2008학년도 2학기(445.206.001)

교과목명 : **결정학개론 (Crystal Structure and Crystallography)**

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학점 : 출석/과제(10%), 중간고사 I (25%), 중간고사 II (25%), 기말고사(40%)

성적 : A(20%), B(30%), C이하(50%) or A(30%), B(30%), C이하(40%)

참고서적 :

1. 결정학개론, 정 수진 저, 피어슨 에듀케이션 코리아,2nd Ed., 2001.
2. W. B. Ott, Crystallography, 2nd Ed., Springer, 1995.
3. B. D. Cullity, Elements of X-ray Diffraction, 3rd Ed., Prentice Hall, 2001.

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

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.

결정학 (crystallography)- concerned
with the laws governing the crystalline state 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

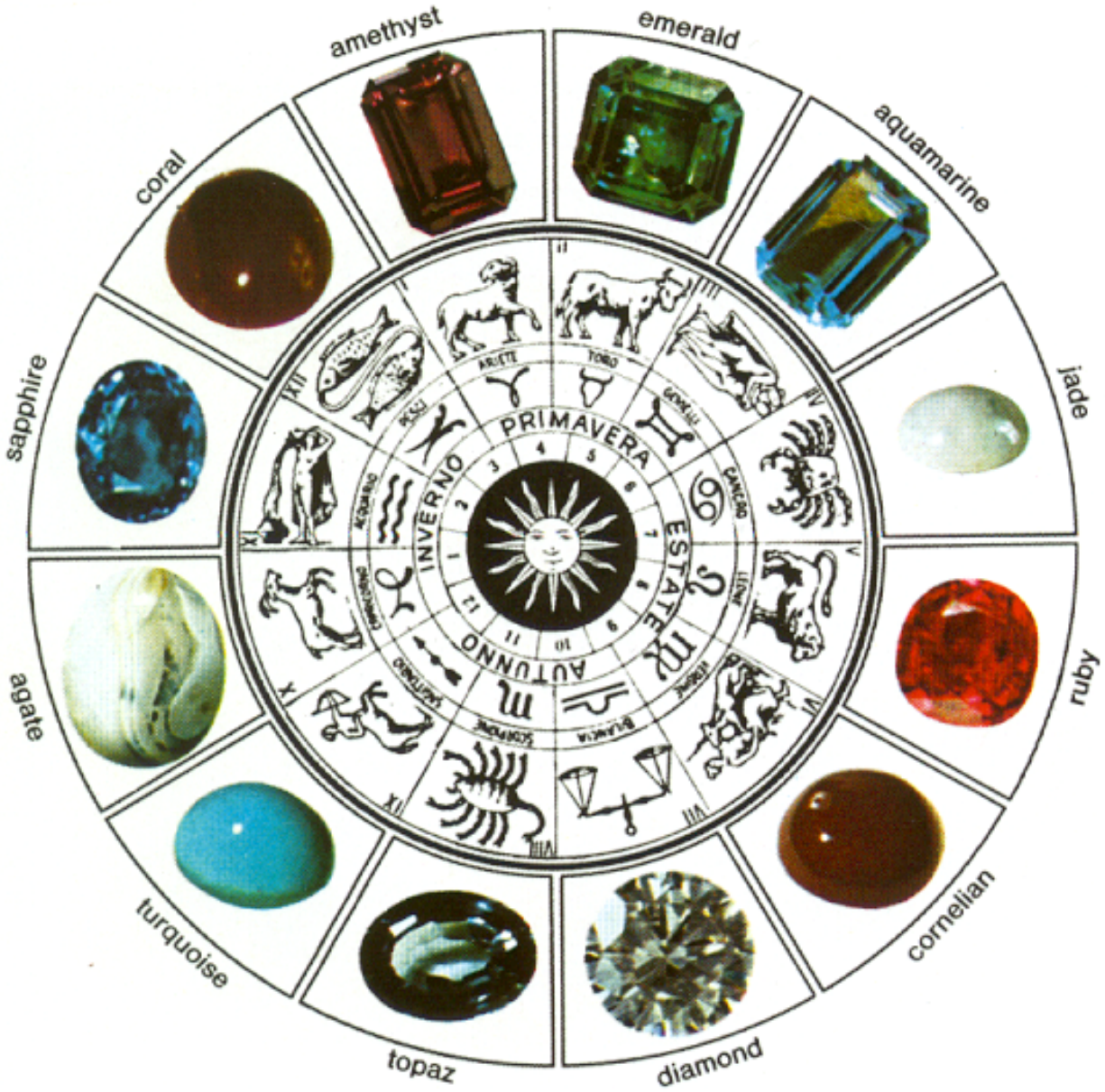
1. Regular geometric shape

form: set of the physically equivalent faces of a crystal, whose presence is controlled by the symmetry of the crystal class

ex)prism, pinacoid planes

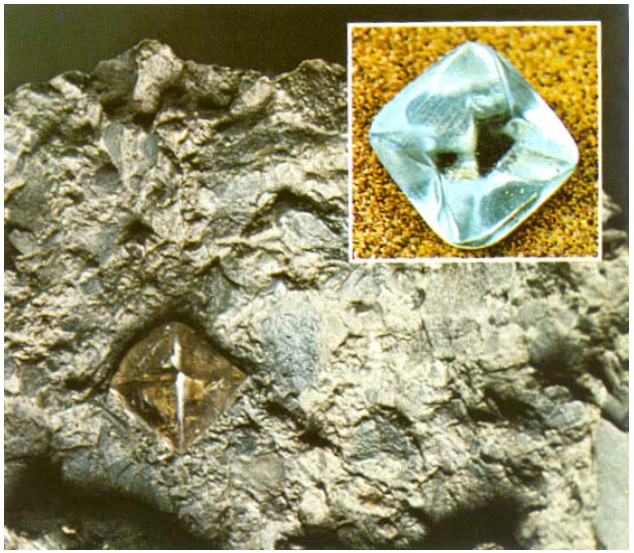
usually not given by a single crystallographic form but by a combination of various forms, each developed to a greater or lesser degree

habit: appearance determined by the predominant form; used to describe the relative sizes of the faces of a crystal

