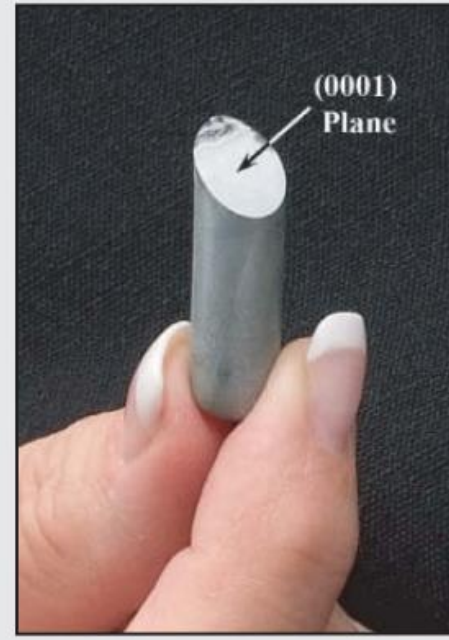
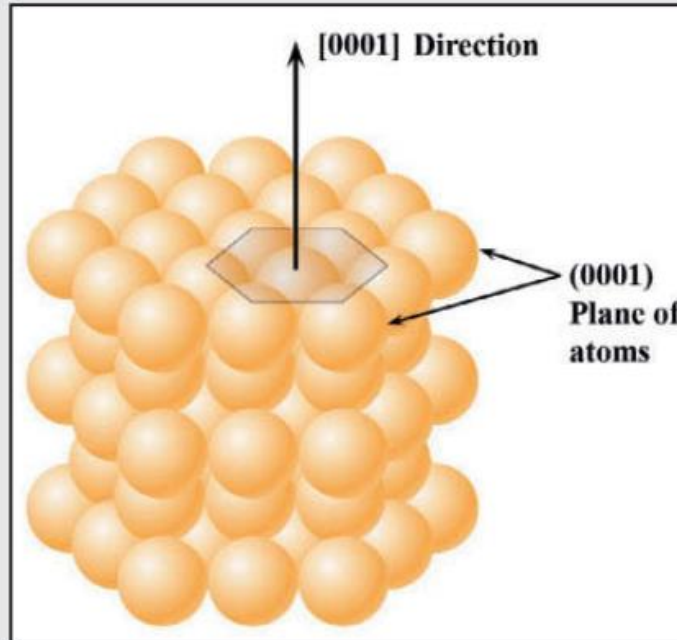
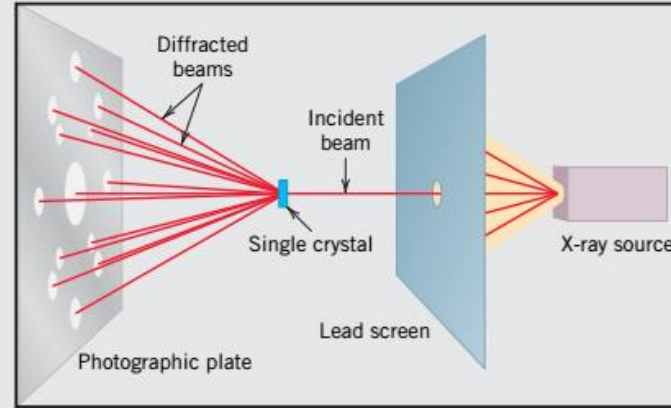
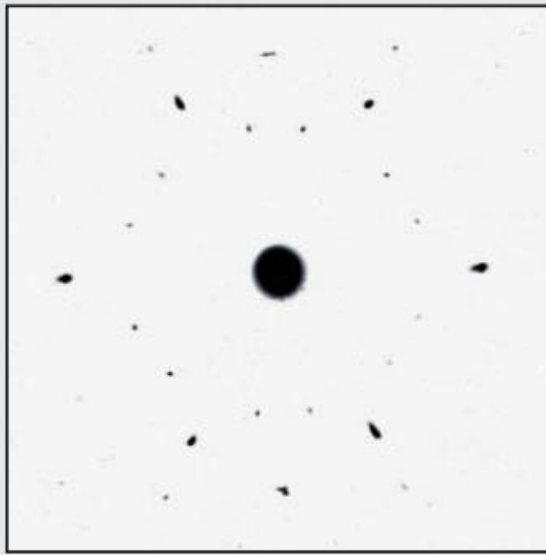




Malzeme I

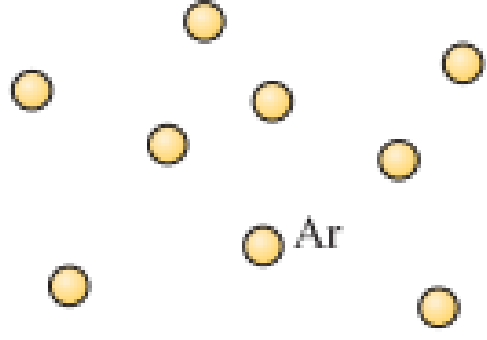
Katılarda Kristal Yapılar

Courtesy of J. G. Byrne

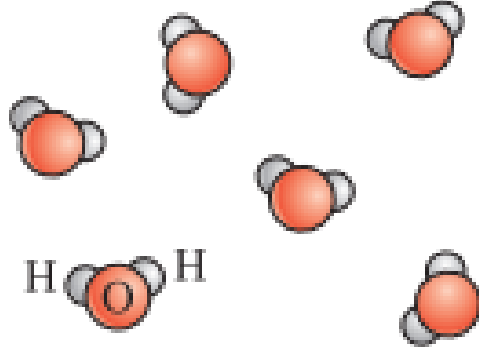


© William D. Callister, Jr.

