결정학개론
(Crystallography)

2006년 2학기

홍성현교수

교과목명 : **결정학개론 (Crystallography)**

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학점 : 출석/과제(10%), 중간고사Ⅰ(20%), 중간고사Ⅱ(20%), 기말고사(50%)

참고서적 :

1. W. B. Ott, Crystallography, 2nd Ed., Springer, 1995.
2. 결정학개론, 정 수진 저, 피어슨 에듀케이션 코리아, 2nd Ed., 2001.
3. B. D. Cullity, Elements of X-ray Diffraction, Prentice Hall, 2001.
4. J. F. Nye, Physical Properties of Crystals, Oxford, 1985
5. D. Sherwood, Crystals, X-rays, and Proteins, Longman, 1976

교과목 내용

1. 서론 – 결정, - 결정학

2. 결정격자 - 병진, - 단위포, - 결정면, 밀러지수, 면간거리

3. 결정투영

4. 결정학 - 대칭 및 대칭조작, - 14 Bravais Lattices, - 7 Crystal Systems
   - 32 결정족, - 17 평면군, - 230 공간군

5. 결정의 물성 - 이방성(텐서), - Neumann's Principle
   - 물성(초전성, 열전도도, 전기전도도, 유전성, 자성, 압전성, 탄성, 전왜)

6. 회절물리 (diffraction physics)

7. 역격자 (reciprocal lattice)

8. X-선 회절 - Laue 조건, - Bragg의 방정식, - 역격자와 회절조건
   - Ewad의 구, - 구조인자, - 소멸규칙

Chapter. 1 Crystallography

Reading Assignment:

1. W. B-Ott, Crystallography-chapter 1
2. D. Sherwood, Crystals, X-rays, and Proteins-chapter 1

Contents

Crystallography

(from the Greek words *crystallon*=cold drop/frozen drop, with its meaning extending to all solids with some degree of transparency, and *graphein*=write)

is the experimental science of determining the arrangements of atoms in solids.

In older usage, it is the scientific study of crystals.

Crystallography

결정학 **(crystallography)-** concerned
with the laws governing the <u>crystalline state</u> of solids materials
with the arrangement of atoms (molecules, ions) in crystals
and with their physical and chemical properties, their synthesis and their growth. (Ott)

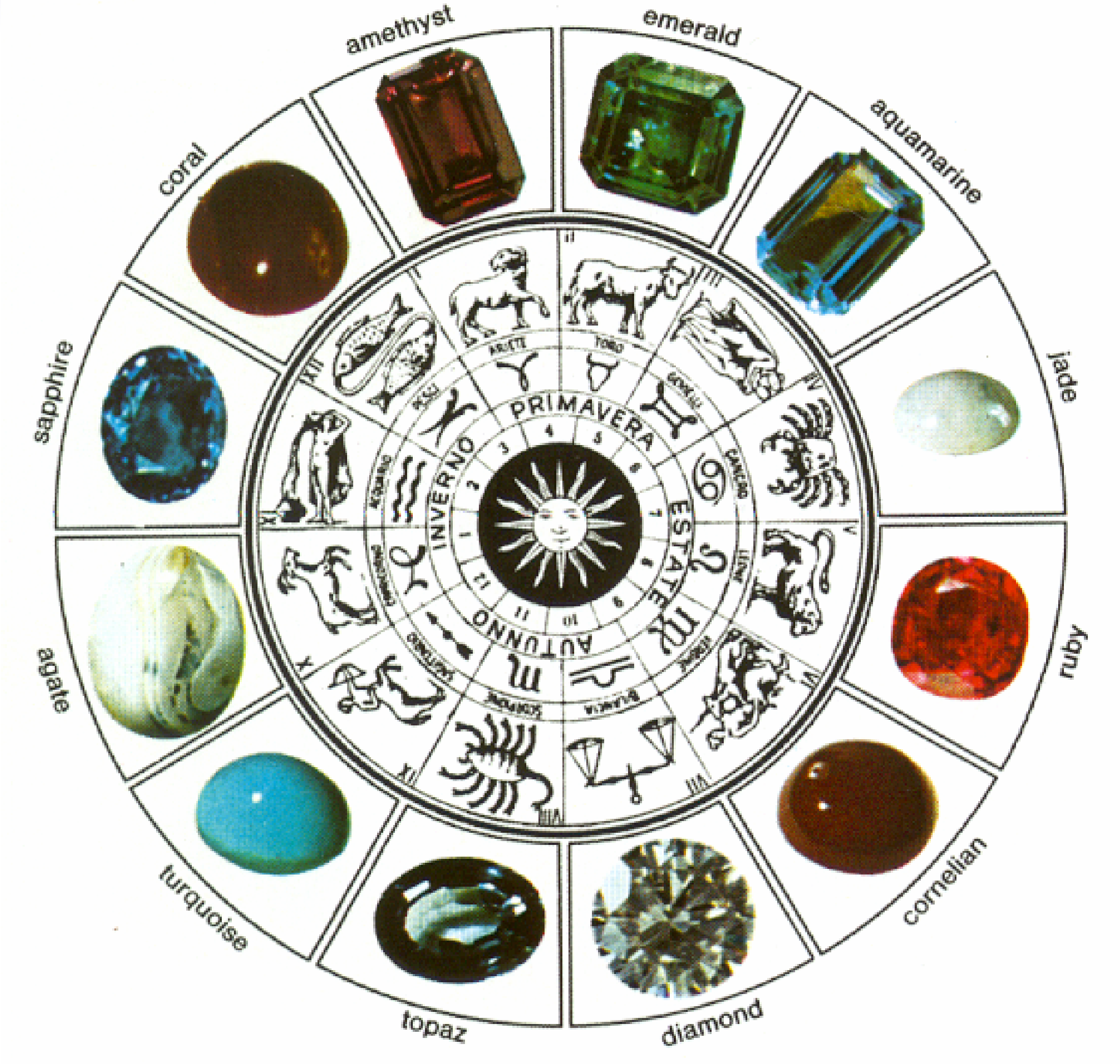
Characteristics of crystals

1. Regular geometric shape

form: set of the physically equivalent faces of a crystal, whose presence is controlled by the symmetry of the crystal class
ex)
usually not given by a single crystallographic form but by a combination of various forms, each developed to a greater or lesser degree

trait: characteristic combination of forms

habit: appearance determined by the predominant form



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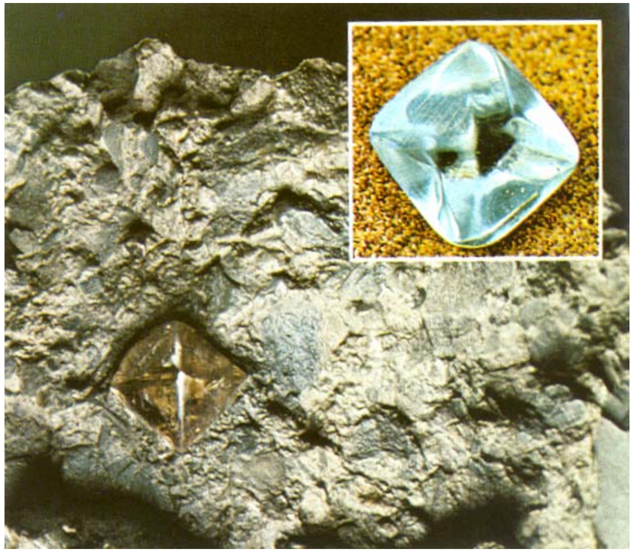
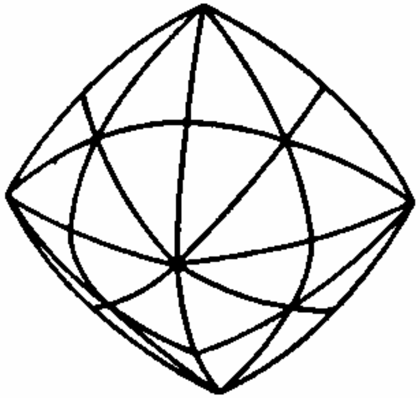
Diamond (C)