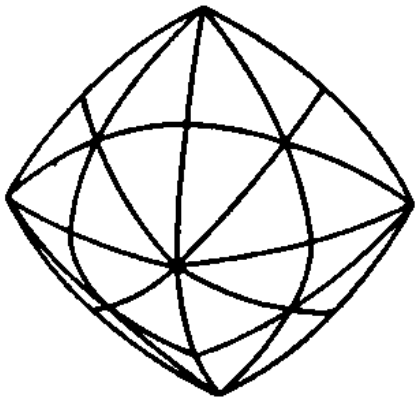


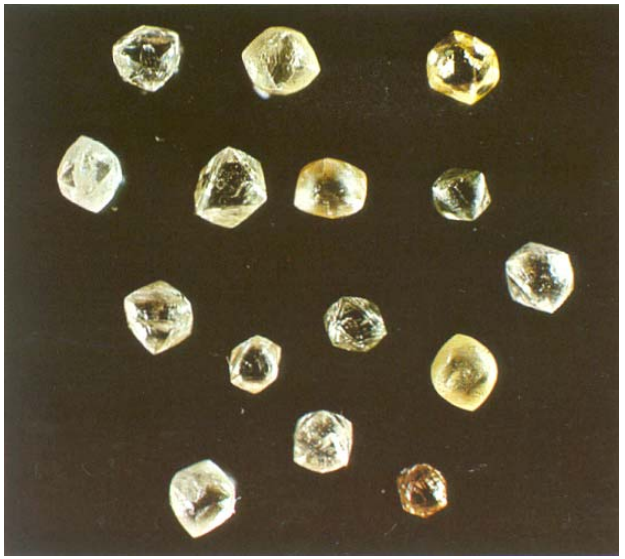
Simon & Schuster's Guide to Gems and Precious Stones

Diamond (C)



