

3.012 Fund of Mat Sci: Structure – Lecture 21

NON-CRYSTALLINE MATERIALS

Images of a silicon nanocrystal removed for copyright reasons.

Light amplification for crystalline silicon in a glassy SiO_2 matrix

Homework for Fri Dec 2

- Study: Chapter 2 of Allen-Thomas until 2.3.1

Last time:

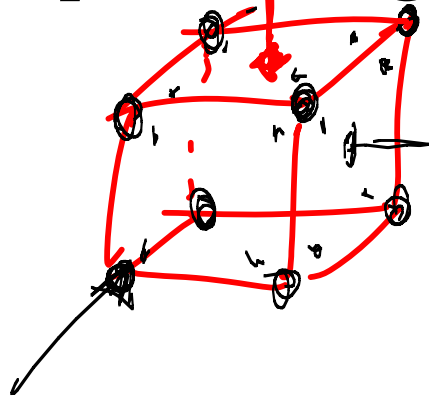
1. Tensors, and their transformations
2. Orthogonal matrices
3. Neumann's principle
4. Symmetry constraints on physical properties
5. Curie's principle

Physical properties and their relation to symmetry

- Density (mass, from a certain volume)
- Pyroelectricity (polarization from temperature)
- Conductivity (current, from electric field)
- Piezoelectricity (polarization, from stress)
- Stiffness (strain, from stress)

Curie's Principle

- a crystal under an external influence will exhibit only those symmetry elements that are common to both the crystal and the perturbing influence*



432

4



Loss of periodic order

- Liquids (“fluid”)
- Glasses (“solid”)
 - Oxide glasses (continuous random networks)
 - Polymeric glasses (self-avoiding random walks)
- Oddballs
 - Quasicrystals
 - Superionics

Table of the applications of noncrystalline materials removed for copyright reasons.

Principle of operation of a CD-RW

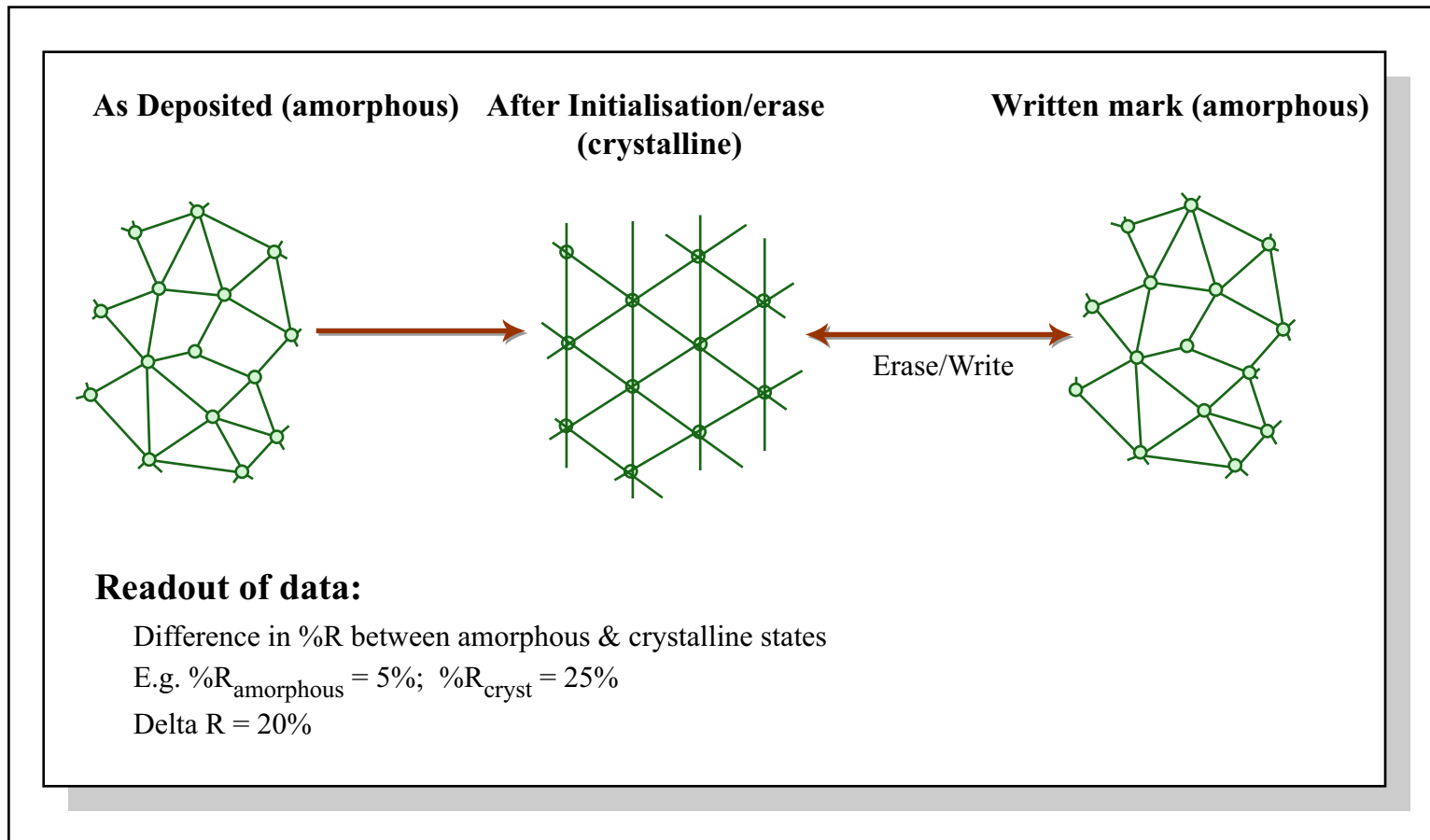


Figure by MIT OCW.