Cubic, Octahedron



Simon & Schuster's Guide to Rocks and Minerals

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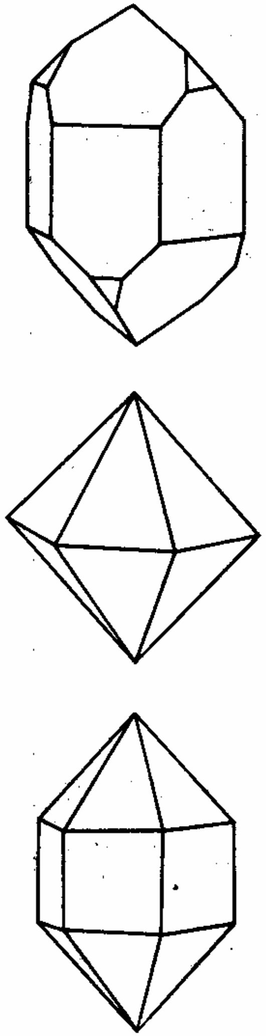
Quartz (SiO_2)

Hexagonal, Prismatic



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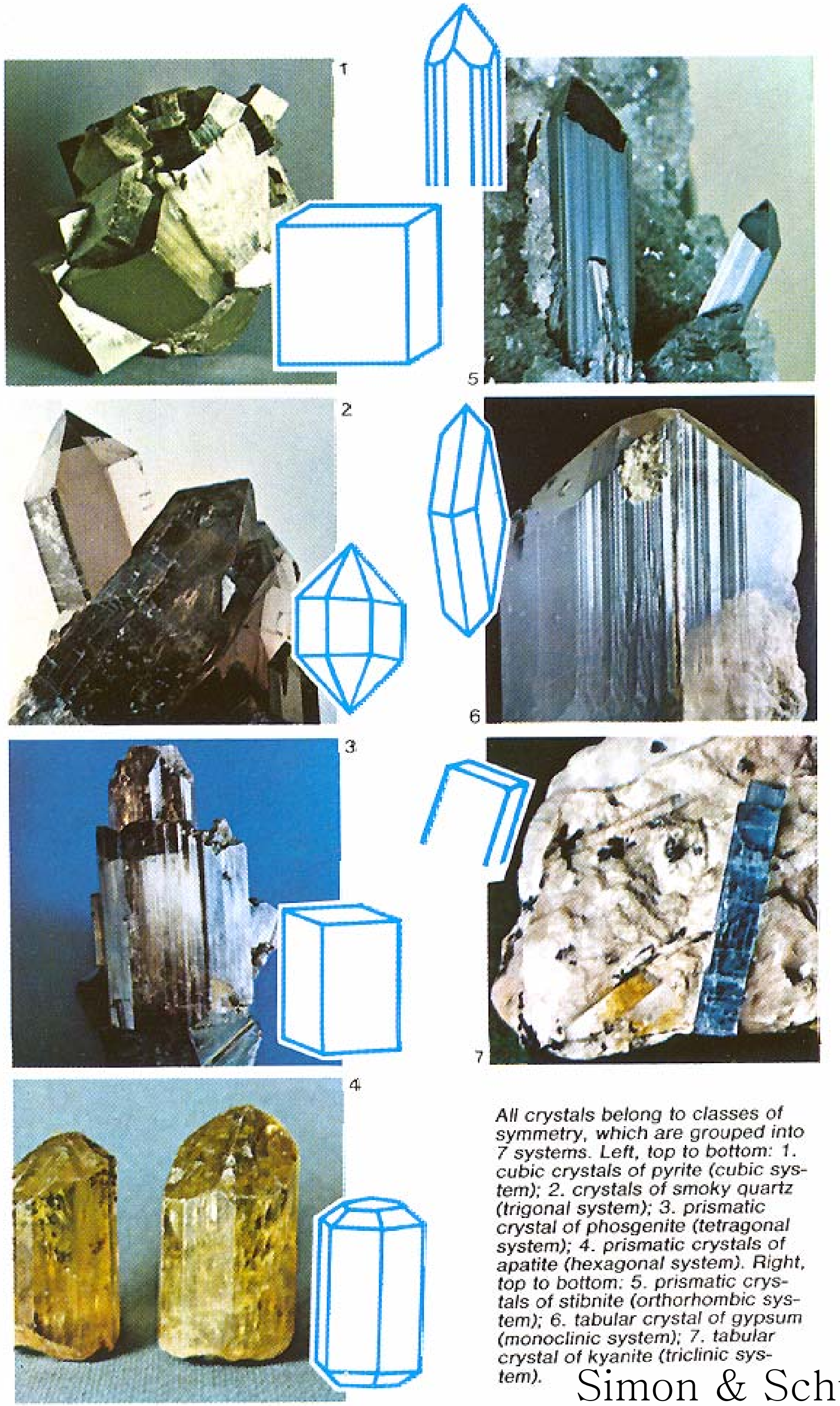

All crystals belong to classes of symmetry, which are grouped into 7 systems. Left, top to bottom: 1. cubic crystals of pyrite (cubic system); 2. crystals of smoky quartz (trigonal system); 3. prismatic crystal of phosgenite (tetragonal system); 4. prismatic crystals of apatite (hexagonal system). Right, top to bottom: 5. prismatic crystals of stibnite (orthorhombic system); 6. tabular crystal of gypsum (monoclinic system); 7. tabular crystal of kyanite (triclinic system).

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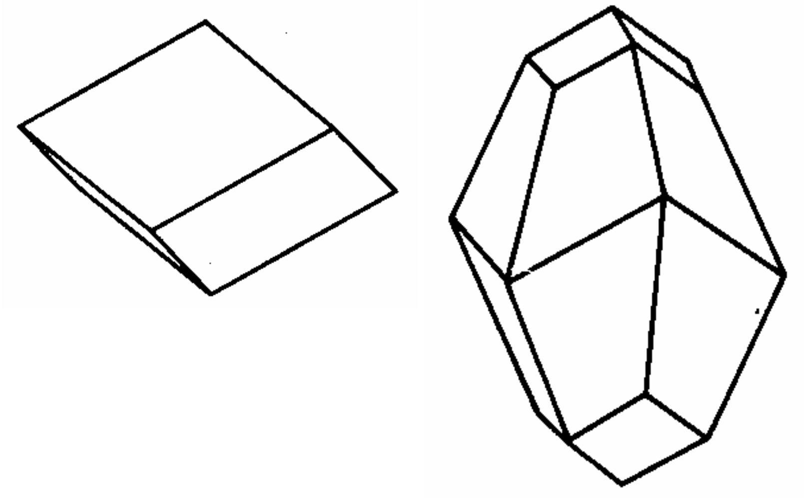
Crystal

2. Cleavage (벽개)- flat surfaces, parallel to crystallographic planes

fracture- irregularly shaped pieces

ex) rhombohedral cleavage of calcite ($CaCO_3$)