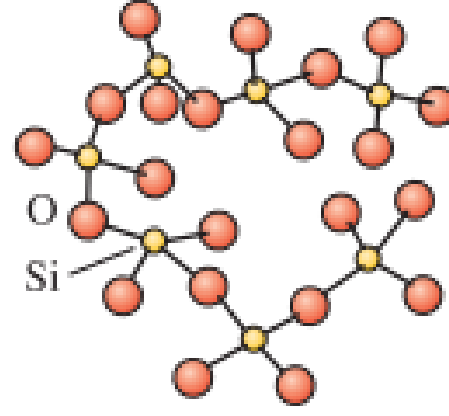
Atomik Yapılarda Düzen



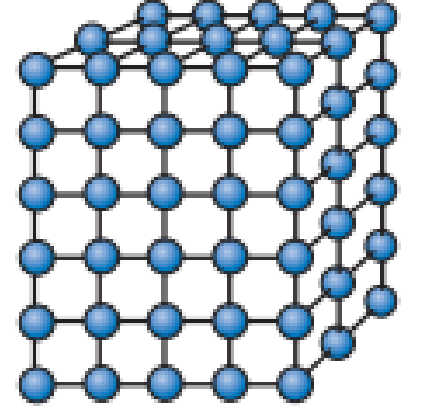
(a)



(b)



(c)



(d)

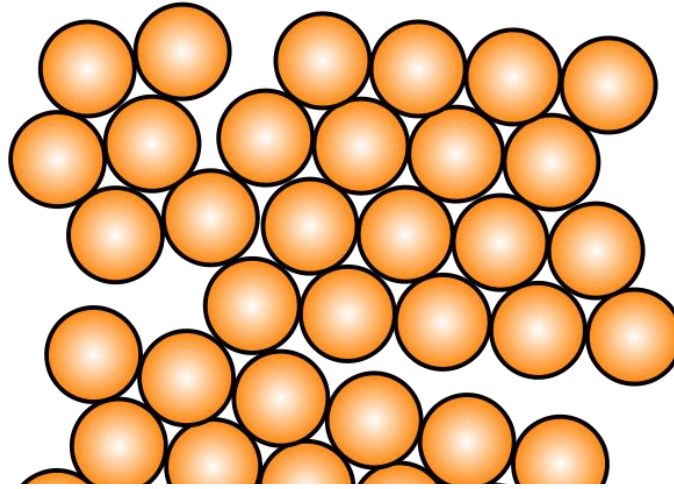
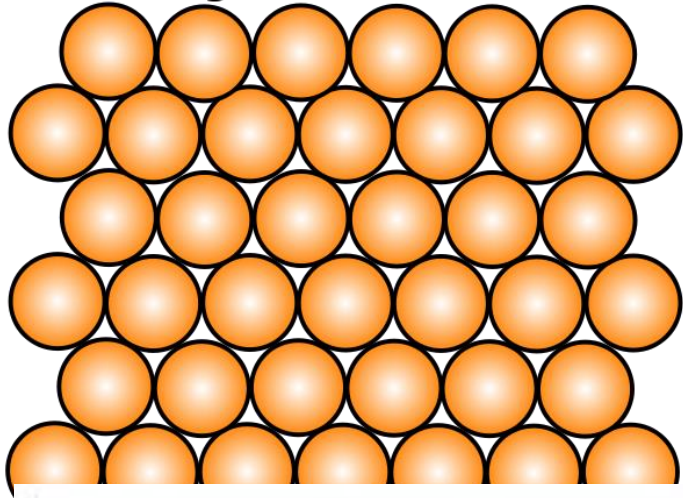
a) Düzensiz yapı: Atomların dağılımında herhangi bir düzen yoktur. Asal gazlarda görülür.

b-c) Kısa aralıklı düzen: Atomların dağılımında düzen yalnızca birbirlerine en yakın olan atomlar arasındadır. Su moleküllerinde, camlarda, polimerlerde görülür.

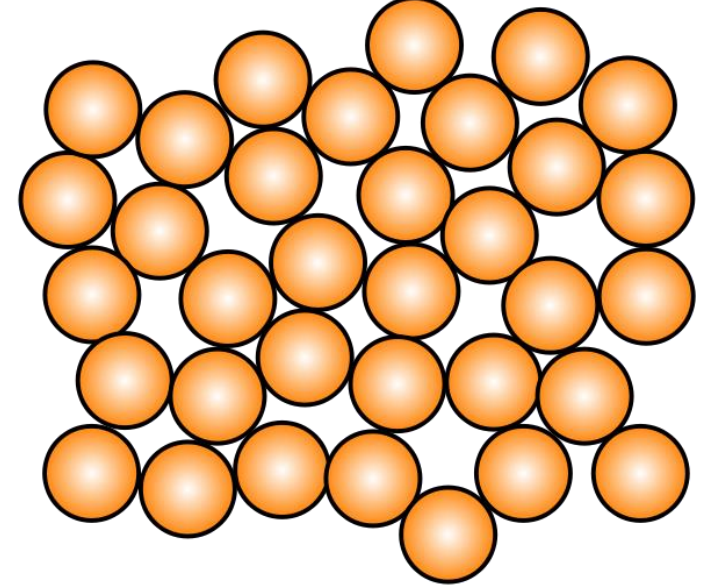
d) Uzun aralıklı düzen: Atomların dağılımında düzen 100 nm'den daha uzun ise bu atomik dizilime uzun aralıklı düzen ve bu tip yapılara kristal yapılar denir. Metal ve metal alaşımlarında, seramiklerde, yarıiletkenlerde ve bazı polimerlerde görülür.