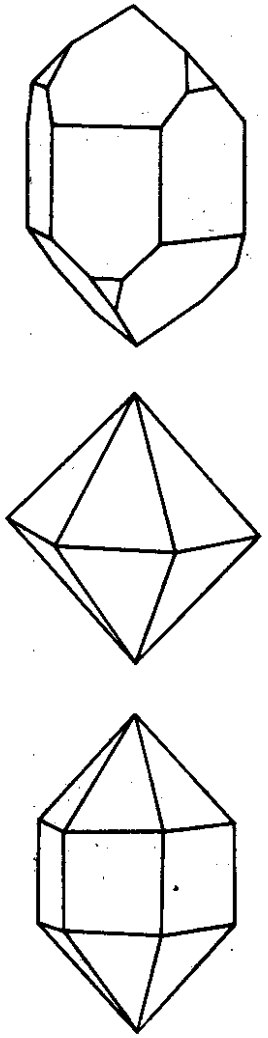
Cubic, Octahedron

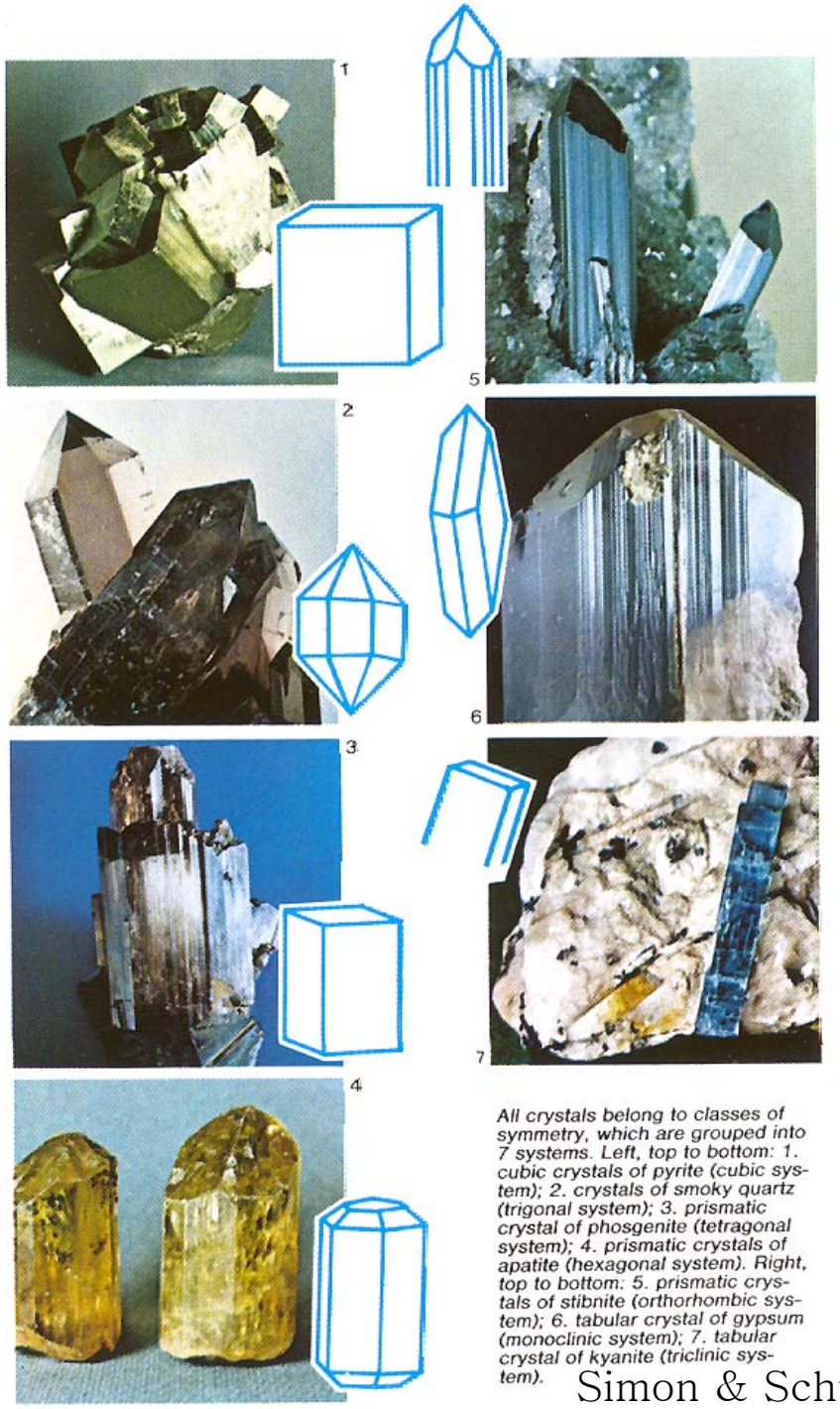




Quartz (SiO_2)

Hexagonal, Prismatic





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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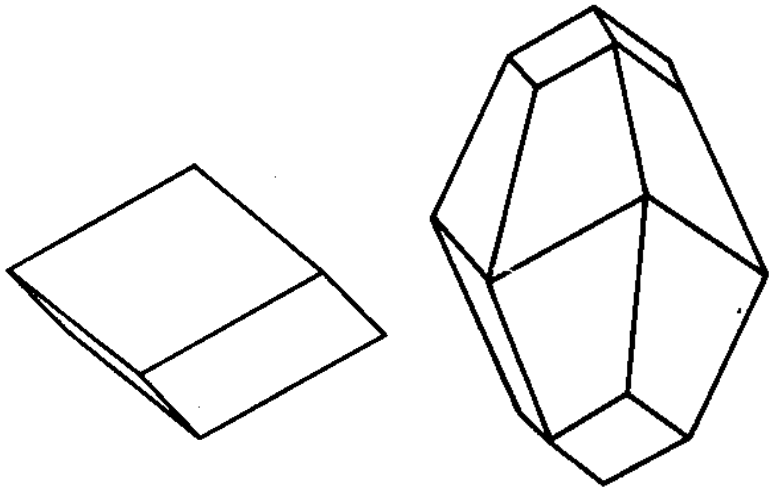
2. Cleavage (벽개)- flat surfaces, parallel to crystallographic planes
fracture- irregularly shaped pieces

ex) rhombohedral cleavage of calcite ($CaCO_3$)