Hexagonal, Rhombohedral



glass

http://www.cchs.carroll.k12.ky.us/instruction/forensiclabs/glass.htm

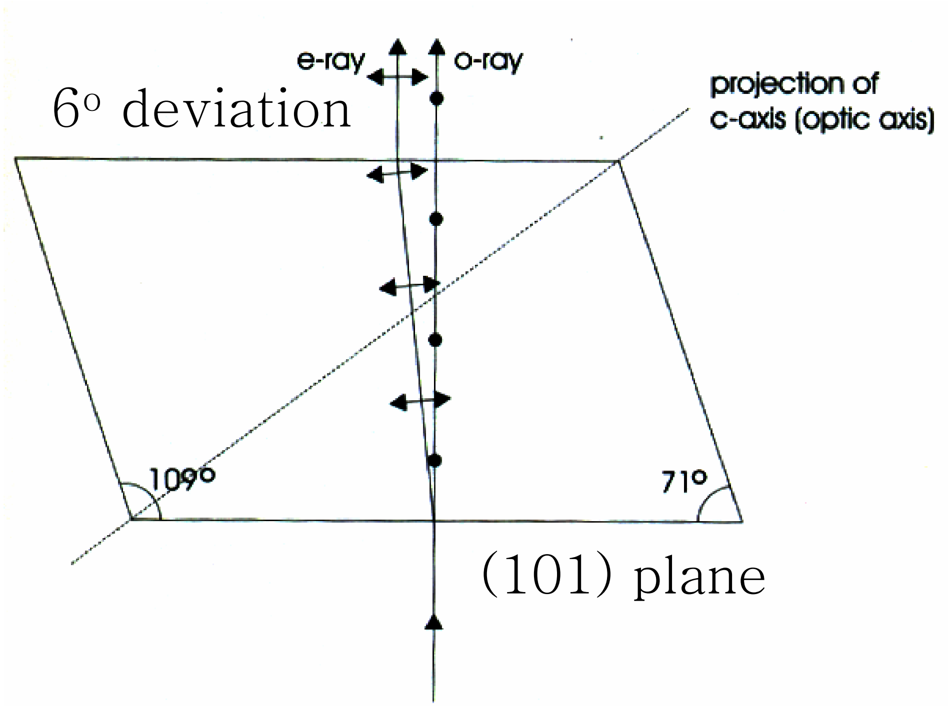
Crystal

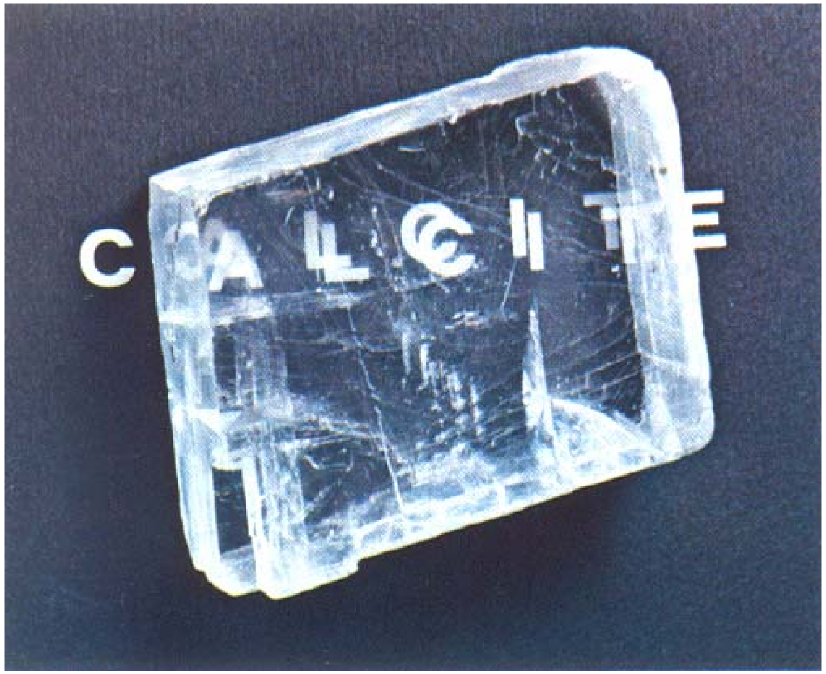
3-1. Birefringence (복굴절)- formation of two polarized light waves

traveling in different directions,

i.e. production of two rays of polarized light

ex) calcite ($CaCO_3$) Hexagonal

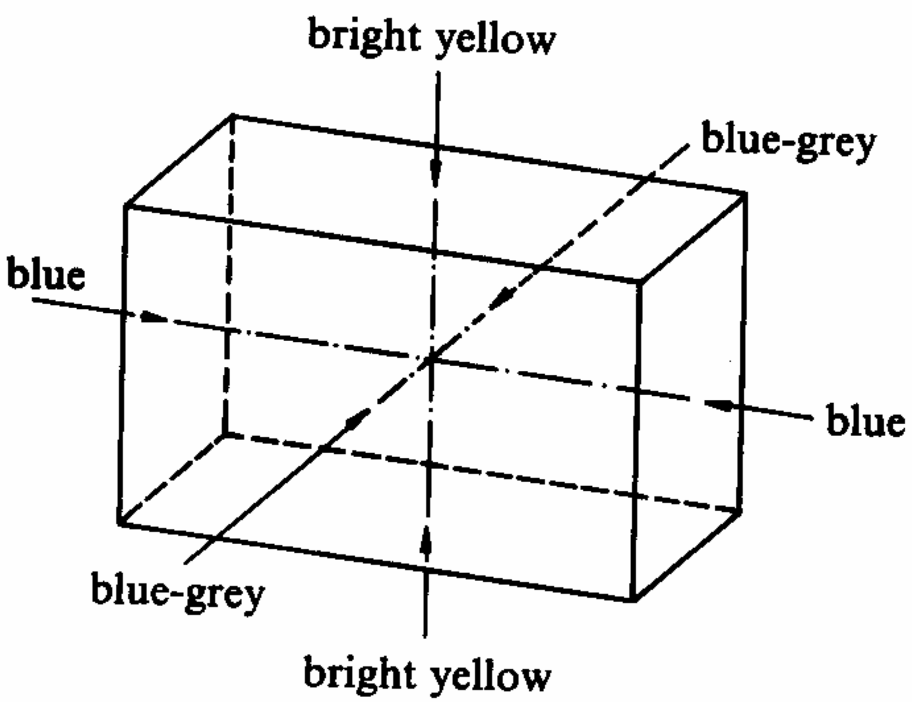


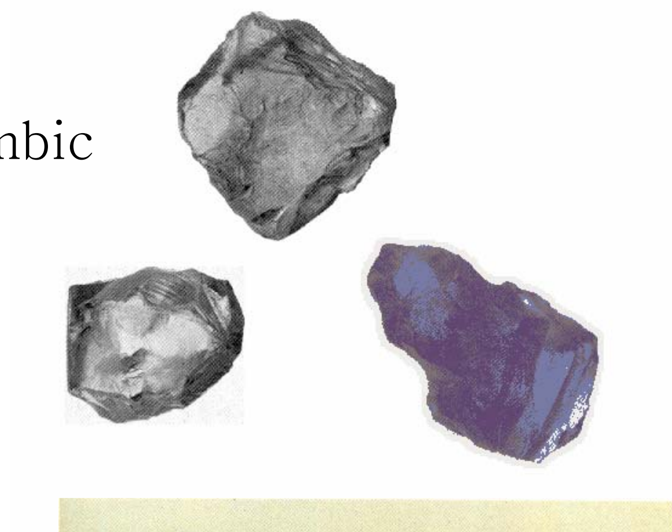


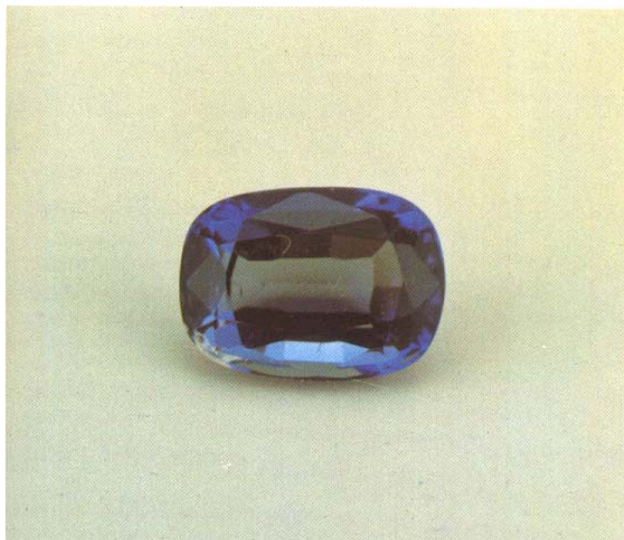
n_o=1.658, n_e=1.486, $n_o - n_e$=0.172

3-2. Pleochroism (다색성)- display more than one color due to the different absorption of light in different directions (dichroism, trichroism)