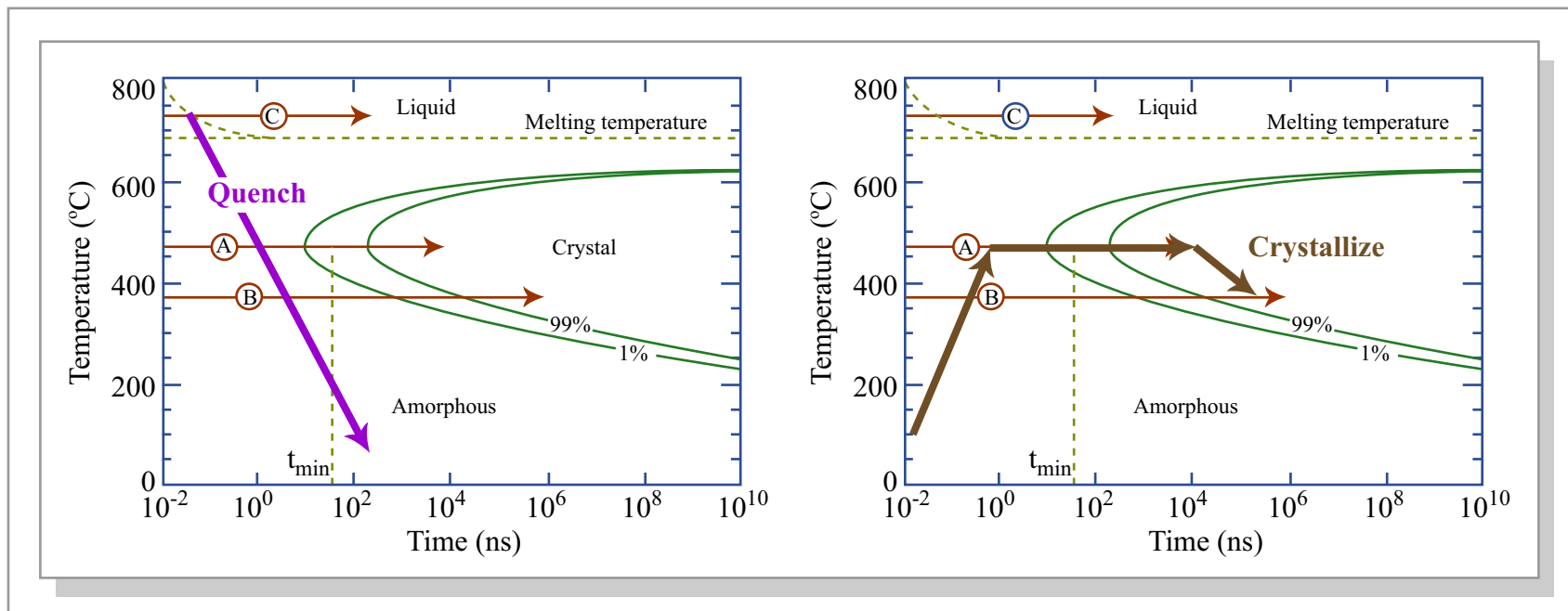
Principle of operation of a CD-RW

Writing - Amorphous

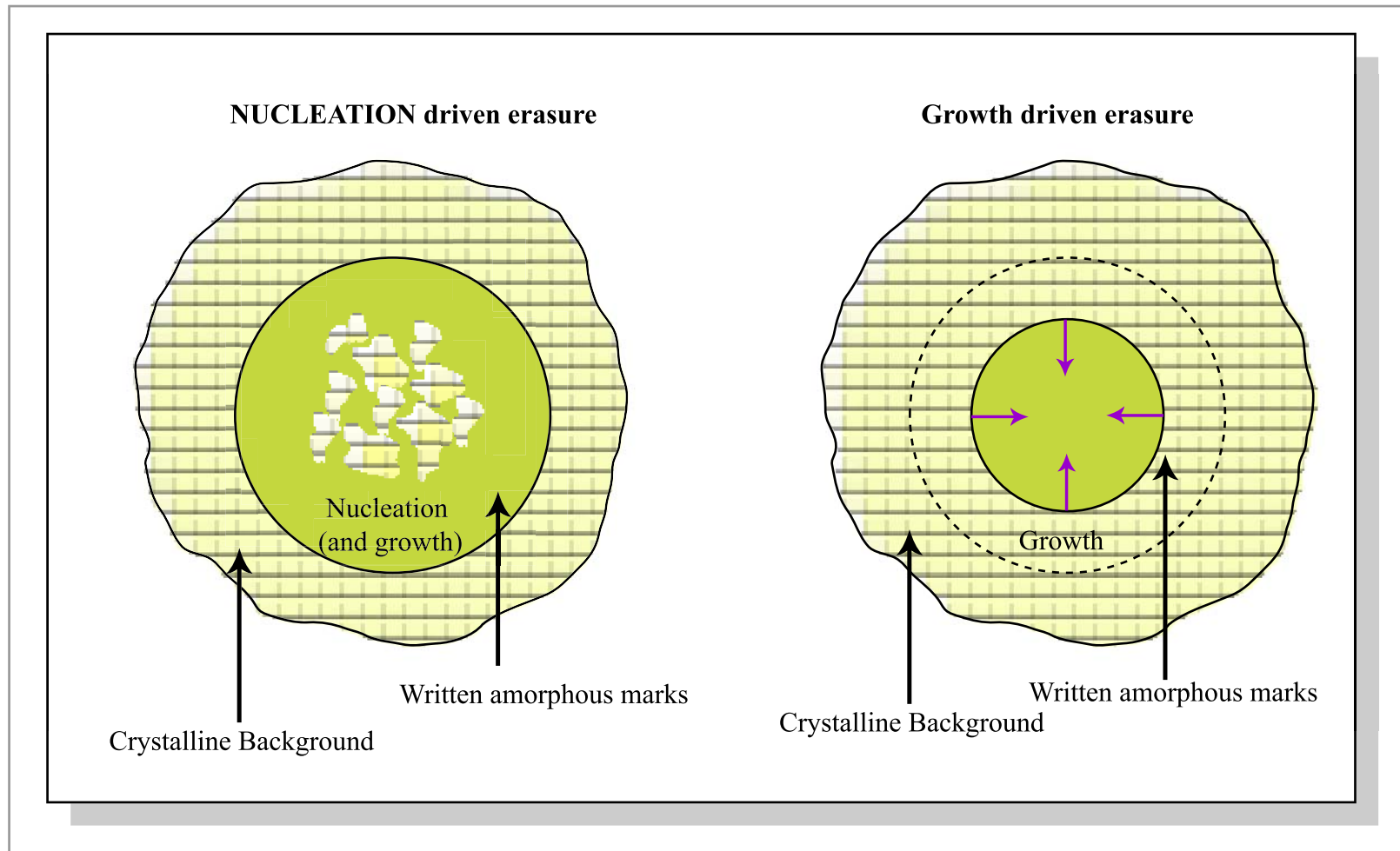
The active layer is heated above its melting point and quenched into the amorphous phase with a short laser pulse to produce marks.

Erasure – Crystalline

Intermediate laser power is used, so that the active layer does not melt, but rather remains within the crystallization temperature region long enough that the amorphous marks re-crystallize.



Erasure: nucleation and growth of crystalline material



Te-Sb-Ge Alloy

Nucleation dominated:
4.7 GB DVD-RAM
(Sb_2Te_3 to GeTe)

Growth dominated: CD-
RW, DVD-RW, Blu-ray
($\text{Sb}_{69}\text{Te}_{31}$ eutectic)

