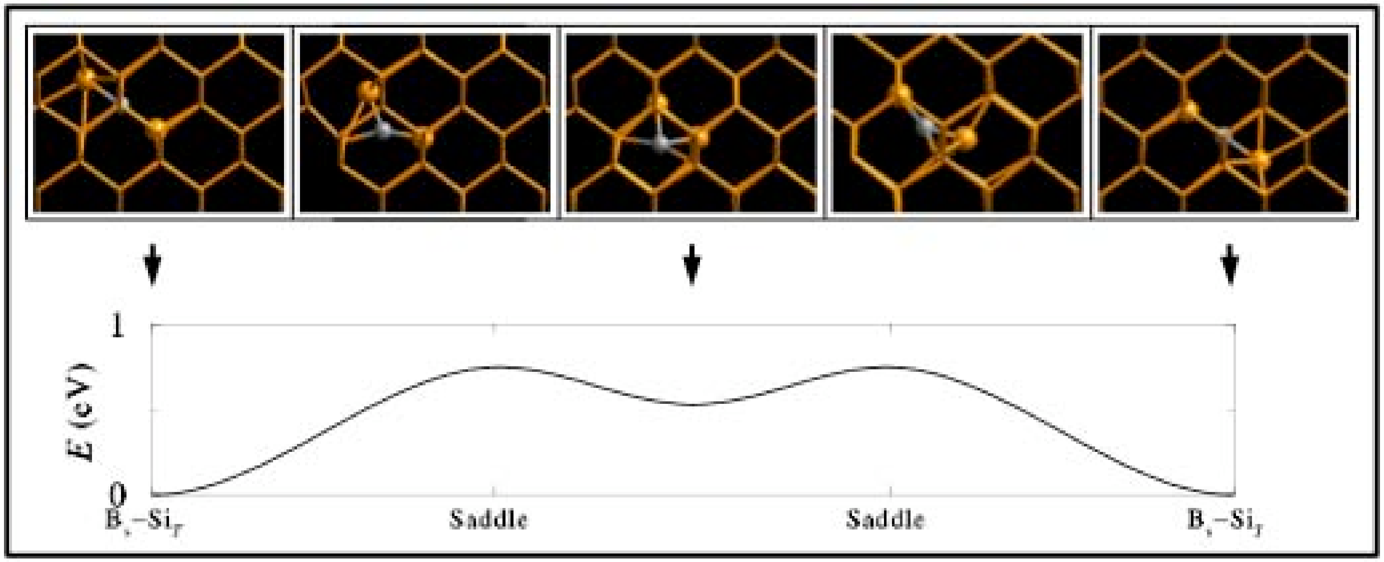
- Diffusion studied by observation of profile
- Investigation of characteristic spectra
- Which path is followed?
- What are the energies to create and move B interstitial?
- Is the only one mechanism?



Plot from N.E.B Cowern, B. Colombeau, J. Benson, A.J. Smith, W. Lerch, S. Paul, T. Graf, F. Cristiano, X. Hebras, and D. Bolze Appl. Phys. Lett. V86 P101905 (2005).

Computational study of diffusion

- Study of diffusion pathways and energies by computational methods



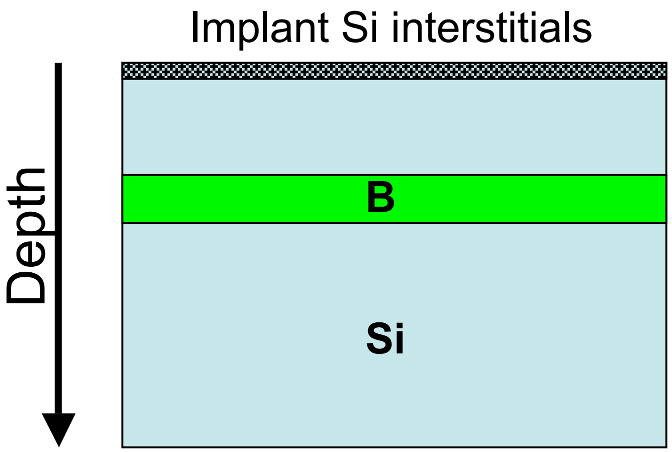
W. Windl, M.M. Bunea, R. Stumpf, S.T. Dunham, and M.P. Masquelier Phys. Rev. Lett. V83 P4345 (1999).

Diffusion mechanism

- Diffusion by kick-out mechanism
  - B sitting on Si site
  - Si interstitial kicks B out of site
  - B diffuses through empty interstitial paths
  - B leave interstitial region
- Long range mechanism
- Multiple energies
  - Kick-out energy
  - Migration energy
  - Kick-in energy

Enhanced diffusion

- Diffusion enhancement not due to P, but Si “interstitial wind”