Atomik Yapılarda Düzen

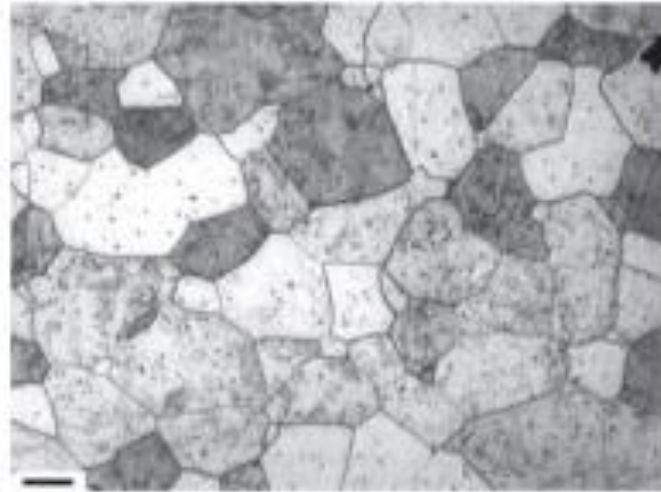
Kristalin?



Amorf?



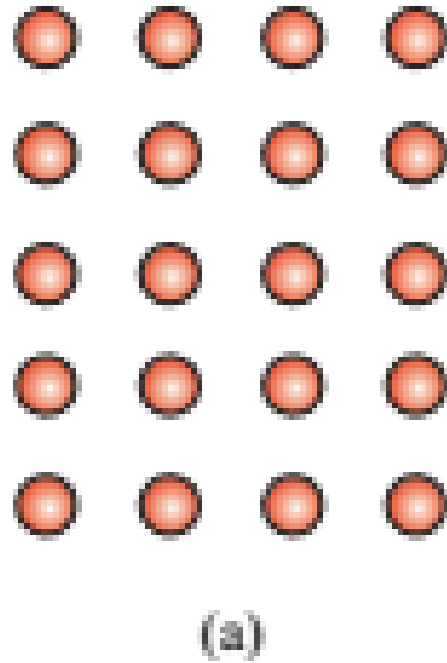
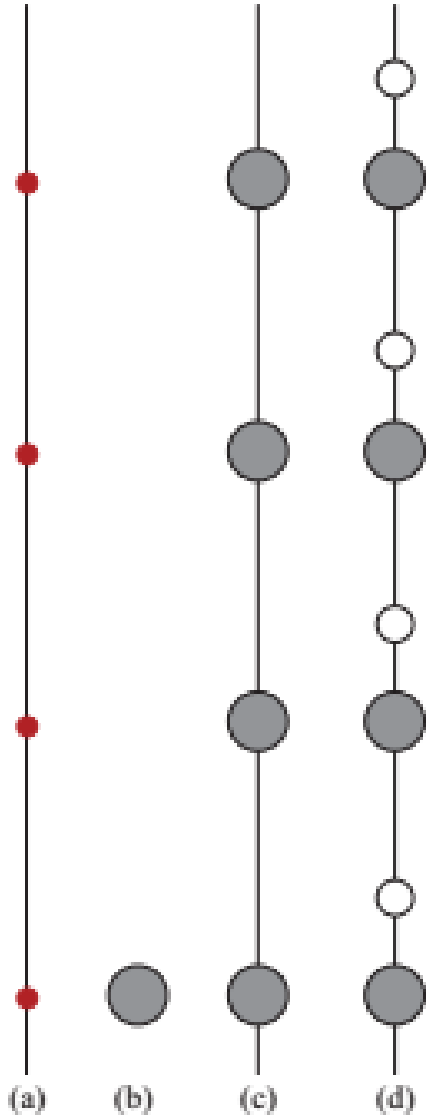
(a) Tek kristalli yapı



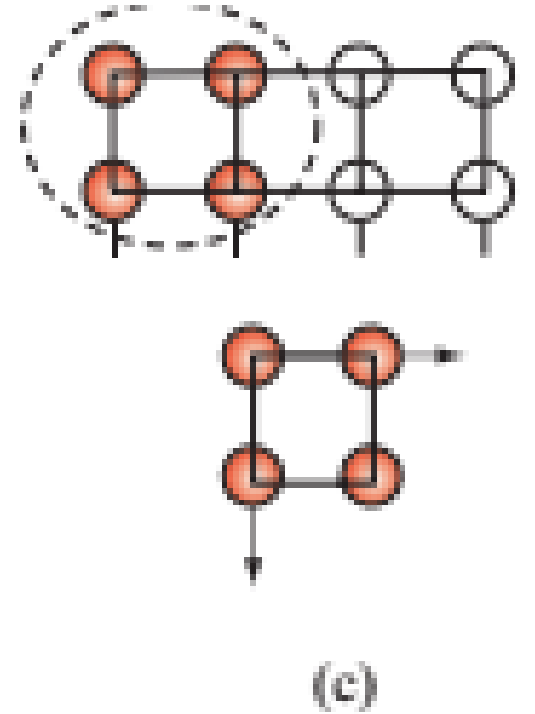
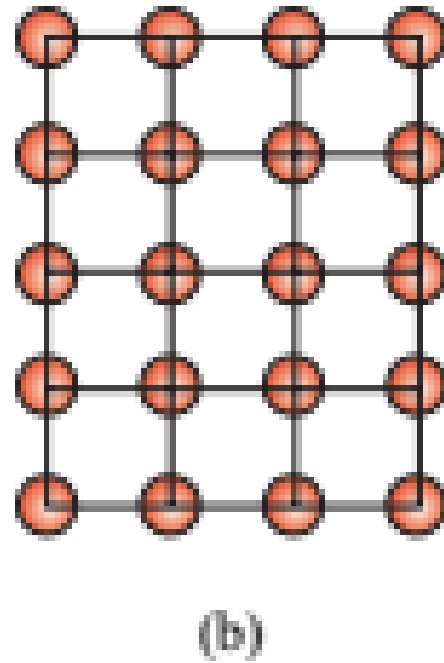
(b) Çok kristalli yapı (polikristalin)