ex) cordiertite ($Mg_2Al_4Si_5O_8$) Orthorhombic







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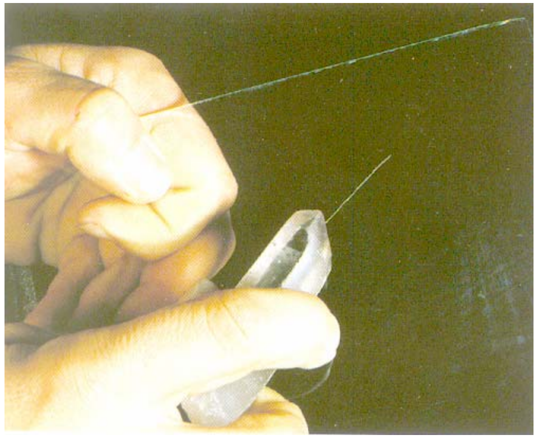
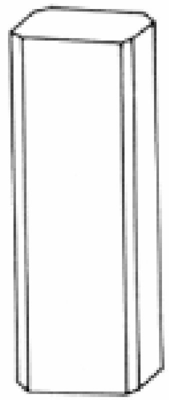
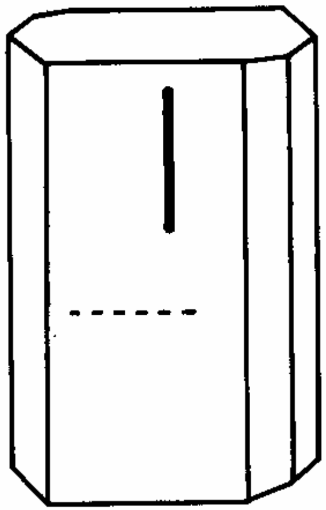
Crystal

4. Hardness (경도)- resistance to external stresses in one direction (scratching), in two (abrasion), and in three (penetration)

ex) kyanite (Al_2SiO_6) Triclinic



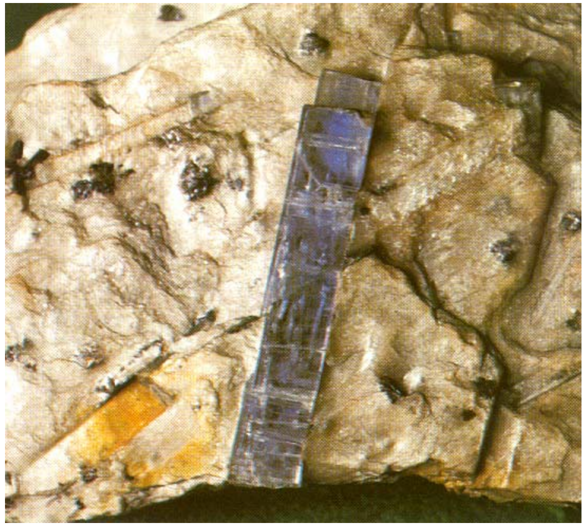




Semihard 4~5

Hard 6~7

* Mohs' scale



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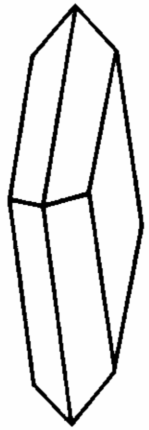
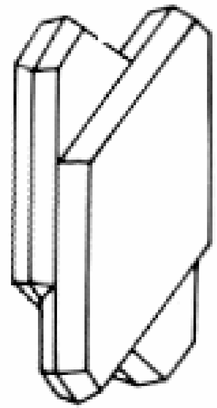
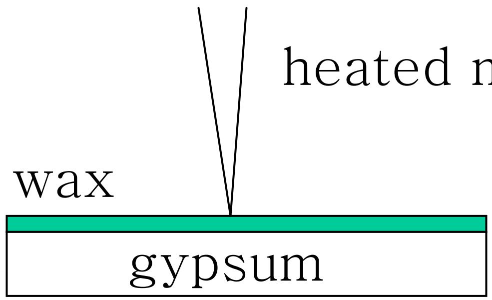
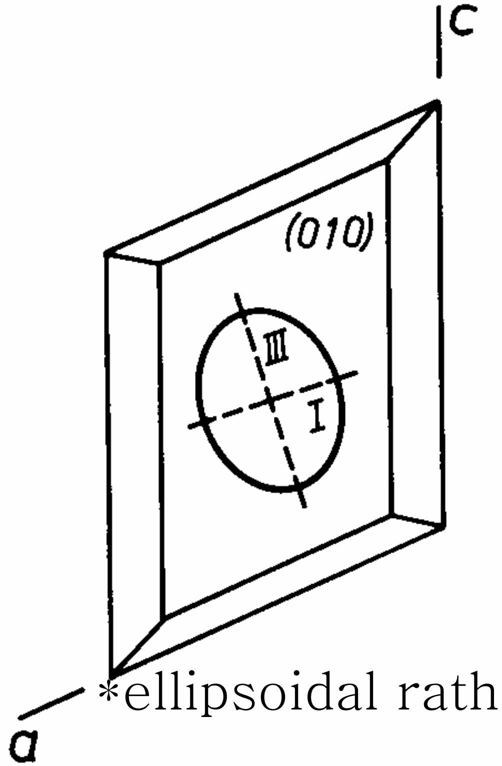
5. Thermal conductivity (열전도도)

ex) gypsum ($CaSO_4 2H_2O$)

Monoclinic





*ellipsoidal rather than circular

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6. Thermal expansion

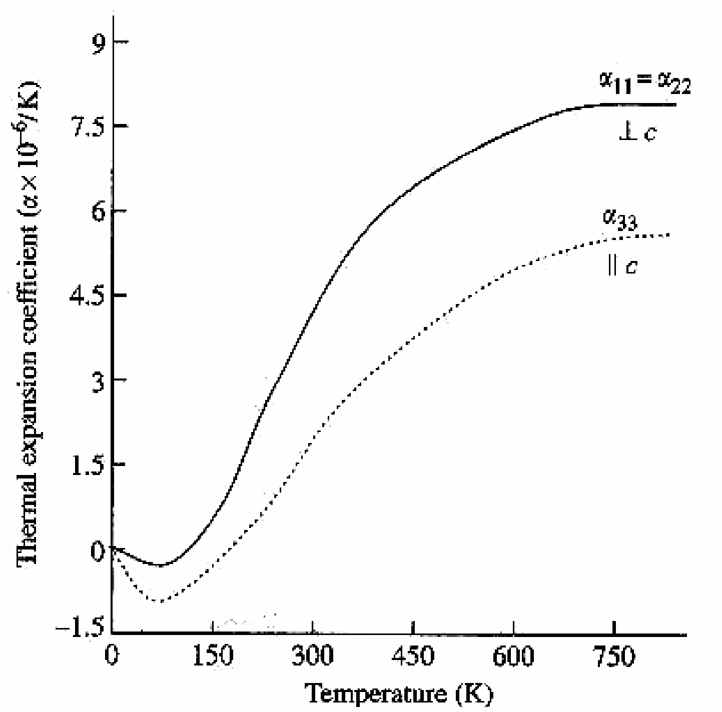


Fig. 11.1 Zinc oxide is a hexagonal crystal with tetrahedrally bonded zinc and oxygen atoms. The thermal expansion coefficients approach zero at 0 K. Anisotropy also changes sign at low temperatures with both coefficients becoming slightly negative.

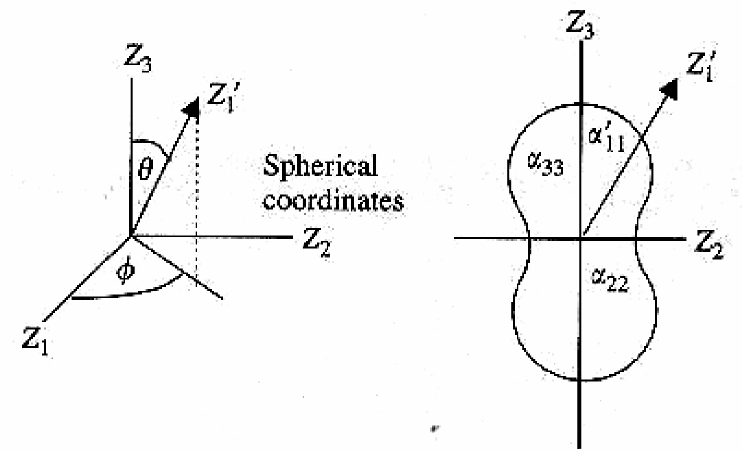


Fig. 11.2 Anisotropy surface for the thermal expansion coefficient of low symmetry crystals.