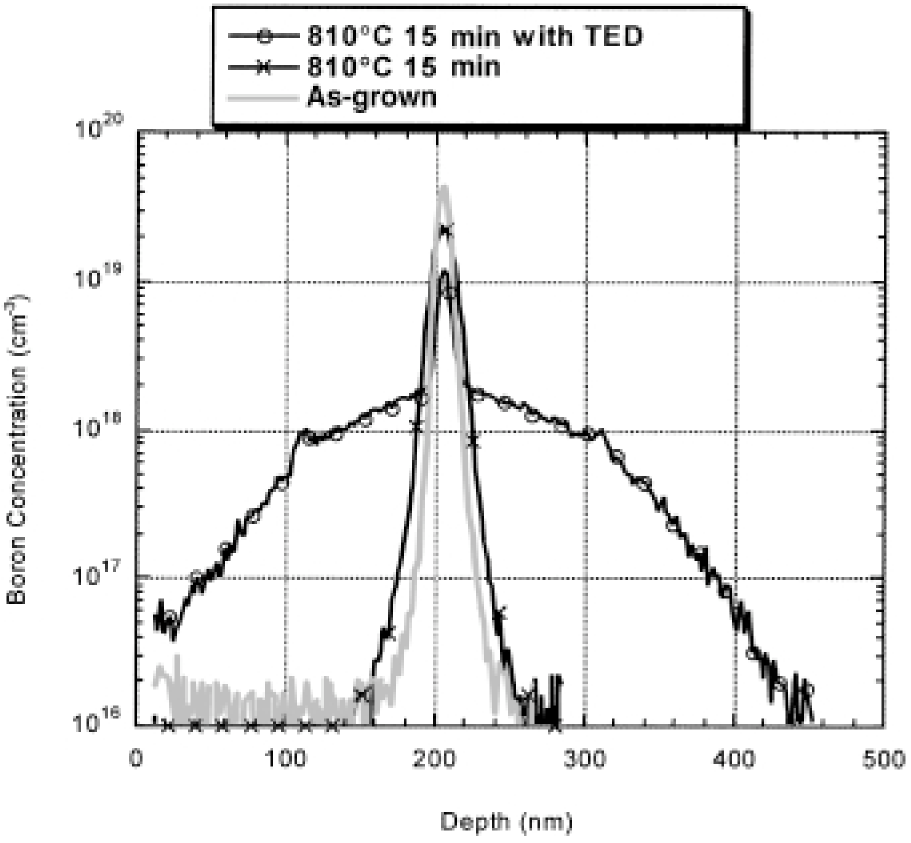
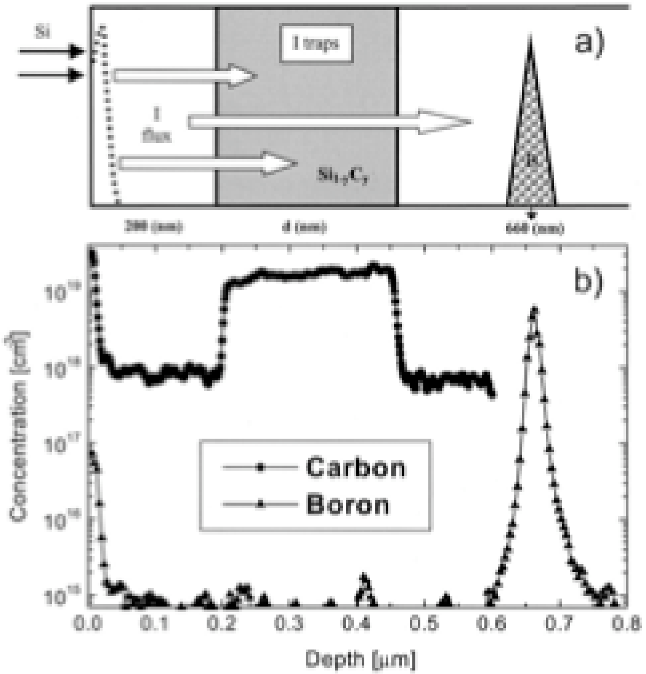


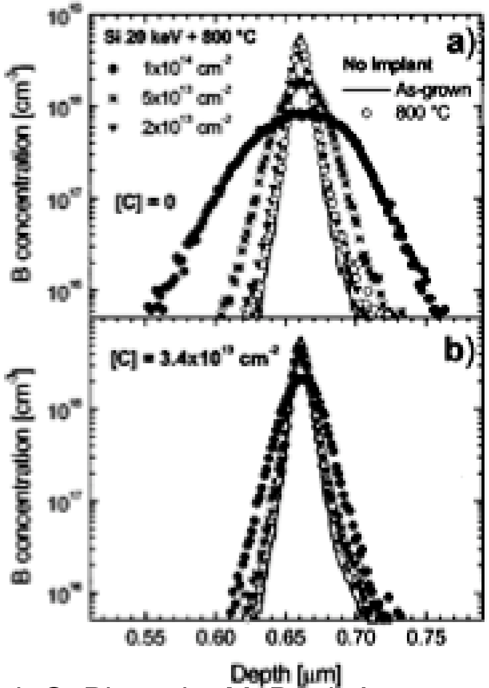
Figure 5. Secondary ion mass spectrometry profiles of boron before and after annealing. Thermal diffusion is small at this temperature, but with surface damage, a huge broadening of the marker layer is seen. TED is transient-enhanced diffusion.

Plot from Nicholas Cowern and Conor Rafferty MRS Bulletin June 2000 P39

Problem solved?

- Carbon can act to trap Si interstitials
- How does this happen? Exchange Si_I for C_I?
- Why does the C interstitials not enhance B diffusion ?





S. Mirabella, A. Coati, D. De Salvador, E. Napolitani, A. Mattoni, G. Bisognin, M. Berti, A. Carnera, A.V. Drigo, S. Scalese, S. Pulvirenti, A. Terrasi, and F. Priolo Phys. Rev. B. V65 P045209 (2002).

Carbon trapping

- C interstitial diffuses until is meets second C on Si site
- C_I $+C_{Si}$ lock together and become immobile
- C is smaller than Si so strain around C_{Si}
- Interstitial defects have strain around interstitial atom
- The C_I and C_{Si} strain stabilize one another

Carbon trapping 2

9 April 1990

- Empirical study of C in Si by Tersoff, 1990.
- Experimental studies by G. Watkins research group 1980’s. (Song et al. published in 1988)

Song *et al.*[9]

The Future

- Computer power continue to increase
- The speed, accuracy, and breadth of computational methods continues to increase
- The past ten year has witnessed the rise of *ab inito* computational methods
- In the future increased coupling computation and experiment