Kristal Yapılar

Kristal: Latis + temel : 10^{23} atom/cm³



Birim hücre



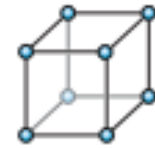
Kristal Yapılar

Bravais Latisleri

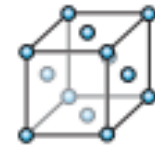


Auguste Bravais
(1811-1863)

Structure	Axes	Angles between Axes
Cubic	$a = b = c$	All angles equal 90° .
Tetragonal	$a = b \neq c$	All angles equal 90° .
Orthorhombic	$a \neq b \neq c$	All angles equal 90° .
Hexagonal	$a = b \neq c$	Two angles equal 90° . The angle between a and b equals 120° .
Rhombohedral or trigonal	$a = b = c$	All angles are equal and none equals 90° .
Monoclinic	$a \neq b \neq c$	Two angles equal 90° . One angle (β) is not equal to 90° .
Triclinic	$a \neq b \neq c$	All angles are different and none equals 90° .



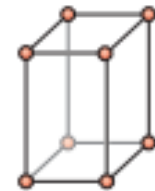
Simple cubic



Face-centered
cubic



Body-centered
cubic



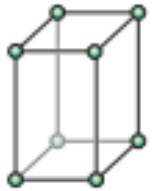
Simple
tetragonal



Body-centered
tetragonal



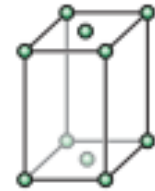
Hexagonal



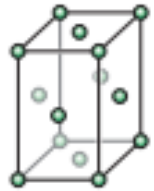
Simple
orthorhombic



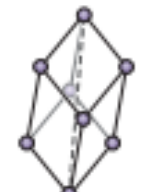
Body-centered
orthorhombic



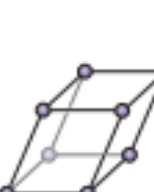
Base-centered
orthorhombic



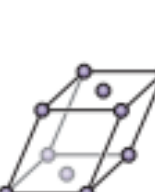
Face-centered
orthorhombic



Rhombohedral



Simple
monoclinic



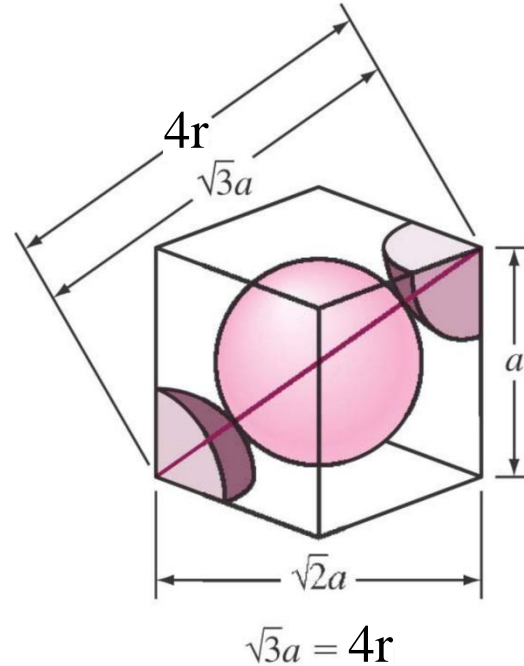
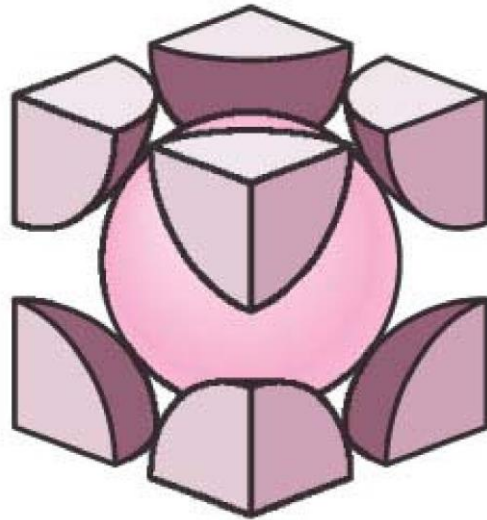
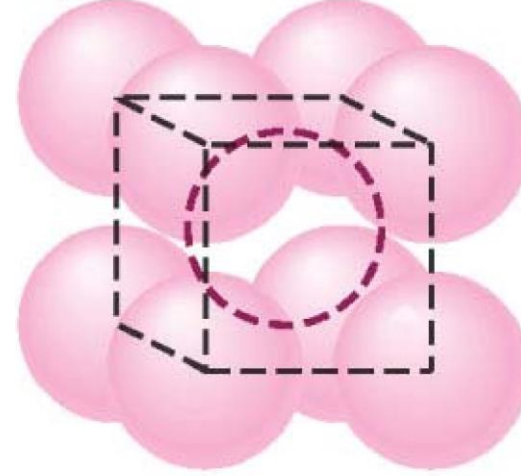
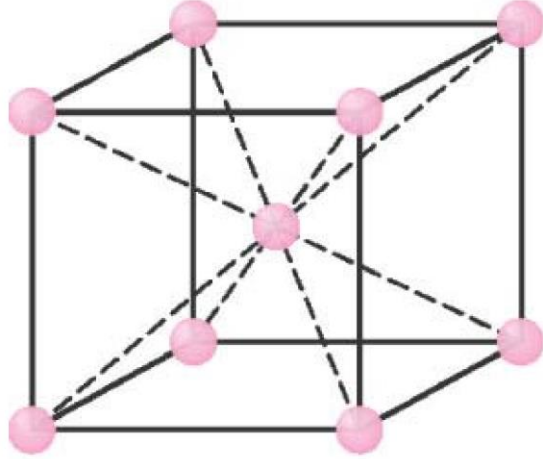
Base-centered
monoclinic