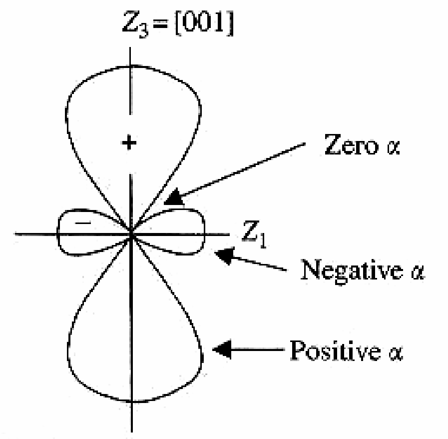
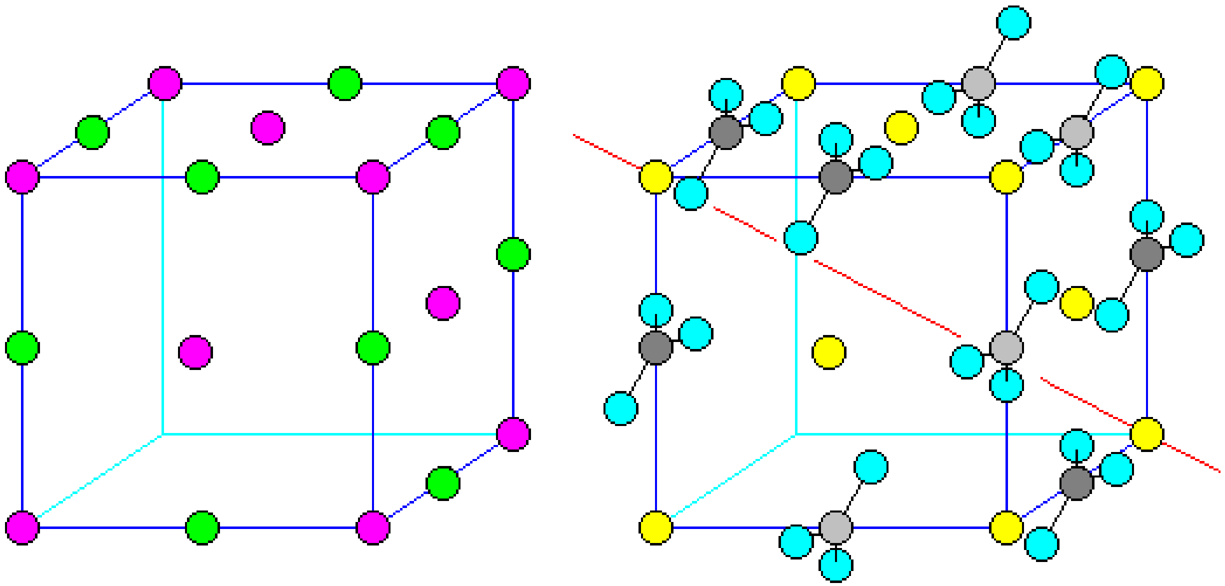


Fig. 11.3 Thermal expansion surface of calcite with circular symmetry about Z_3, the trigonal axis. The maximum expansion is perpendicular to the flat carbonate groups of the structure.

Calcite ($CaCO_3$)

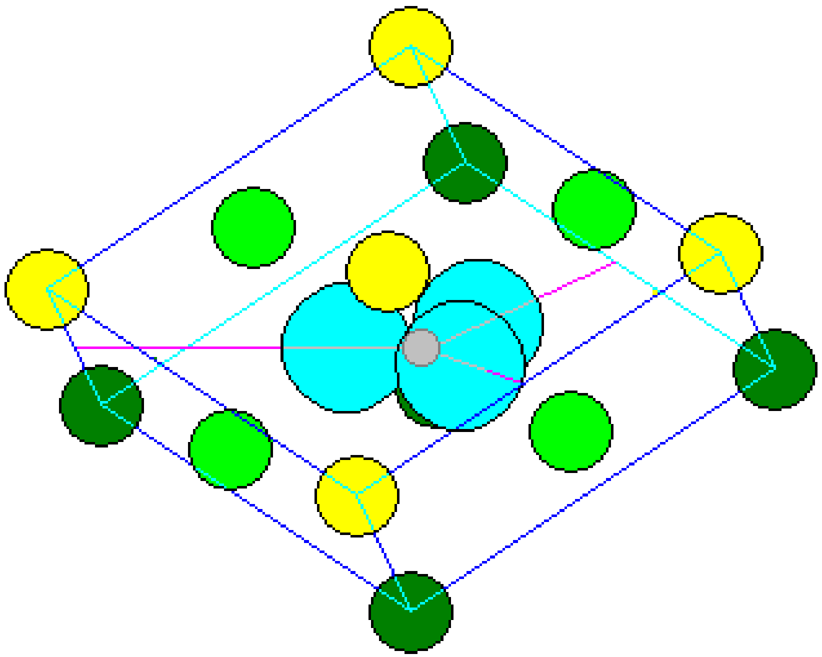


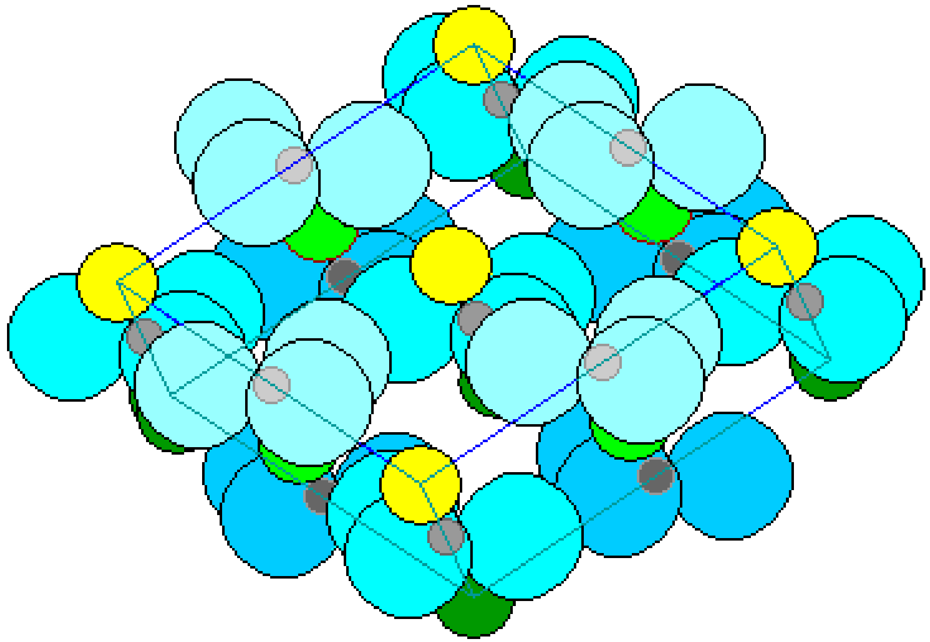

http://mineral.galleries.com/minerals/carbonat/calcite/calcite.htm



http://www.uwgb.edu/dutchs/PETROLGY/Calcite%20Structure.HTM

Calcite ($CaCO_3$)





http://www.uwgb.edu/dutchs/PETROLGY/Calcite%20Structure.HTM

Crystal

- thermal expansion coefficient

Cubic crystals	α		
Diamond (C)	1.4		
Silicon (Si)	4.2		
Germanium (Ge)	5.9		
Copper (Cu)	17		
Silver (Ag)	20		
Gold (Au)	15		
Iron (Fe)	12		
Platinum (Pt)	8.3		
Tungsten (W)	4.3		
Hexagonal crystals	α_{11}	α_{33}	
Magnesium (Mg)	27	28	
Zinc (Zn)	14	61	
Cadmium (Cd)	19	48	
Magnesium Hydroxide ($Mg(OH)_2$)	11	45	
Tetragonal crystals	α_{11}	α_{33}	
Tin (Sn)	46	22	
Titanium Oxide (TiO_2)	7.1	9.2	
Trigonal crystals	α_{11}	α_{33}	
Calcium Carbonate ($CaCO_3$)	−3.8	21	
Sodium Nitrate ($NaNO_3$)	11	120	
Tellurium (Te)	28	−1.7	
Antimony (Sb)	8.2	16	
Aluminum Oxide (Al_2O_3)	5.4	6.6	
Orthorhombic crystals	α_{11}	α_{22}	α_{33}
Iodine (I_2)	133	95	35
Lead Chloride ($PbCl_2$)	34	39	17