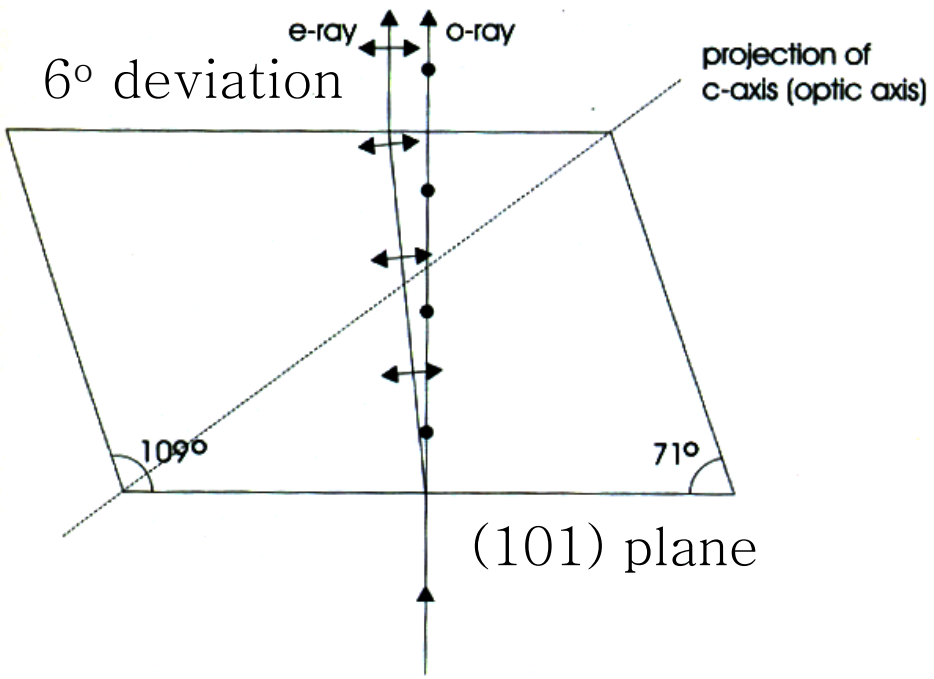
Hexagonal, Rhombohedral

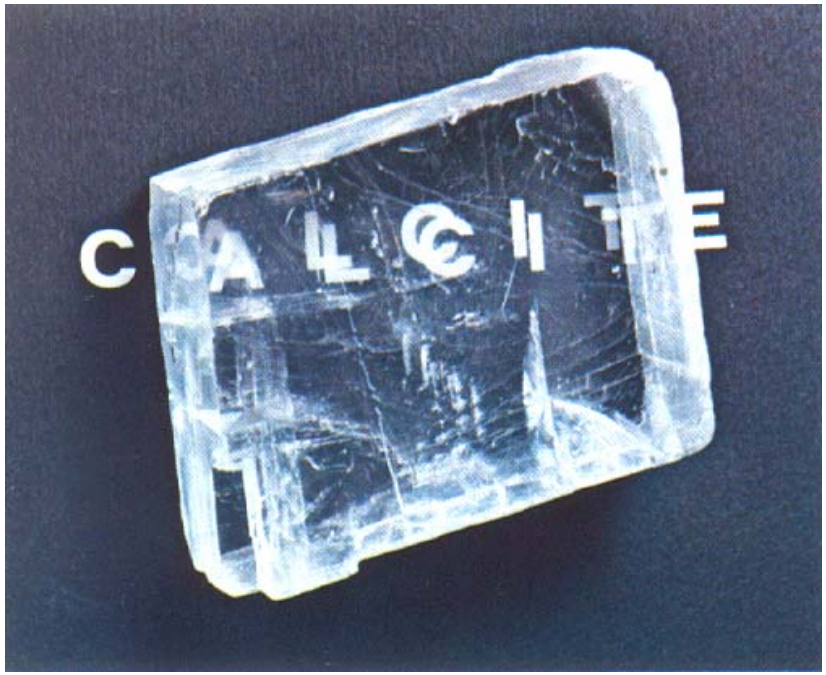


3-1. Birefringence (복굴절)- formation of two polarized light waves traveling in different directions,

i.e. production of two rays of polarized light

ex) calcite ($CaCO_3$) Hexagonal



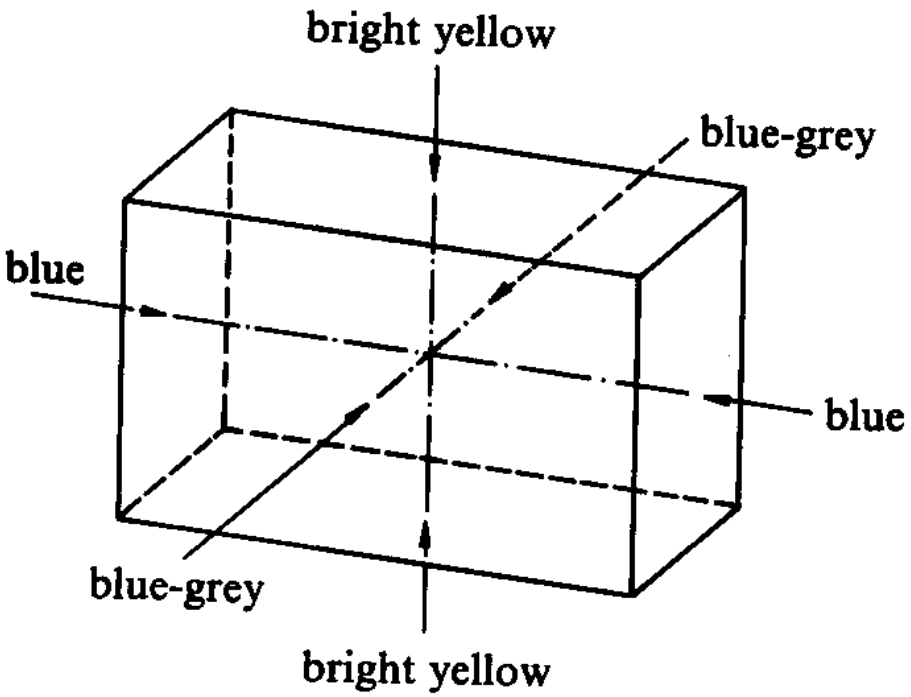


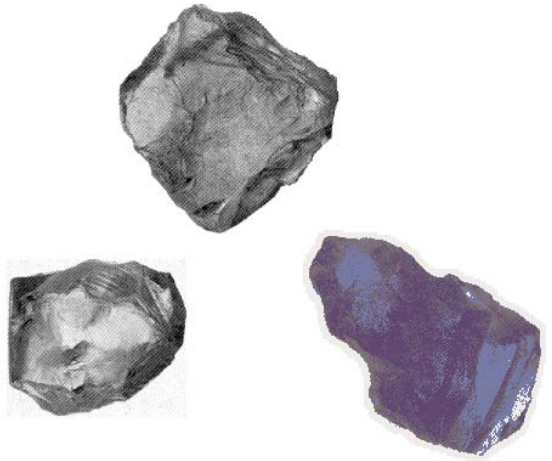
n_o=1.658, n_e=1.486, $n_o - n_e$=0.172

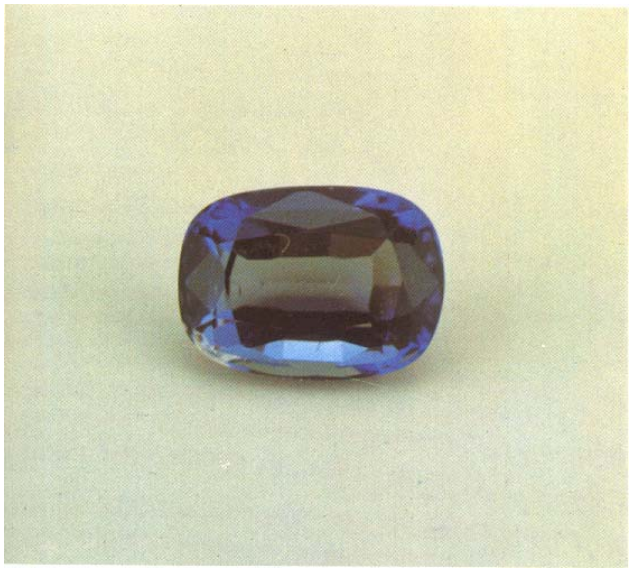
3-2. Pleochroism (다색성)- display more than one color due to the different absorption of light in different directions (dichroism, trichroism)

ex) cordiertite ($Mg_2Al_4Si_5O_8$) Orthorhombic

"Vikings' compass"