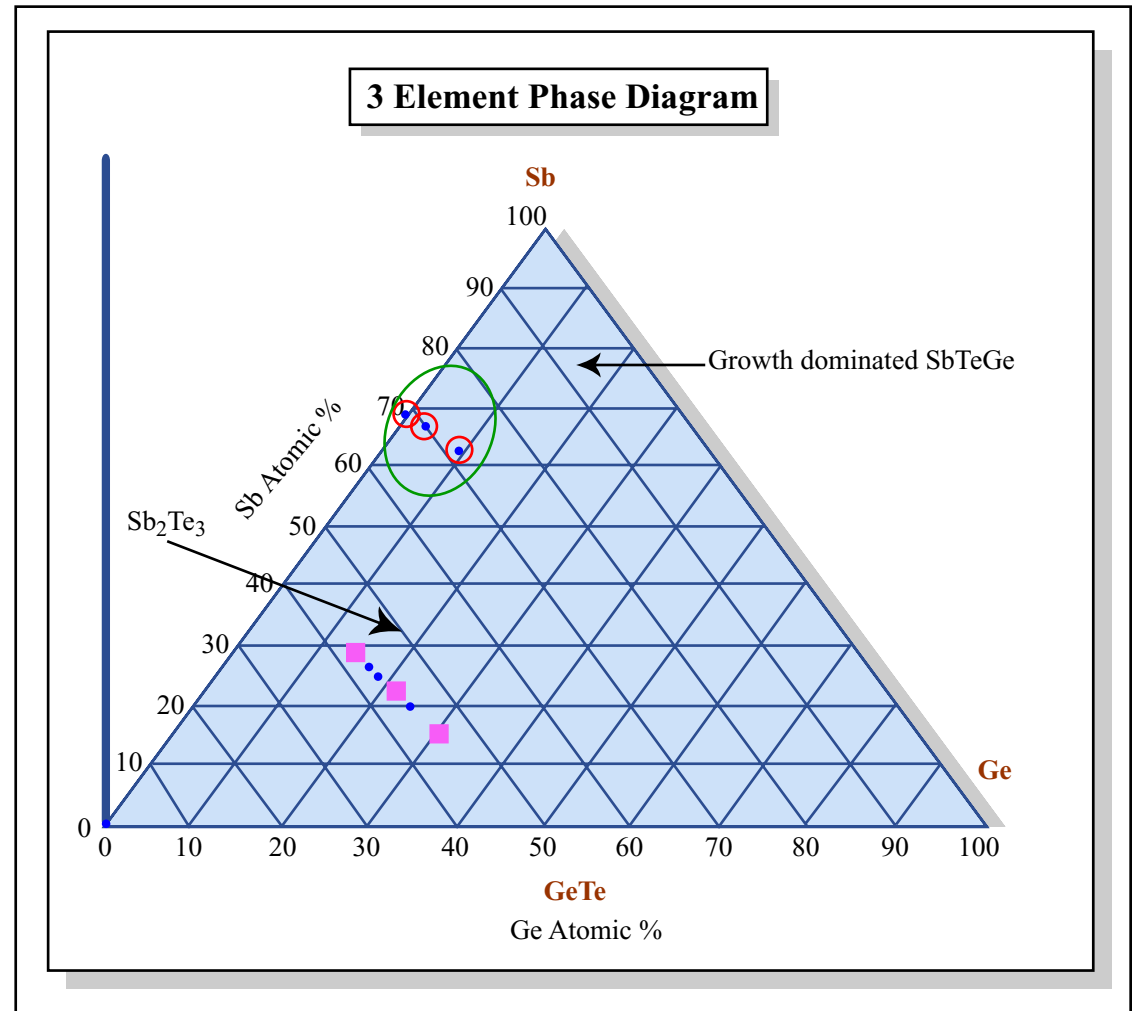
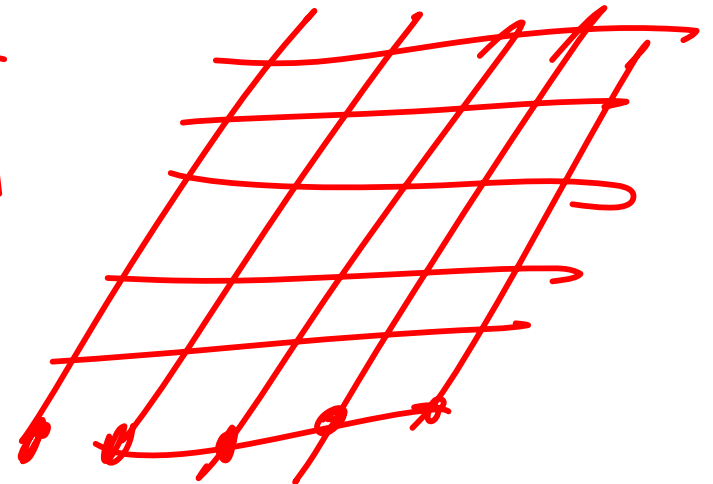
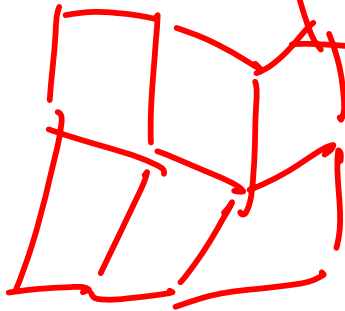


Figure by MIT OCW.

Structural Descriptors

- Long-range order
- Short-range order



What do ice and silicon have in common ?



Source: Wikipedia

What do ice and silicon have in common ?

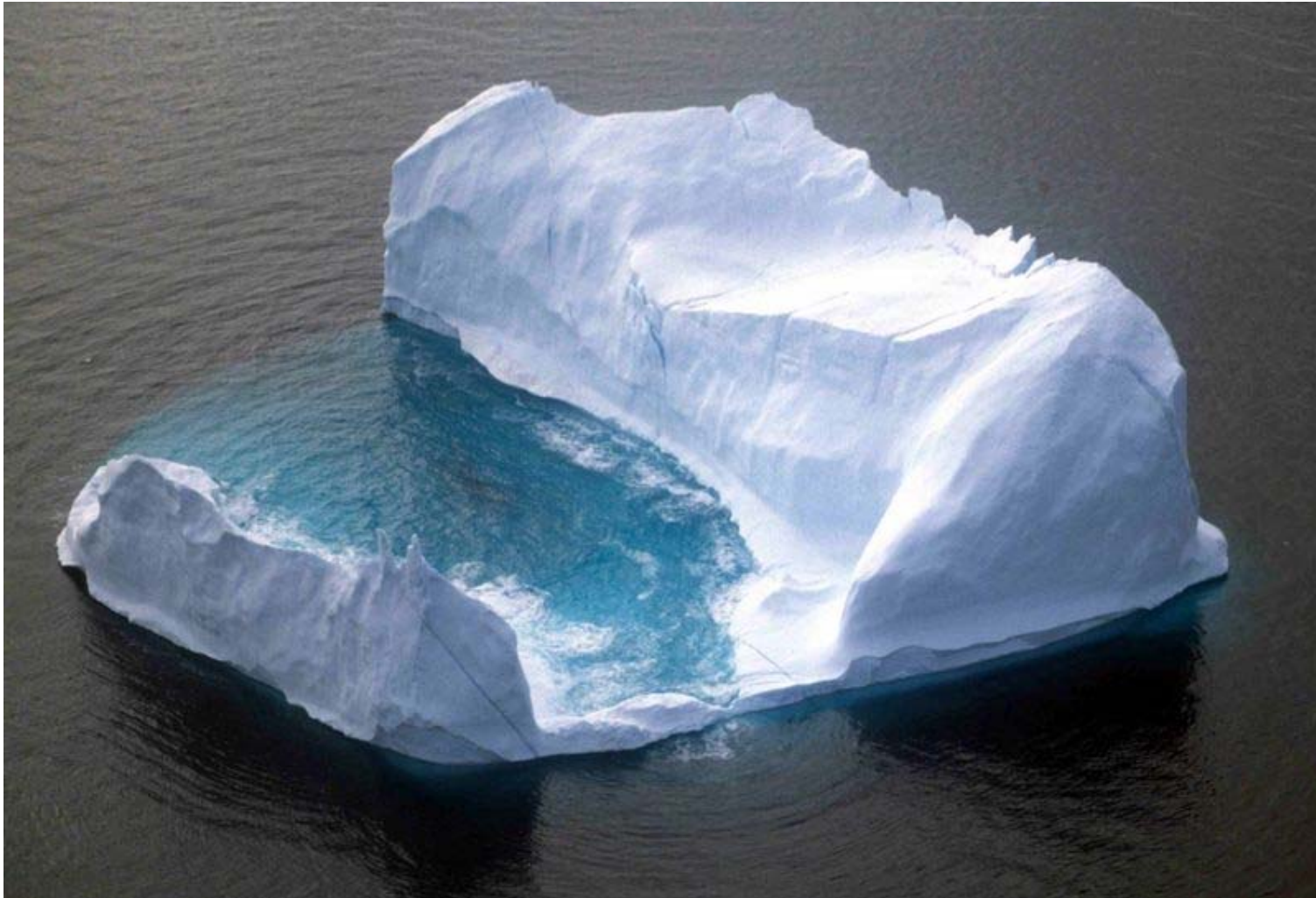


Photo courtesy of Ansgar Walk.