Triclinic

Figure 3-6 The fourteen types of Bravais lattices grouped in seven crystal systems. The actual unit cell for a hexagonal system is shown in Figures 3-8 and 3-13.

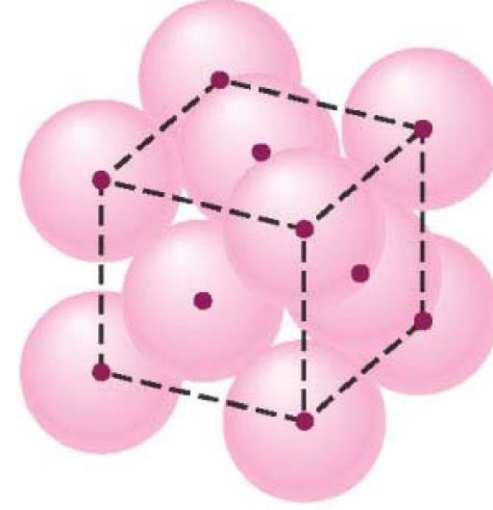
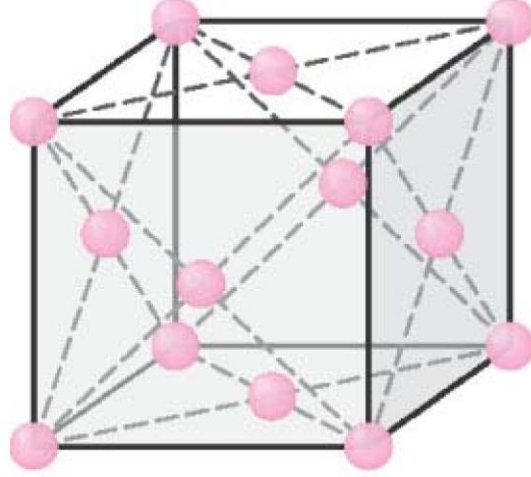
Hacim Merkezli Kübik



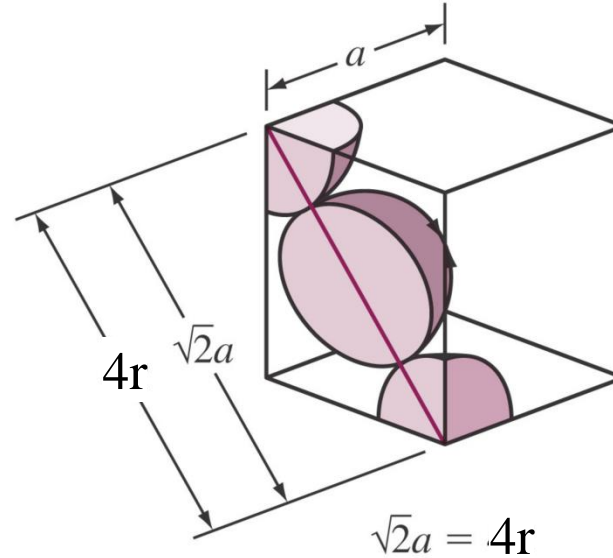
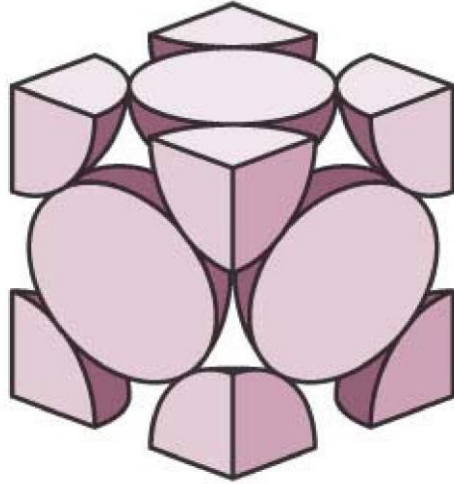
Örnekler:

Baryum (Ba),
Krom (Cr),
Sezyum (Cs),
 α -Demir (Fe),
Potasyum (K),
Lityum (Li),
Molibden (Mo),
Sodyum (Na),
Niyobyum (Nb),
Tantal (Ta),
Vanadyum (V),
Tungsten (W)...