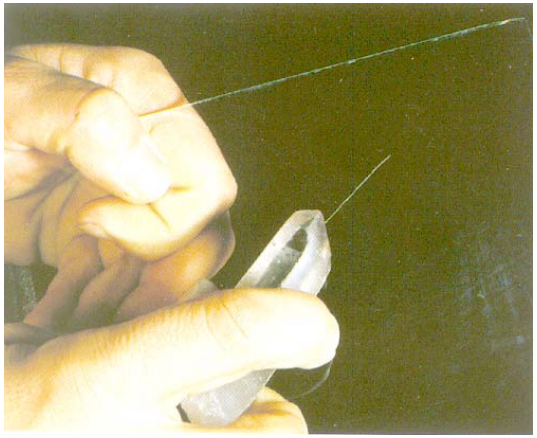


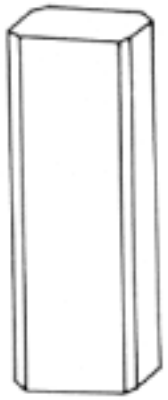


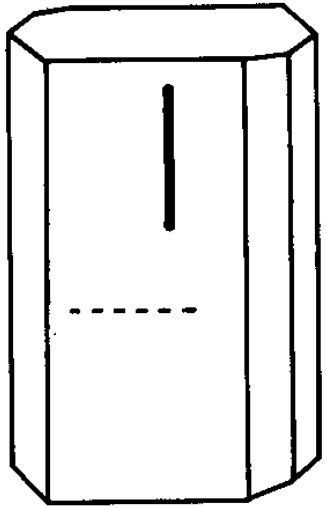


4. Hardness (경도)- resistance to external stresses in one direction (scratching), in two (abrasion), and in three (penetration)