ABAB → WURTZITE
→ ICF HEXAGONAL

FCC [111] ABCABC

What do ice and silicon have in common ?

Si = FCC 2 ATOM BASIS

CUBIC ICE

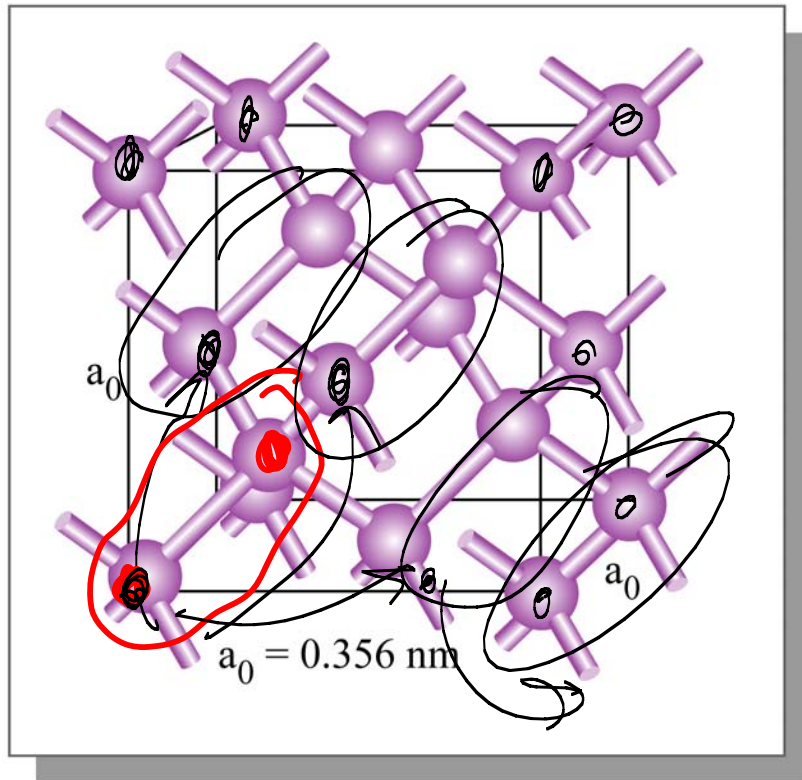


Figure by MIT OCW.

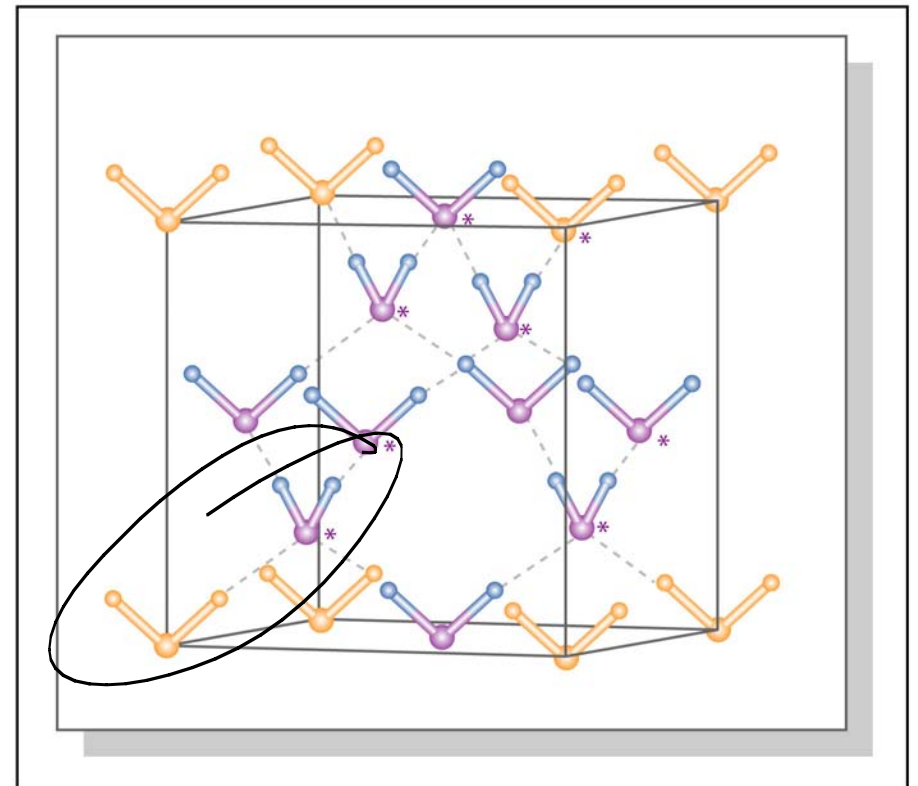
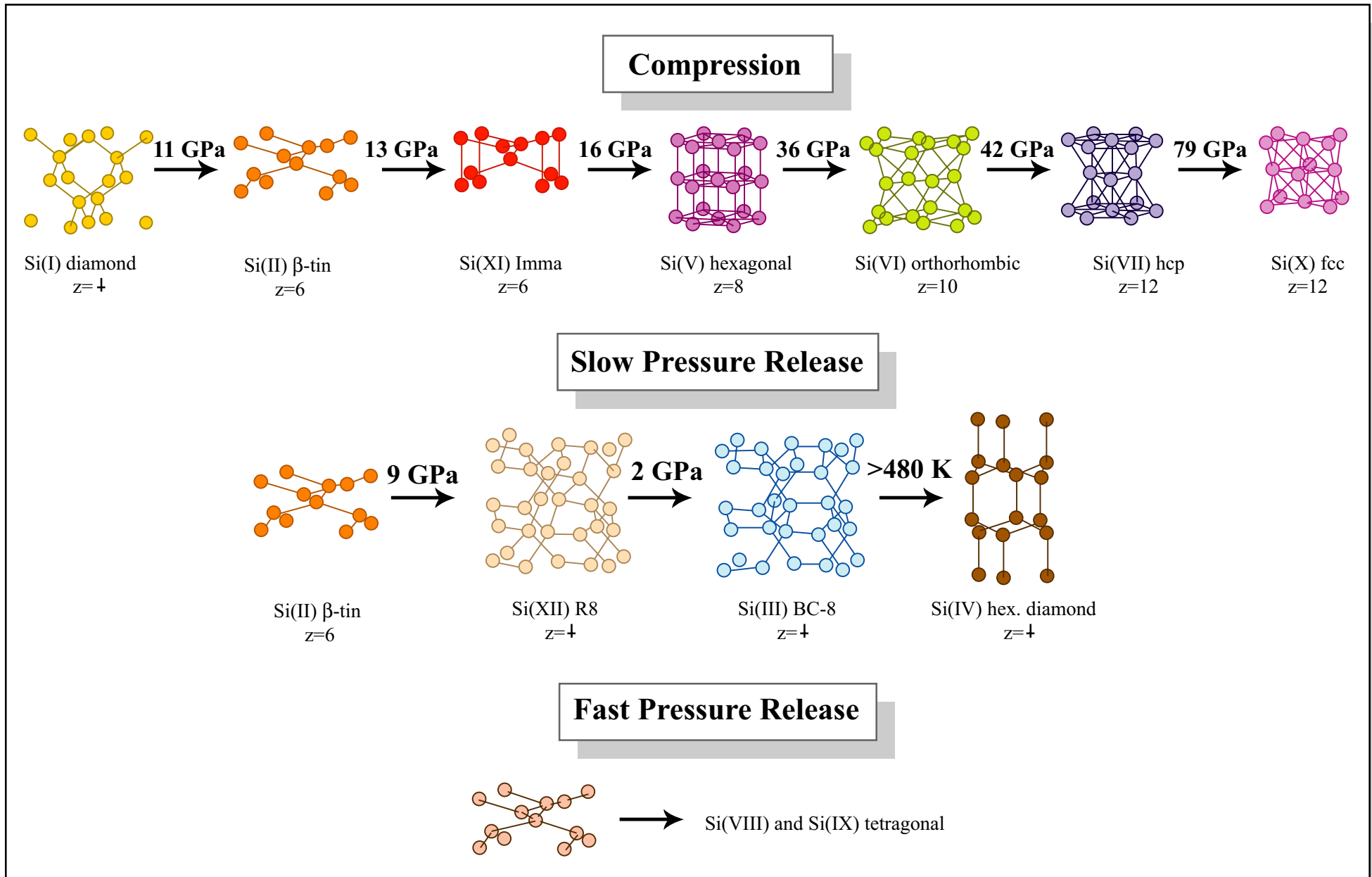