R. E. Newnham, Properties of Materials

Anisotropy

Anisotropy (이방성)- different values of a physical property
in different directions

Isotropy (등방성)- same value of a physical property in all directions

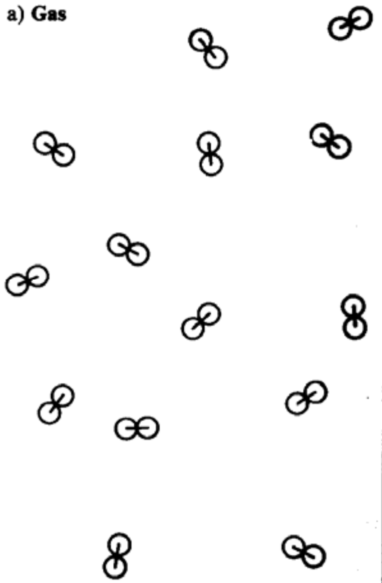
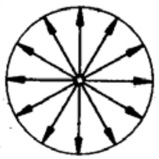
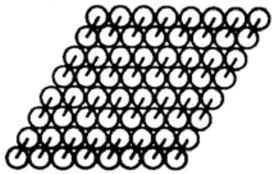
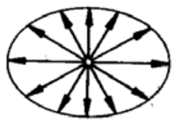
In general, most solids are anisotropic with respect to some physical parameters, but isotropic to others.

ex) solid NaCl is optically isotropic but mechanically anisotropic.

What feature of the structure of the solid state give rise to anisotropy?

- internal structure of crystals

Schematic representation of the states of matter

Representation of the state	Retention of shape	Retention of volume	Distribution of molecules	Physical properties
a) Gas 	No	No	Statistically homo-geneous[1]	 Isotropic[2]
Boiling point				
b) Liquid 	Yes	No		
Melting point				
c) Crystal 	Yes	Yes	Periodically homo-geneous[1]	 Anisotropic[3]

No Yes

[1] Equal physical properties in parallel directions

[2] Equal physical properties in all directions

[3] Different physical properties in different directions

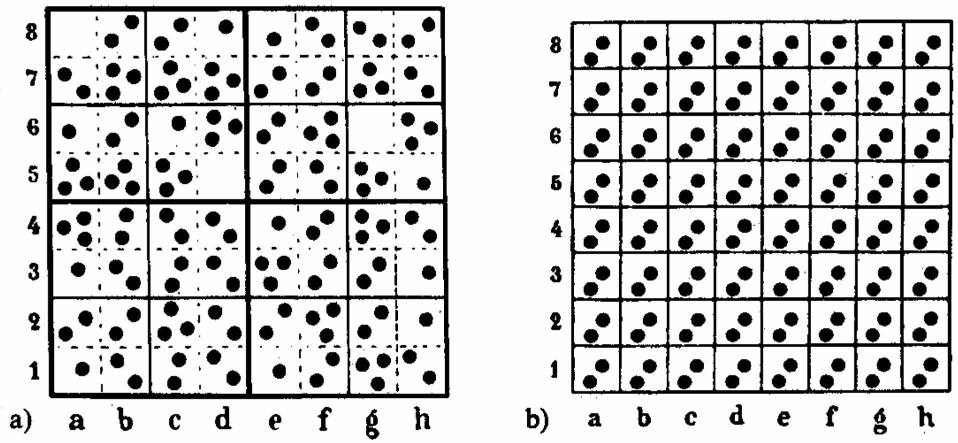
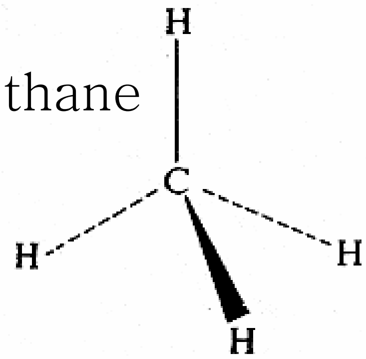
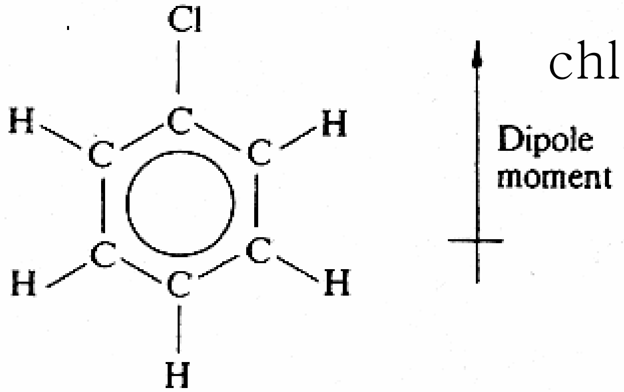


Fig. 1.6 a, b. Statistical (**a**) and periodic (**b**) homogeneity. Johnsen [21]