ex) kyanite (Al_2SiO_6) Triclinic

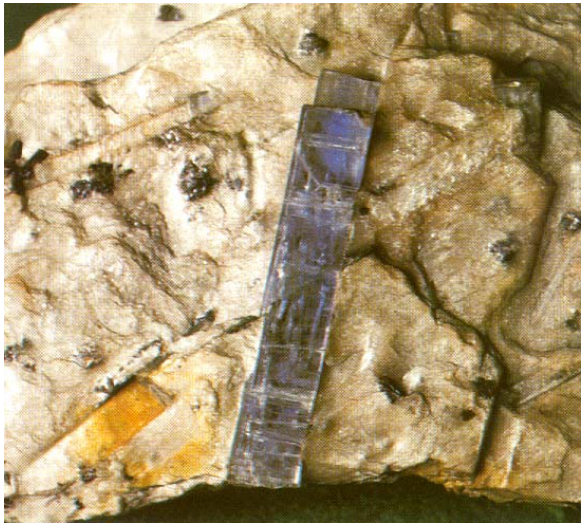






Hard 6~7

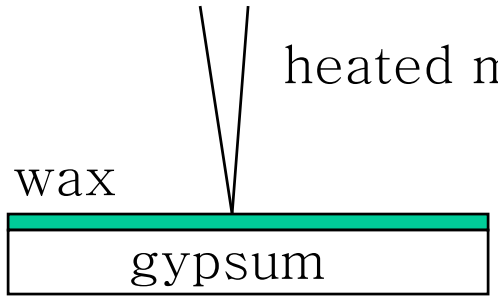
Semihard 4~5

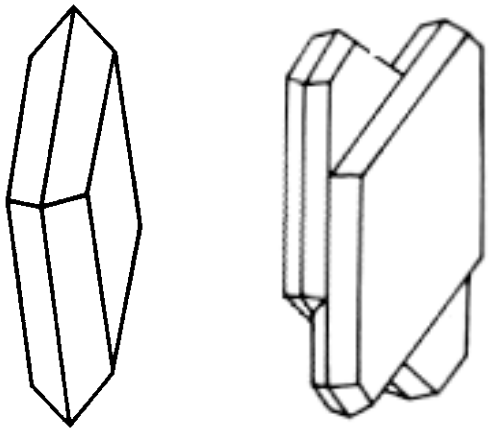


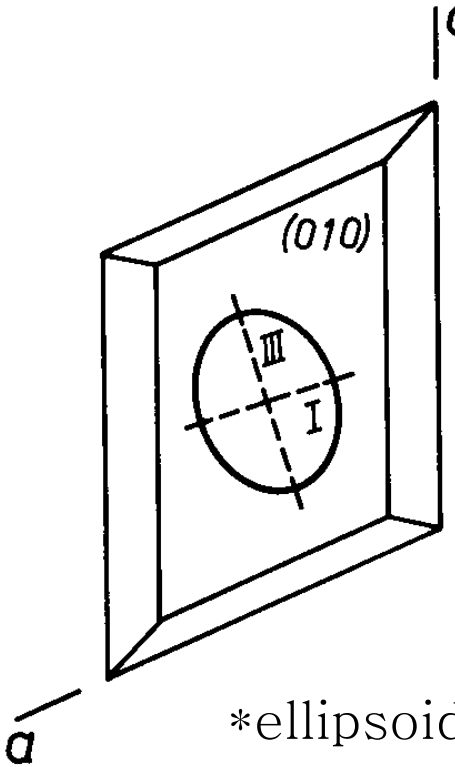
* Mohs' scale

5. Thermal conductivity (열전도도)

ex) gypsum ($CaSO_4 2H_2O$) Monoclinic







*ellipsoidal rather than circular

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 homogeneous[1]	Isotropic[2]
Boiling point				
b) Liquid	Yes	No		
Melting point				
c) Crystal	Yes	Yes	Periodically homogeneous[1]	Anisotropic[3]

[1] Equal physical properties in parallel directions ⟹
[2] Equal physical properties in all directions
[3] Different physical properties in different directions

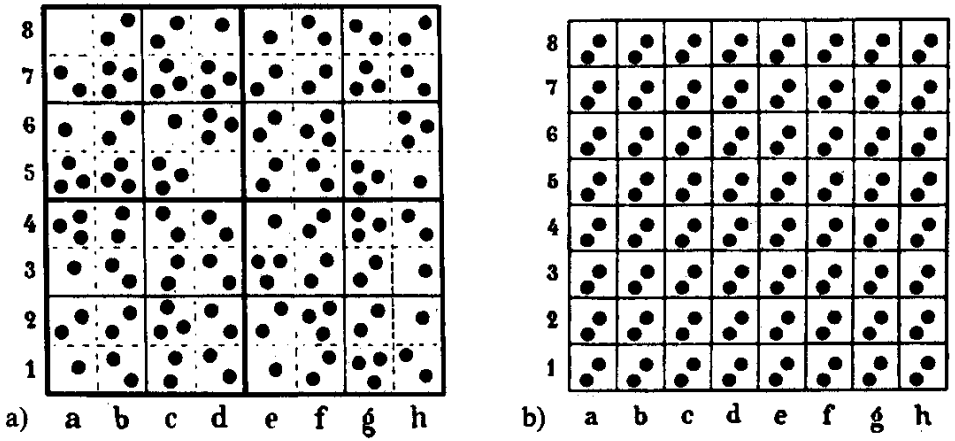
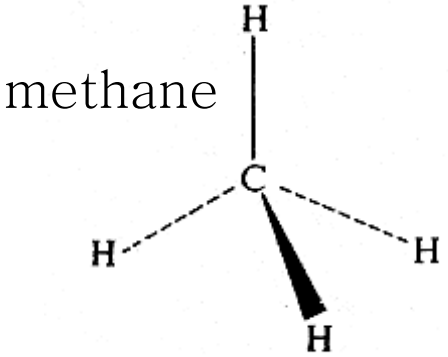


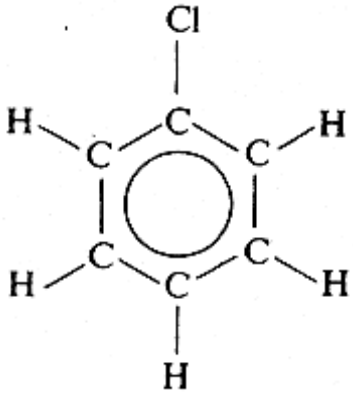
Fig. 1.6a, b. Statistical (a) and periodic (b) homogeneity. Johnsen [21]

미국 펜실베이니아주립대 김은성(金恩成·33·사진) 박사는 세계적인 과학저널 '사이언스' 인터넷판인 '사이언스 익스프레스' 2일자에 "고체 헬륨을 대기압의 26배인 고압상태에서 -273도에 가깝게 냉각시켰더니 전체 원자 중 1.5%가 마치 물이 흐르듯 다른 원자들 사이를 움직이는 현상을 확인했다"는 논문을 발표했다.

액체 헬륨의 초유체현상을 발견해 지난해 노벨 물리학상을 수상한 안소니 레깃 박사는 사이언스 익스프레스에 발표한 논평에서 "레코드판 위에 동전을 얹고 돌려도 레코드판과 동전이 따로 움직일 수 있음을 증명한 것"이라며 "고체에 대한 기존의 설명을 극적으로 변화시킬 것"이라고 평가했다.