Figure by MIT OCW.

What do ice and silicon have in common ?



What do ice and silicon have in common ?

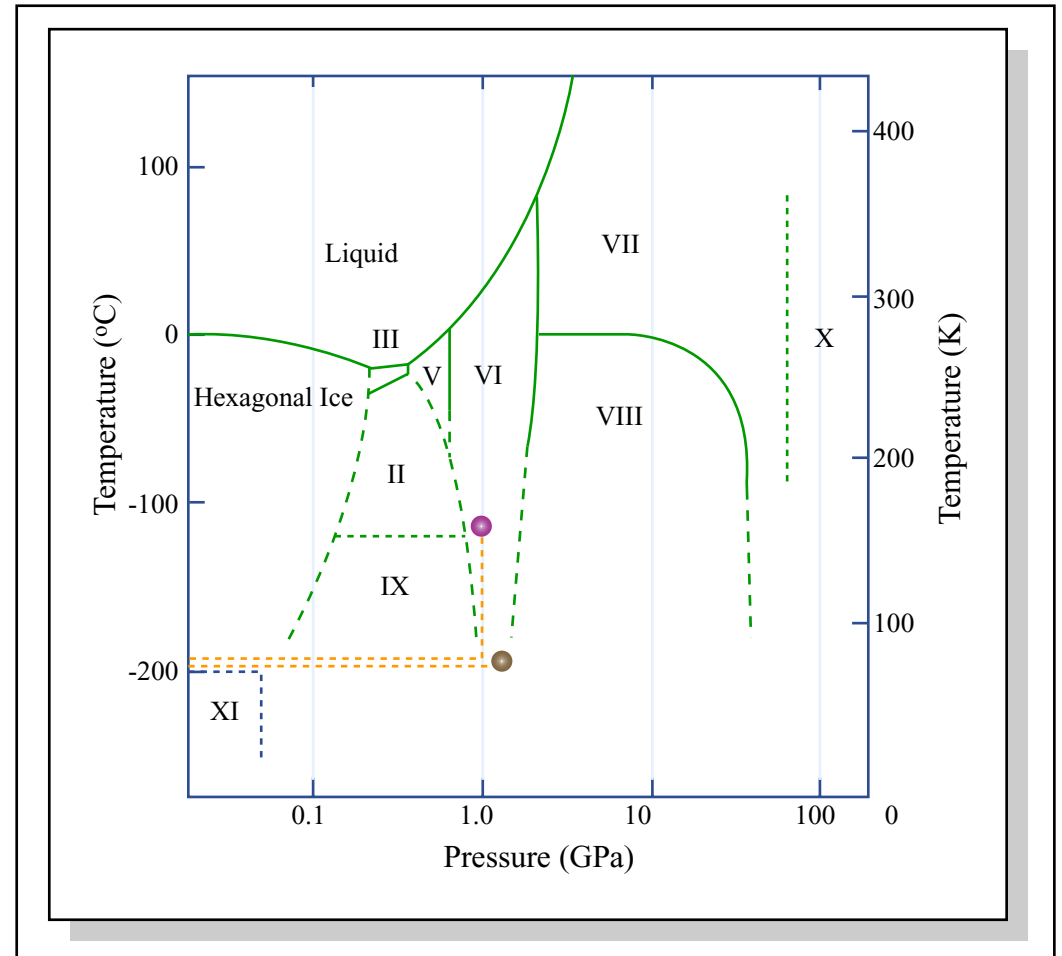
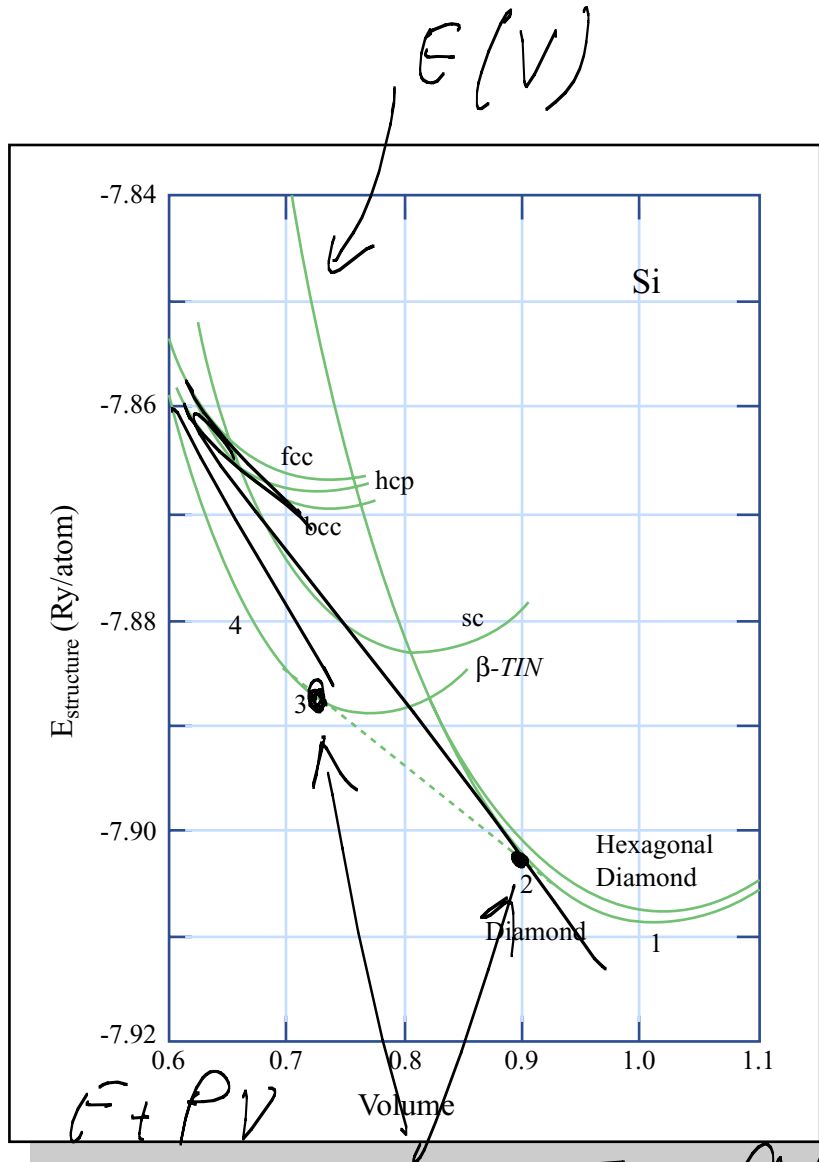
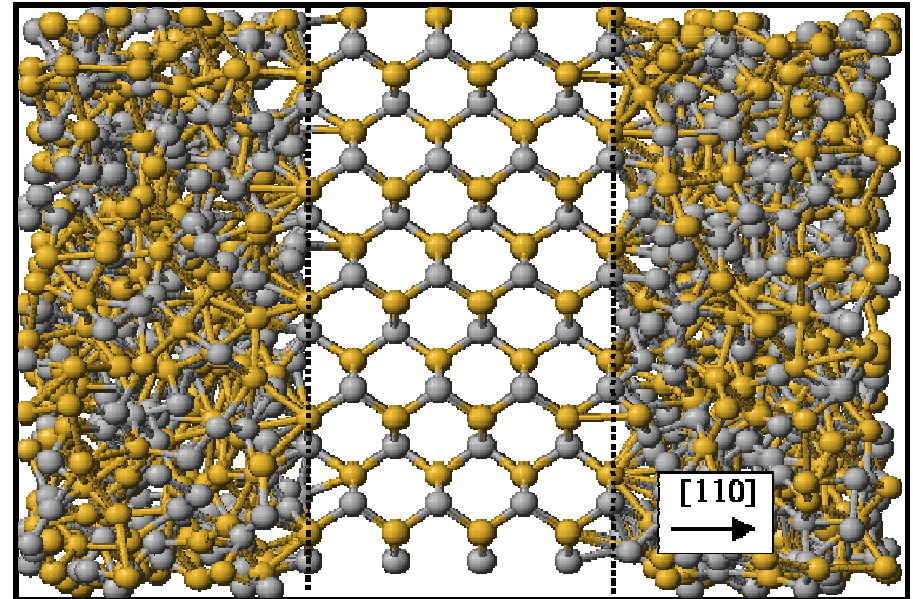
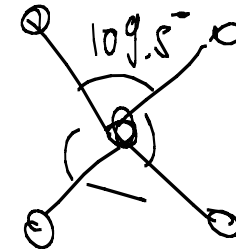
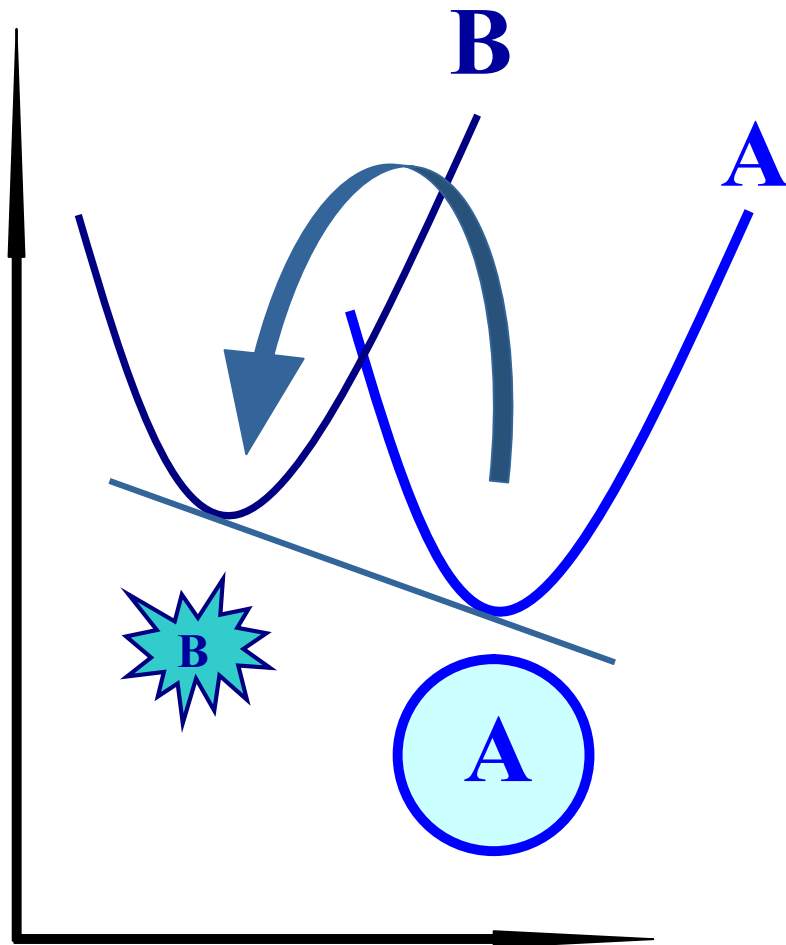