Yüzey Merkezli Kübik

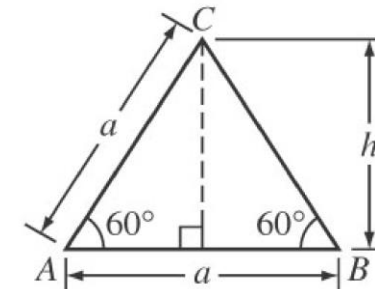
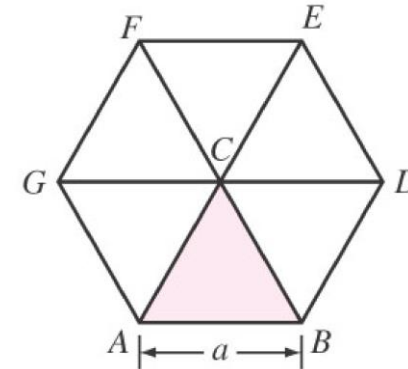
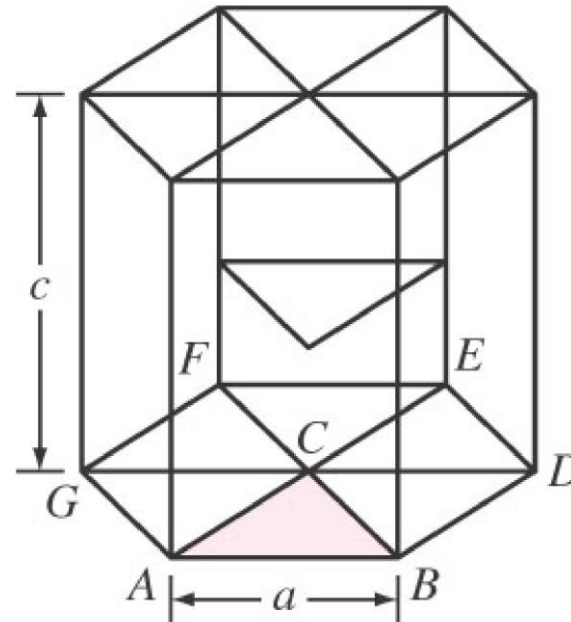
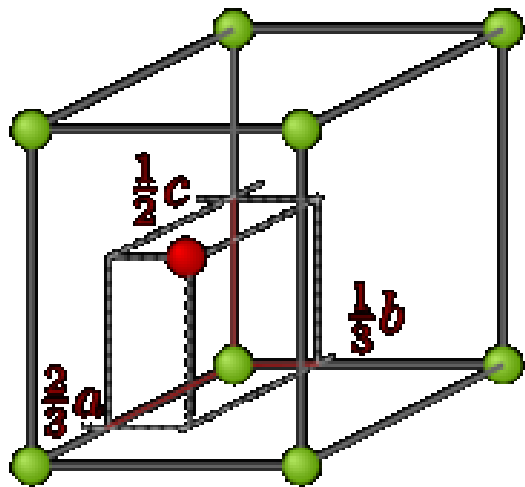
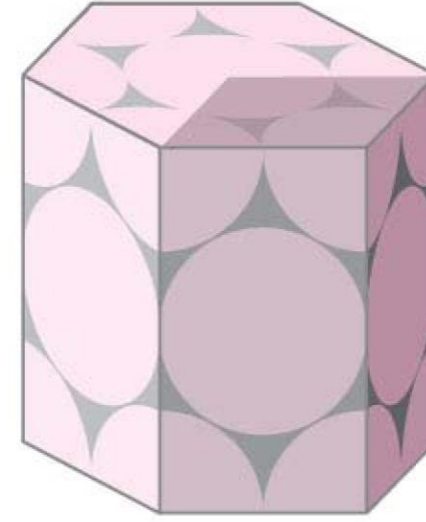
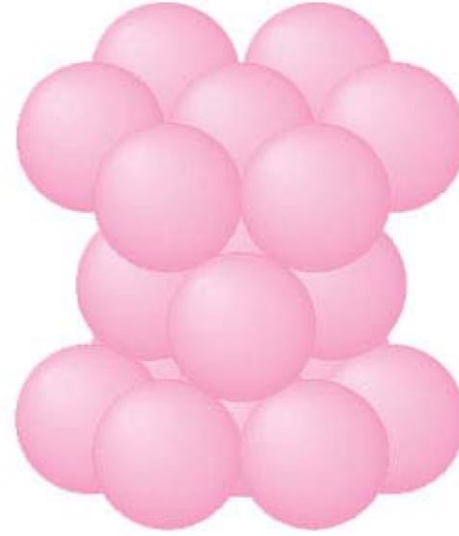
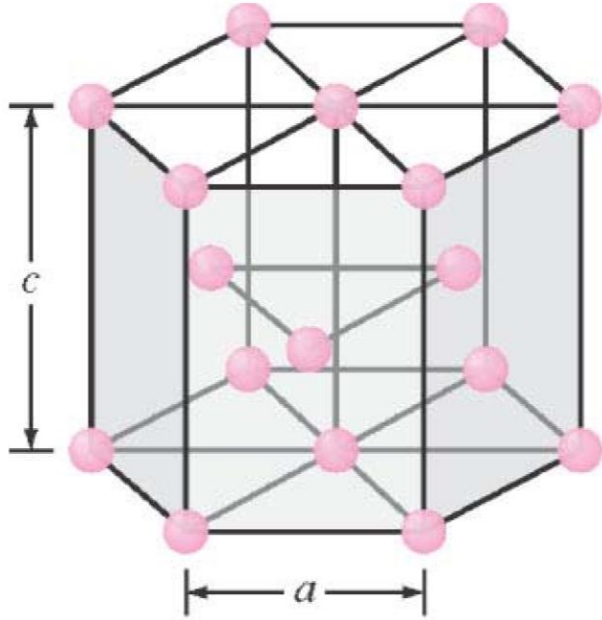


Örnekler:
Gümüş (Ag),
Alüminyum (Al),
Altın (Au),
Kalsiyum (Ca),
Bakır (Cu),
İridyum (Ir),
Nikel (Ni),
Kurşun (Pb),
Paladyum (Pd),
Platin (Pt),
Stronsiyum (Sr)...