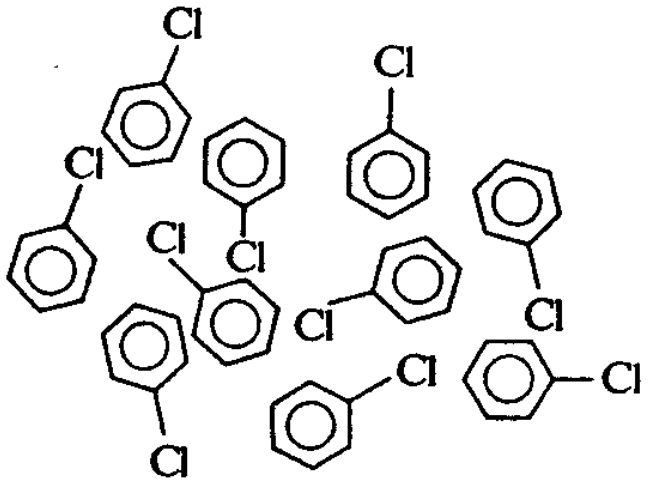
조선일보 2004. 9.3





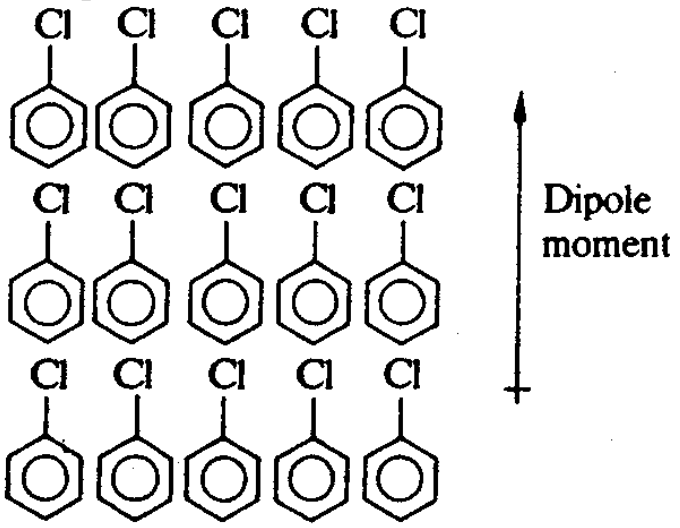
chlorobenzene

Molecular structure can give rise to anisotropy



(a)

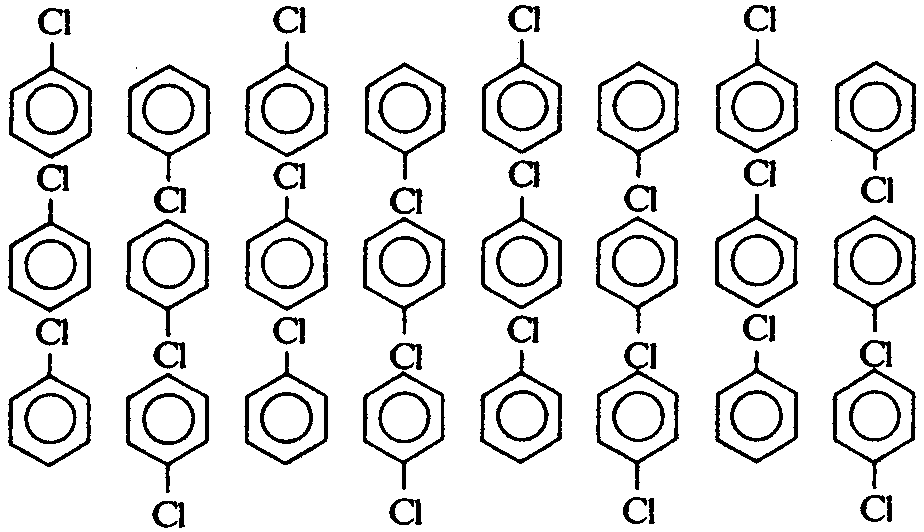
A random array,
no net dipole moment



(b)

A regular array,
a net dipole moment exists

Which of these structures is anisotropic?



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

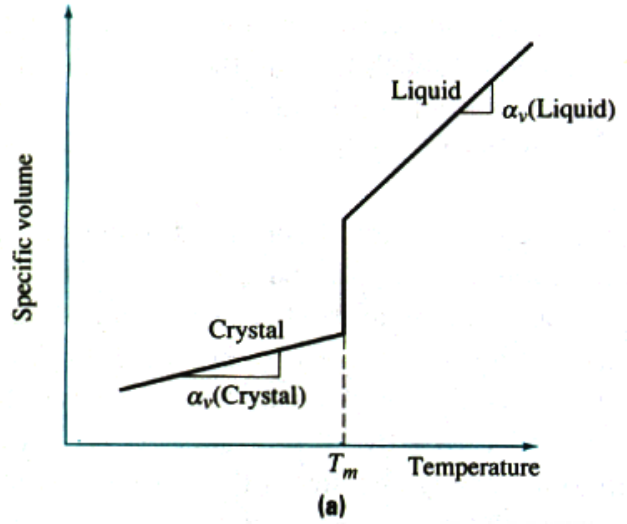
$$P = Np = N\alpha E$$

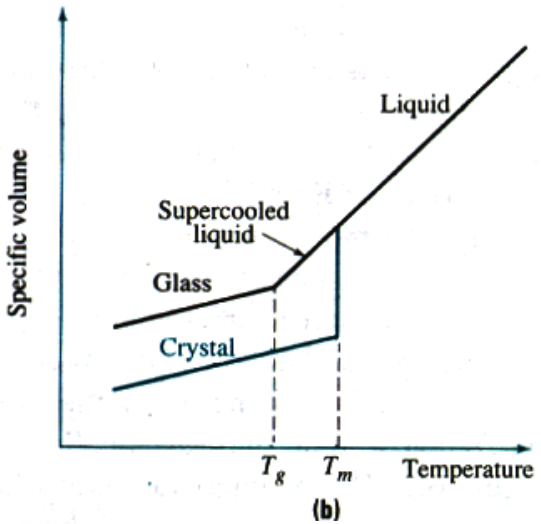
Order, but no anisotropy.
Isotropic with respect to its dielectric constant

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.