Figure by MIT OCW.

$$E_1 + PV_1 = E_2 + PV_2$$

Phase transitions in silicon

Energy



Volume

Order Parameters for Silicon

THE σ OF AVERAGE OF ANGLES

VARIANCE

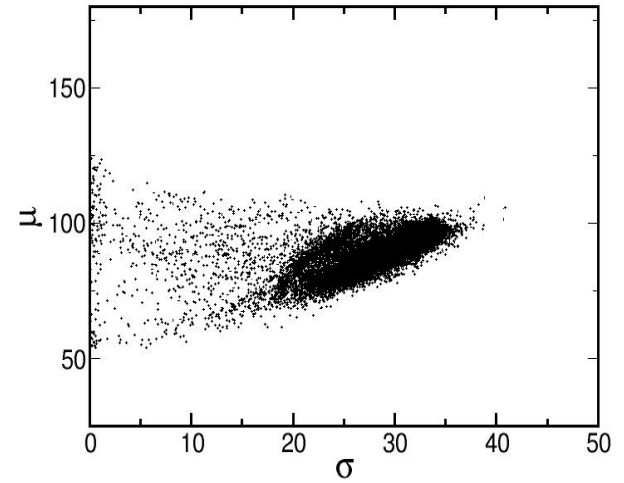
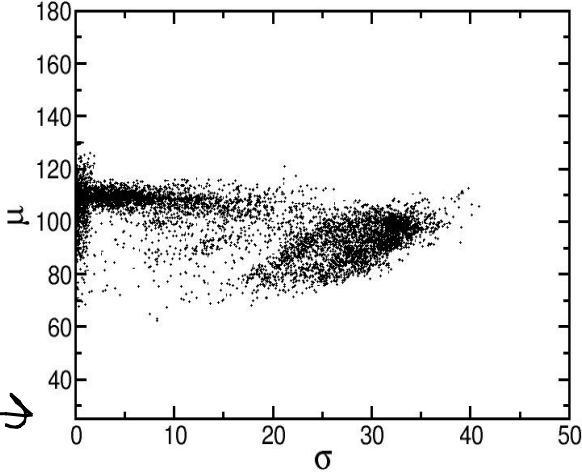
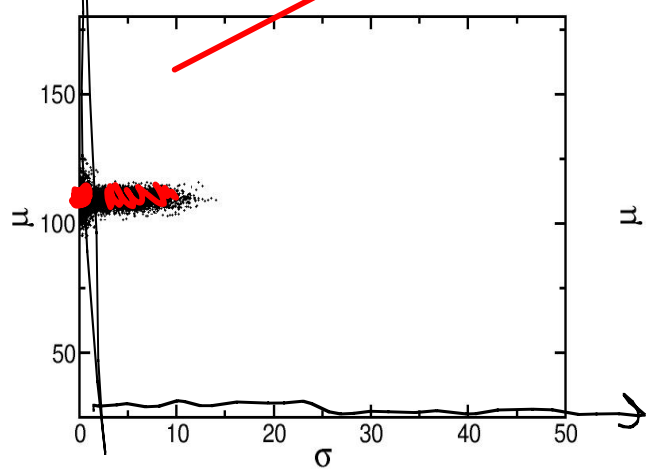
$$\mu = \frac{1}{N} \sum_i \theta_i$$