Hekzagonal Sıkı Paket

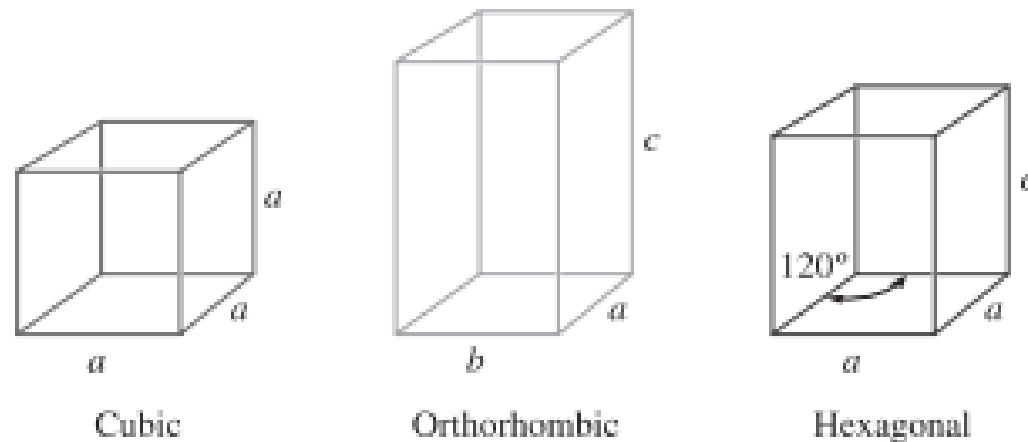
Örnekler:
Berilyum (Be),
Kadmiyum (Cd),
Kobalt (Co),
Hafniyum (Hf),
Magnezyum (Mg),
Osmiyum (Os),
Rodyum (Rh),
Titanyum (Ti),
Çinko (Zn),
Zirkonyum (Zr)...



Kristal Yapılar

<i>Metal</i>	<i>Crystal Structure^a</i>	<i>Atomic Radius^b</i> (nm)	<i>Metal</i>	<i>Crystal Structure</i>	<i>Atomic Radius (nm)</i>
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

^aFCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.