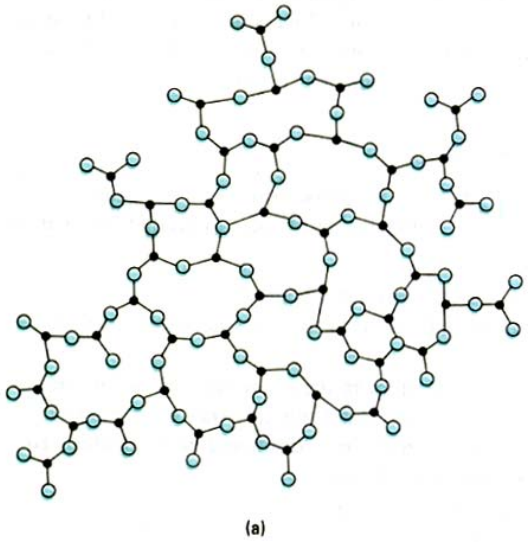
Definition

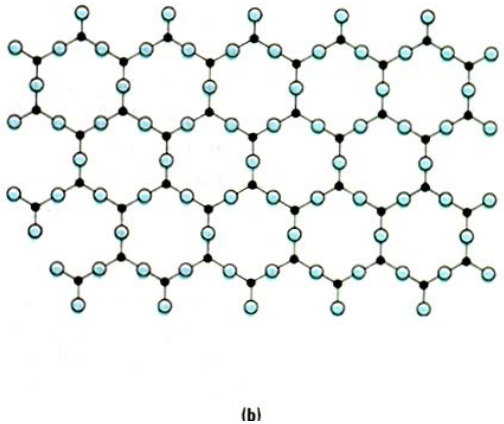
A **crystal** is an anisotropic, homogeneous body consisting of a three-dimensional periodic ordering of atoms, ions, or molecules.



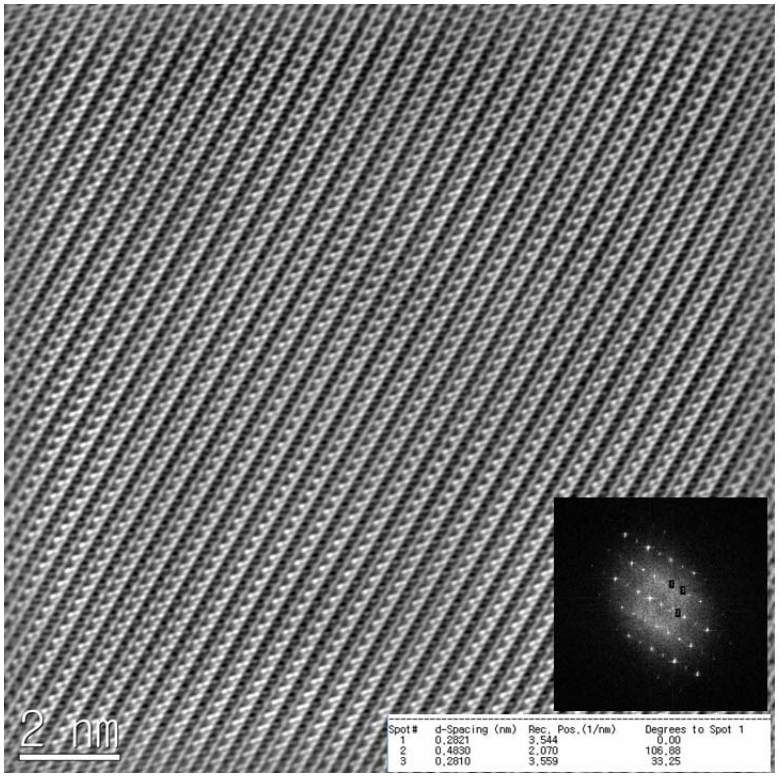


* X-ray diffraction
  crystal
  amorphous

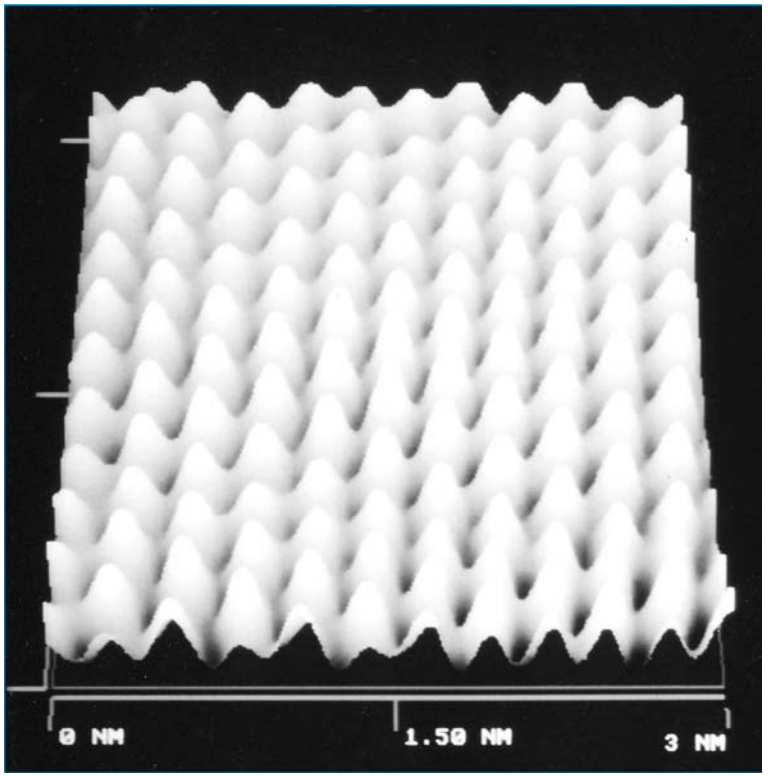




Crystal



$CaCu_3Ti_4O_{12}$
Transmission Electron microscope



Au, (111) surface
Atomic Force Microscope