$$\sigma = \left(\frac{1}{N} \sum_i \theta^2 - \mu^2 \right)^{\frac{1}{2}}$$

Before compression

During compression

P = 40 GPa



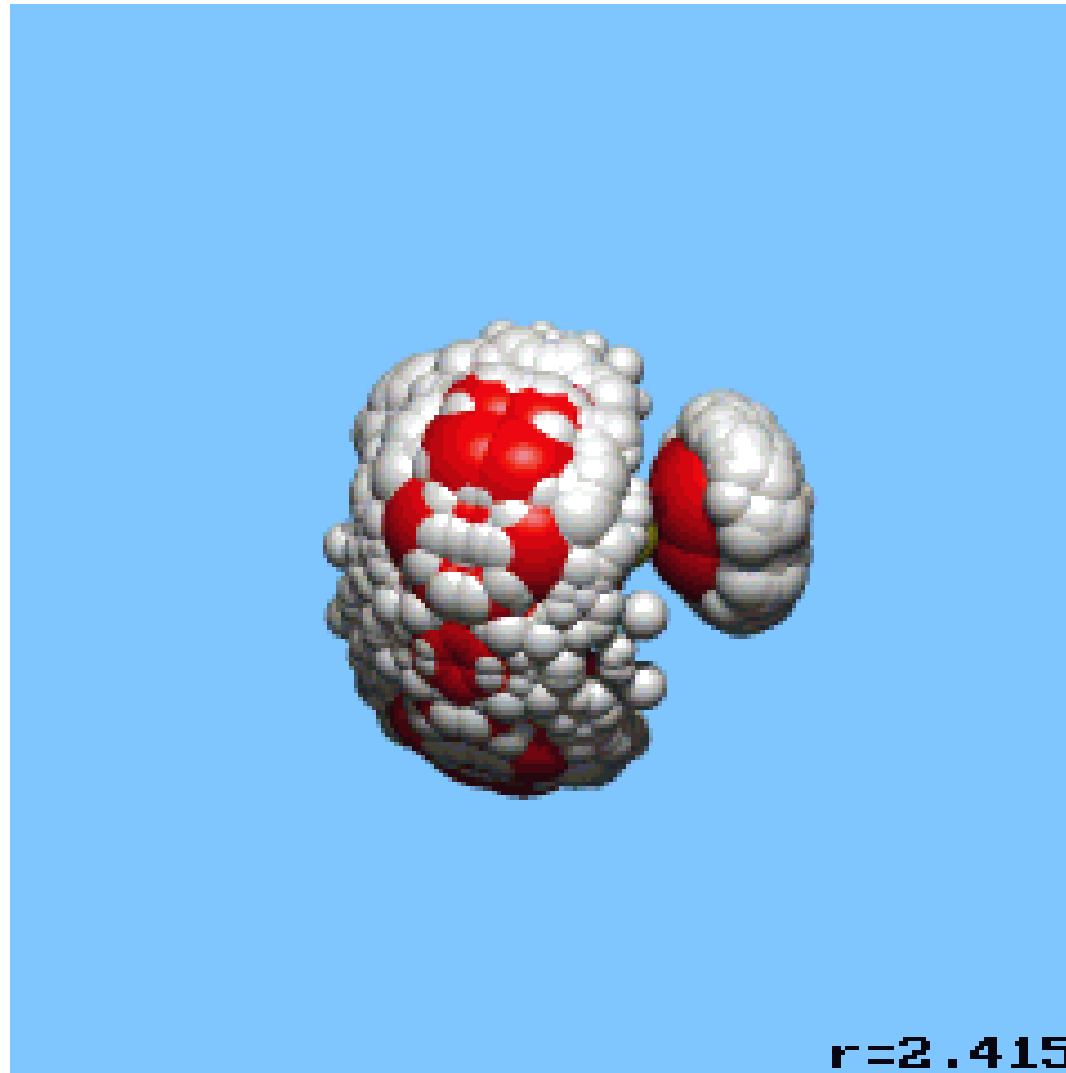
M. J. Demkowicz and A. S. Argon, Phys. Rev. Lett. 93, 25505 (2004)

Pair correlation functions

Graphs of the pair-distribution functions for gas, liquid/gas, and monatomic crystal removed for copyright reasons.
See page 41, Figure 2.5 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

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Pair correlation function: water

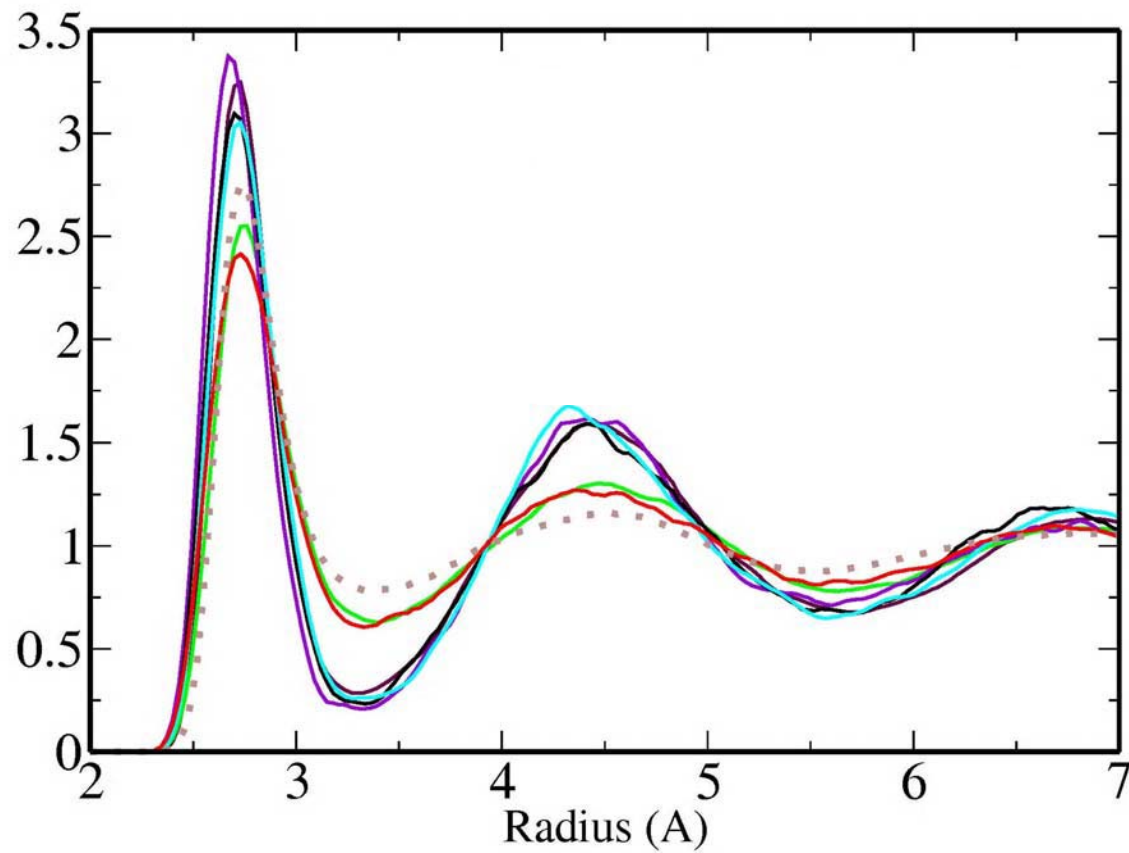


3.012 Fundamentals of Materials Science: Bonding - Nicola Marzari (MIT, Fall 2005)

Courtesy of Dr. J. Kolafa. Used with Permission.