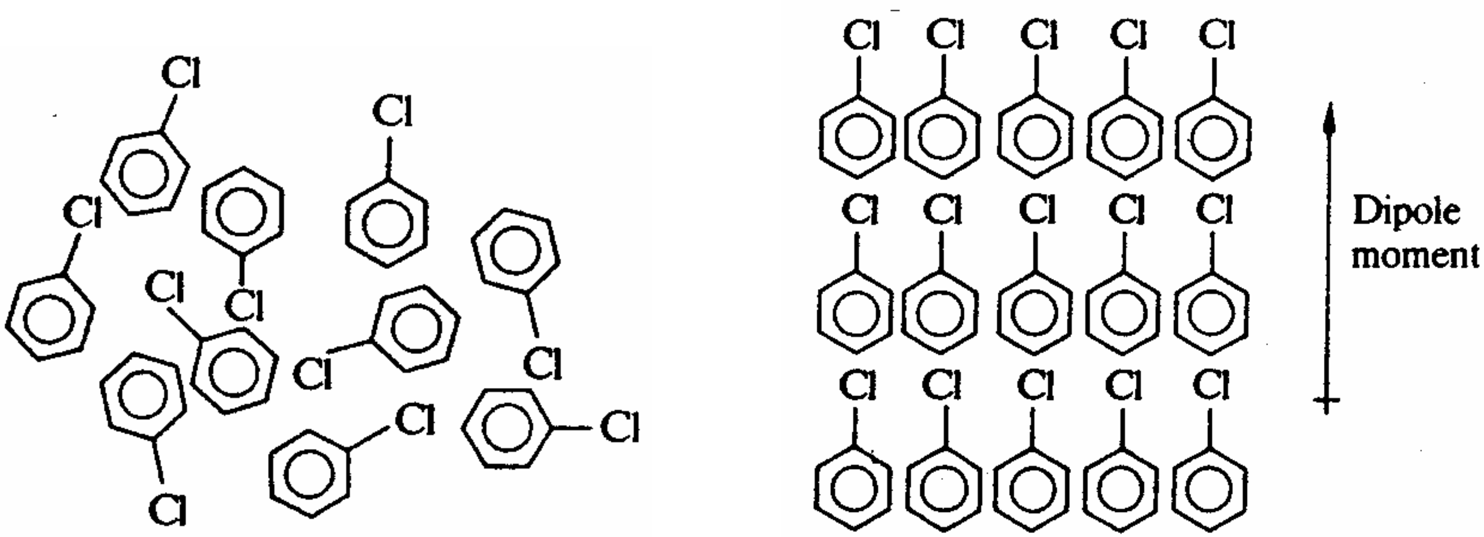
methane



chlorobenzene



Molecular structure can give rise to anisotropy



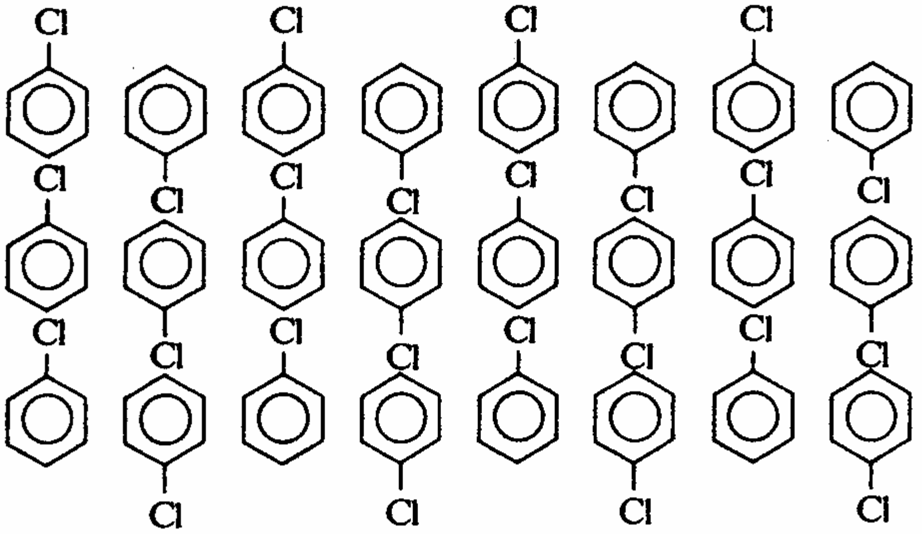
(a)

A random array,
no net dipole moment

(b)

A regular array,
a net dipole moment exists

Which of these structures is anisotropic?



$$\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha}{3\varepsilon_o}$$

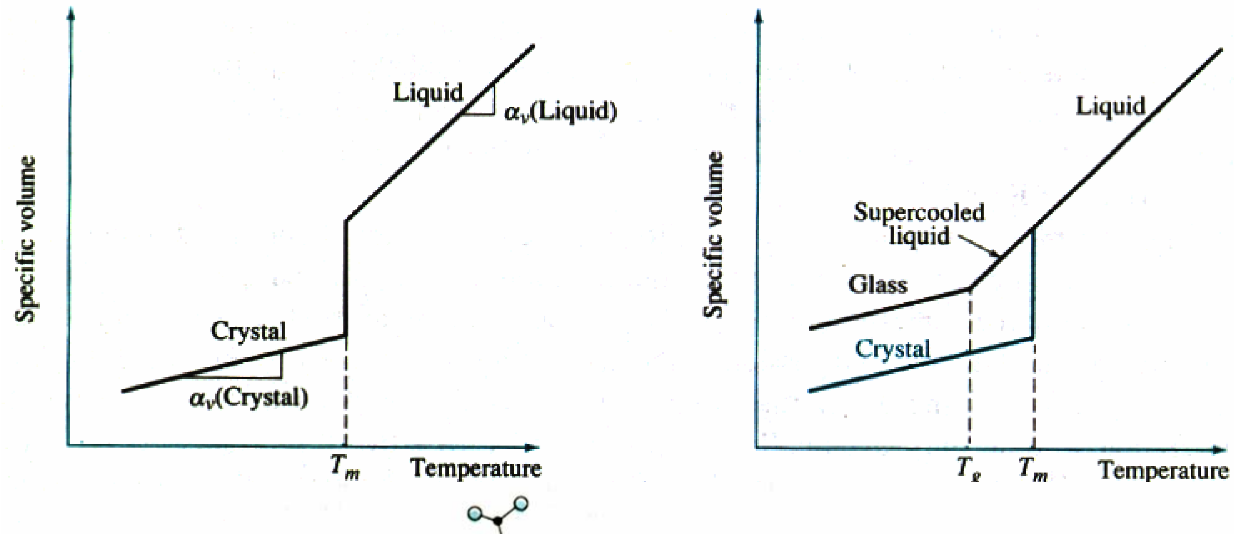
$$P = Np = N\alpha E$$

Order, but no anisotropy.
Isotropic with respect to its dielectric constant

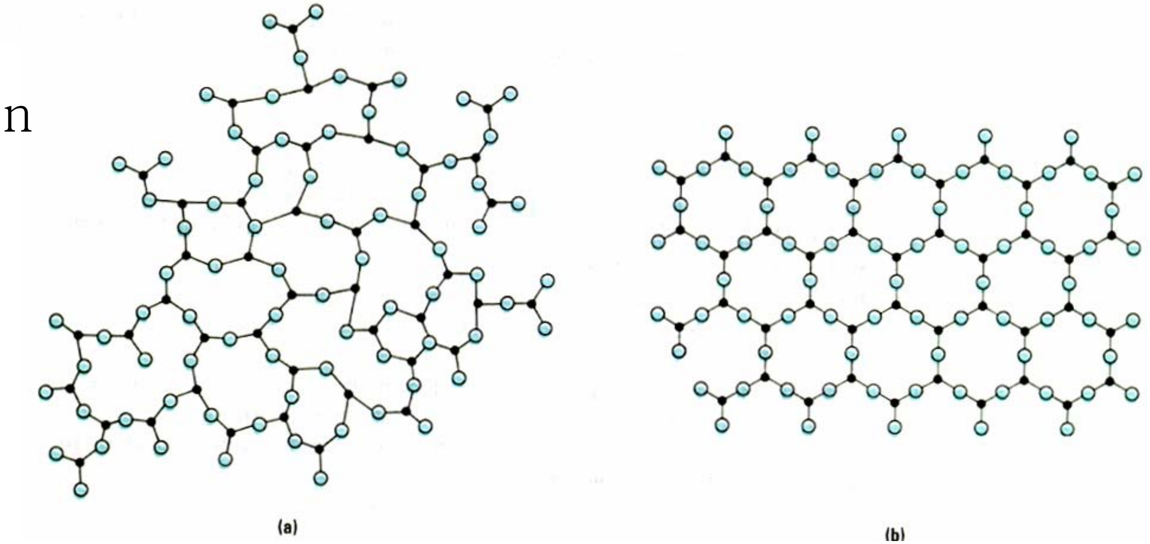
It is therefore fallacious to say that all ordered arrays will be anisotropic, but it is undoubtedly true to say the converse, namely, that all anisotropic materials have an ordered structure.

Definition

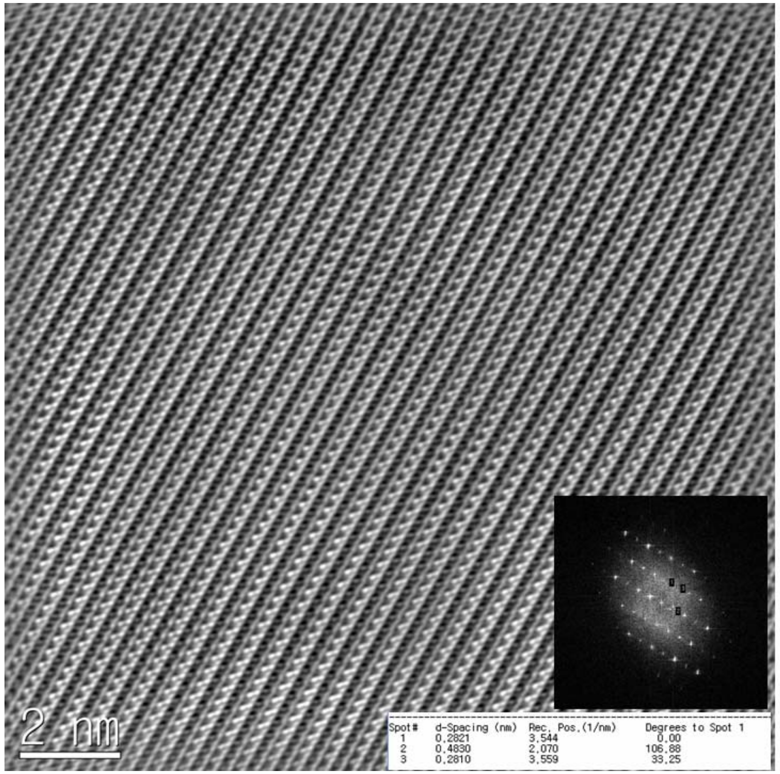
A **crystal** is an anisotropic, homogeneous body consisting of a three-dimensional periodic ordering of atoms, ions, or molecules.