See animation at <http://www.icpf.cas.cz/jiri/movies/water.htm>.

Pair correlation function: water



Count thy neighbours

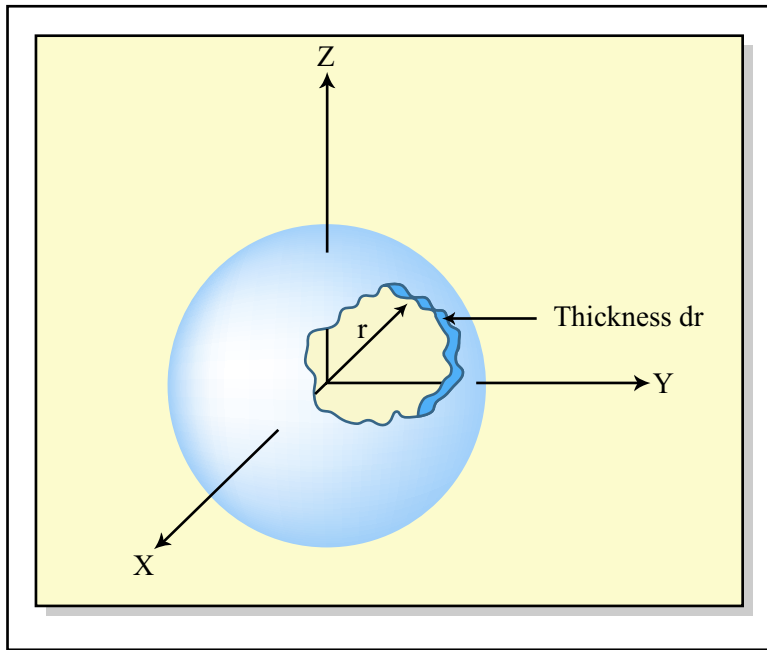
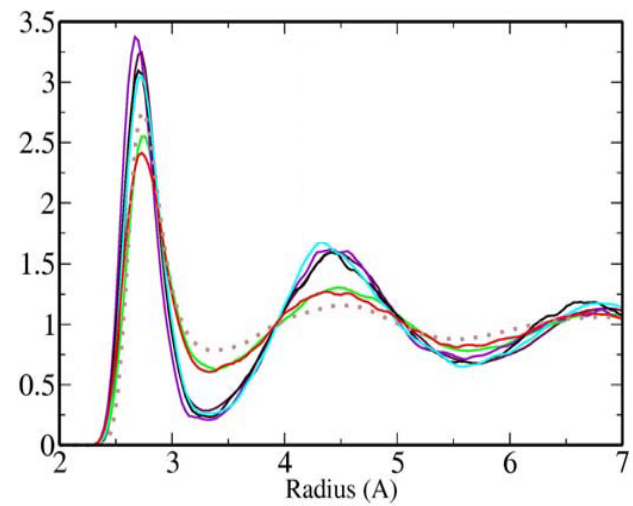


Figure by MIT OCW.



Models of disorder: hard spheres

- Bernal random close packed sphere model

Photos of the Bernal random close-packing model removed for copyright reasons.
See them at the Science & Society Picture Library: [Image 1](#), [Image 2](#).

Models of disorder: hard spheres

- Voronoi polyhedra (in a crystal: Wigner-Seitz cell)

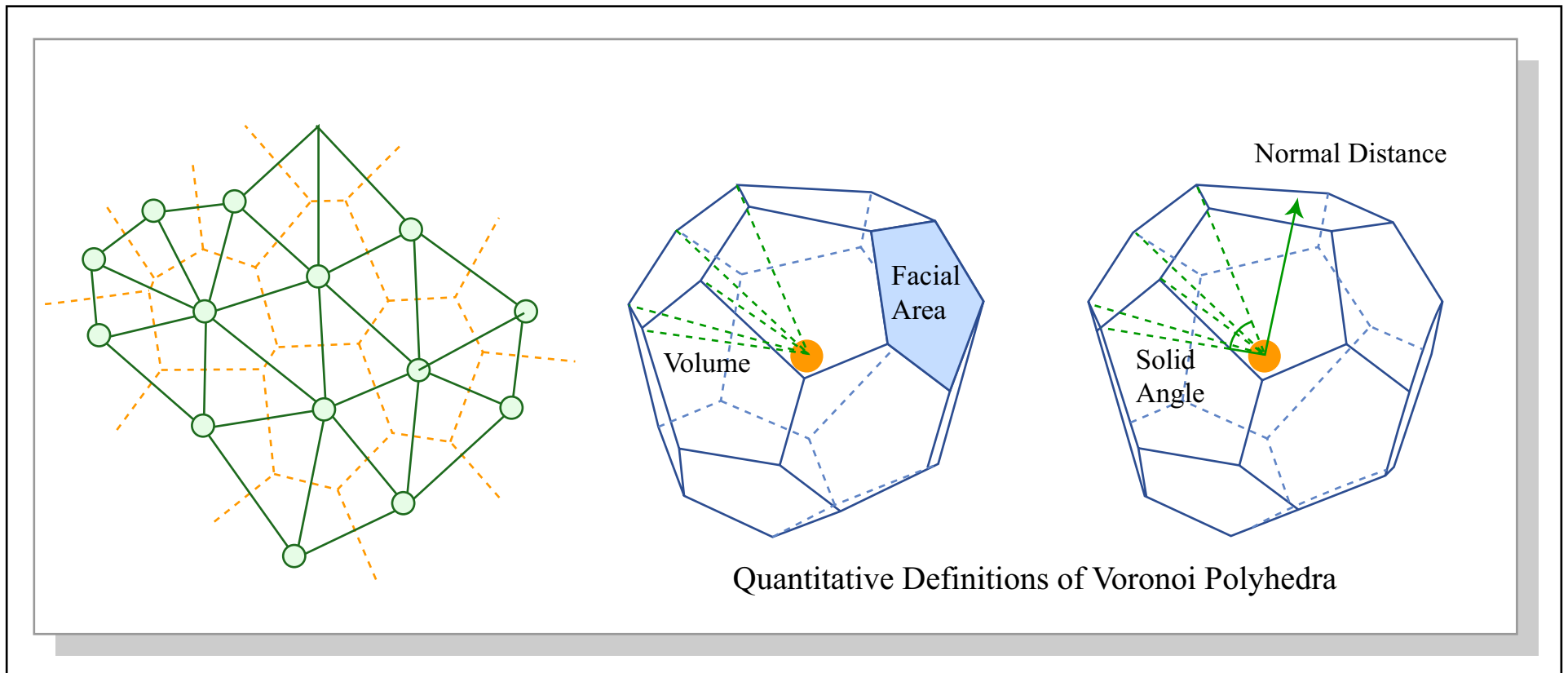


Figure by MIT OCW.

Mean Square Displacements

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