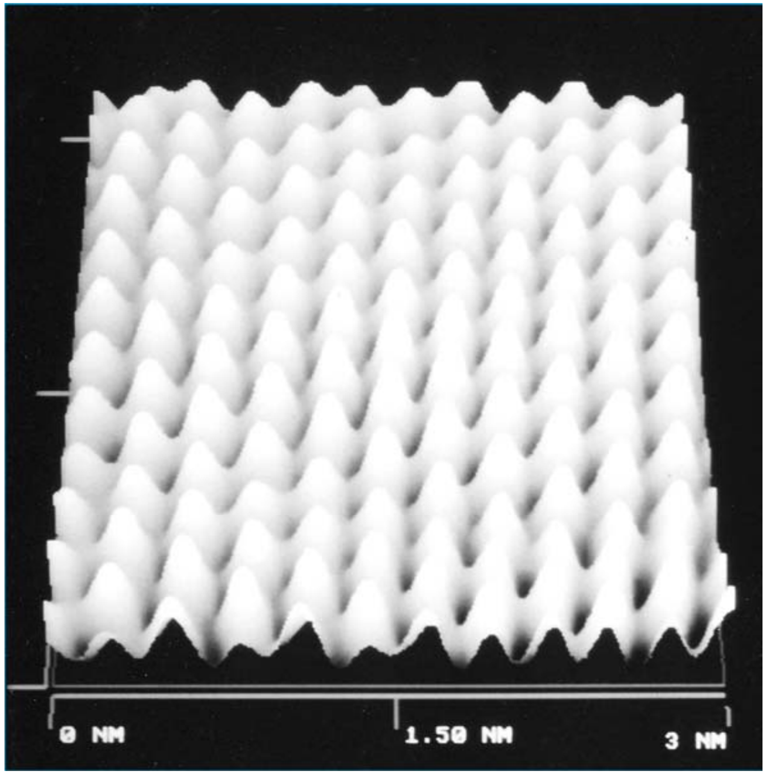
* X-ray diffraction
  crystal
  amorphous



Crystal- Microstructure



$CaCu_3Ti_4O_{12}$
Transmission Electron microscope

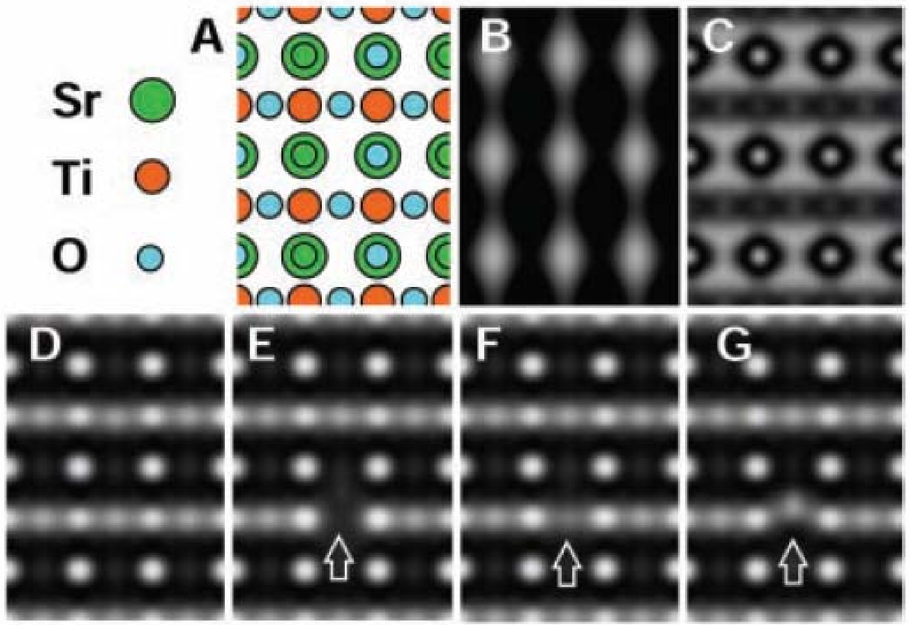


Au, (111) surface
Atomic Force Microscope

Atomic-Resolution Imaging of Oxygen in Perovskite Ceramics

C. L. Jia, M. Lentzen, K. Urban*

experimental



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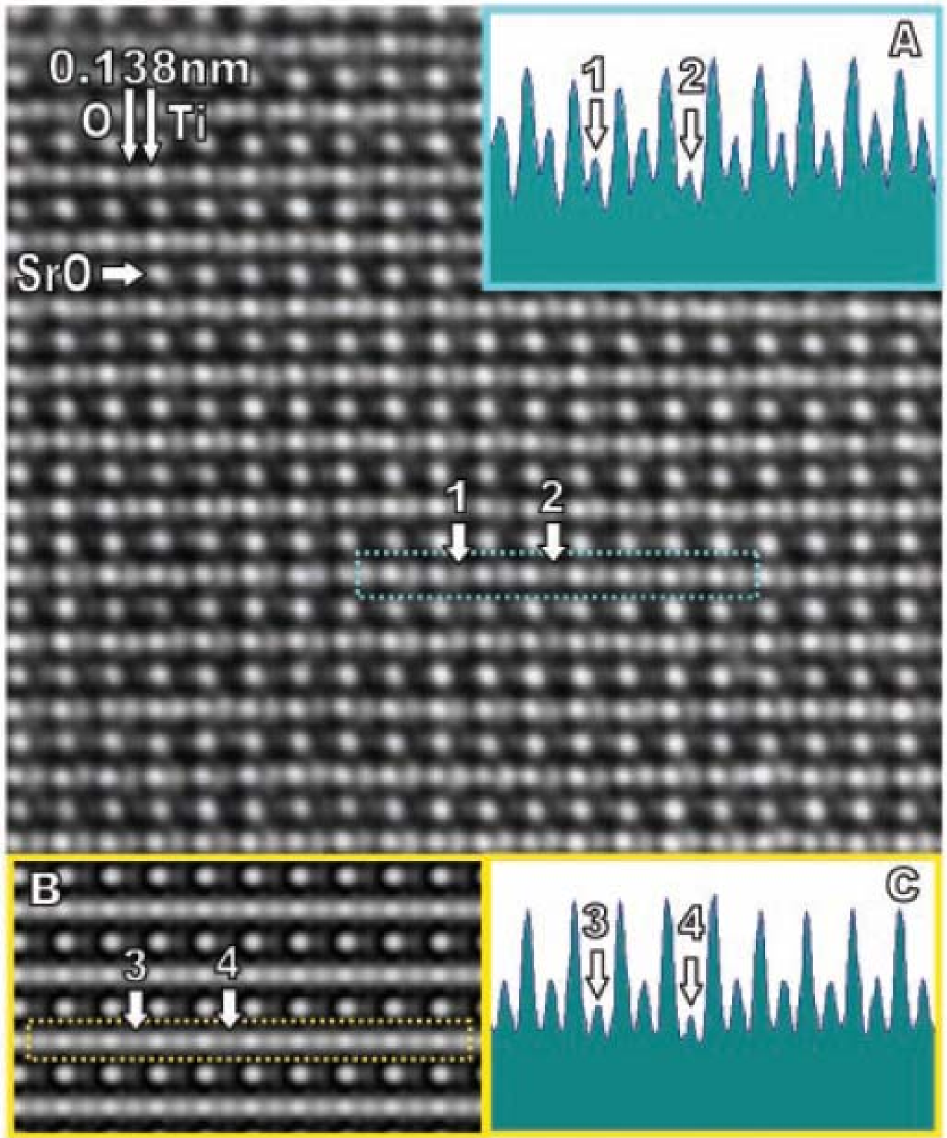

www.sciencemag.org SCIENCE VOL 299 7 FEBRUARY 2003

calculated