Kristal Yapılar

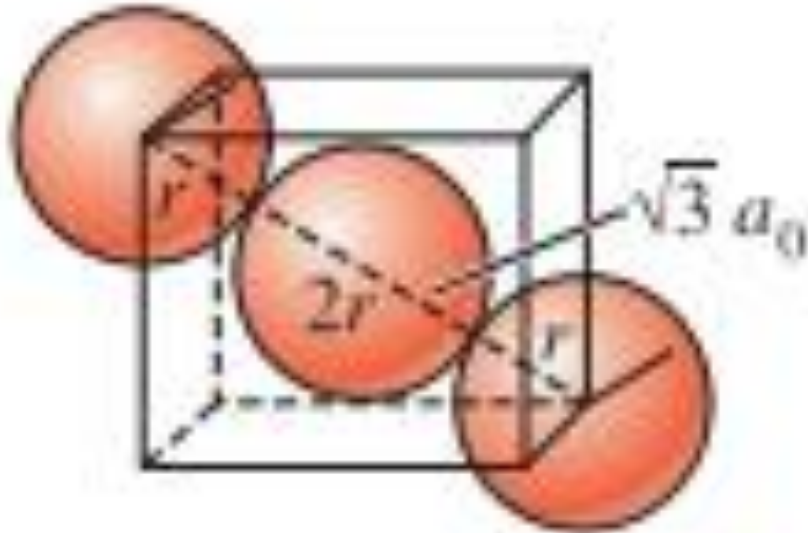
Basit kübik



$$a_0$$

$$a_0 = 2r$$

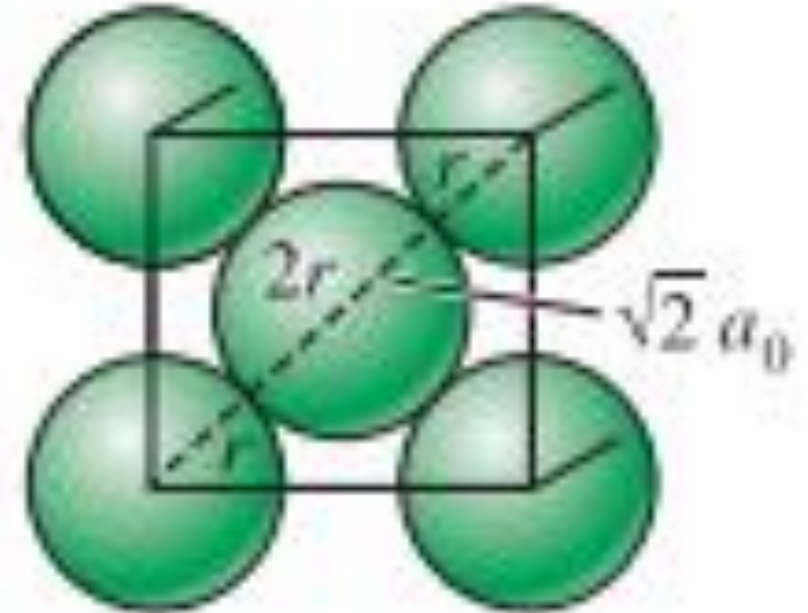
Hacim merkezli kübik



$$a_0$$

$$a_0 = \frac{4r}{\sqrt{3}}$$

Yüzey merkezli kübik



$$a_0$$

$$a_0 = \frac{4r}{\sqrt{2}}$$

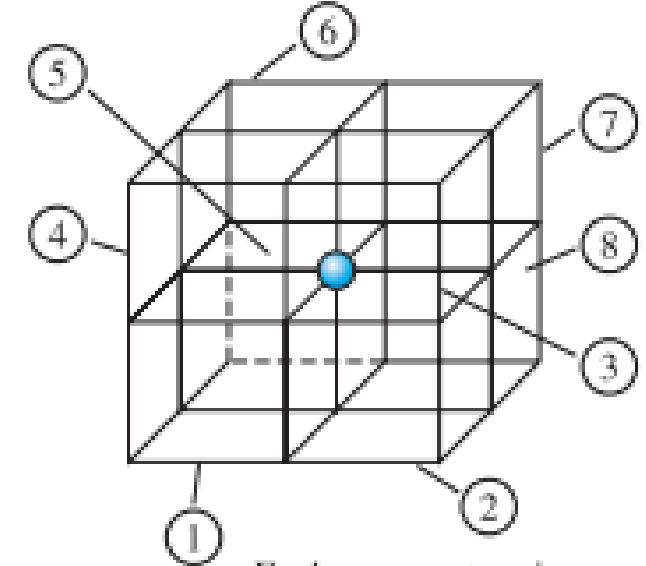
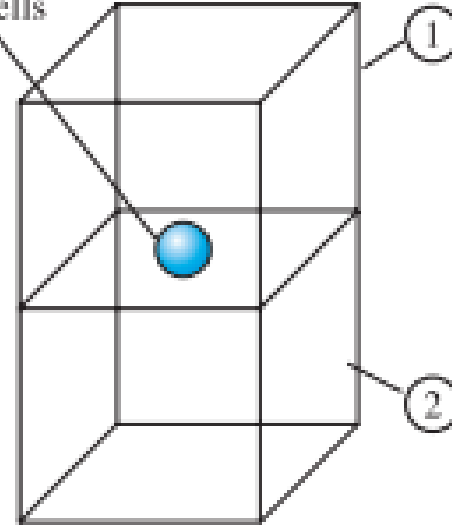
Kristal Yapılar

Birim hücre başına düşen atom sayısı

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

N_i : Kafes içi atomlarının sayısı
 N_f : Yüzey atomlarının sayısı
 N_c : Köşe atomlarının sayısı

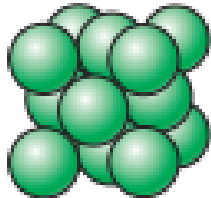
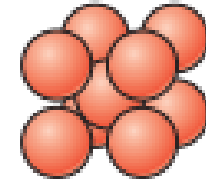
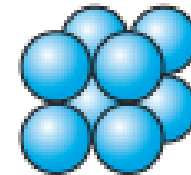
Face center atom
shared between
two unit cells



Each corner atom is
shared by 8 unit cells
(1-4 in front, 5-8 in back)

Basit kübik birim hücrede: $N = (8 \text{ köşe atomu})/8 = 1$

HMK birim hücrede: $N = 1 \text{ iç atom} + (8 \text{ köşe atomu})/8 = 2$



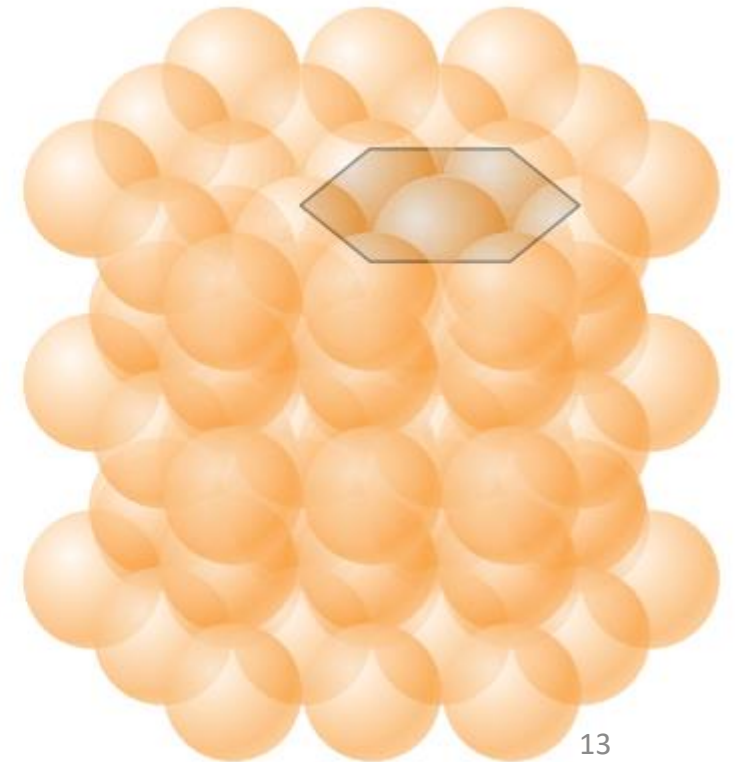
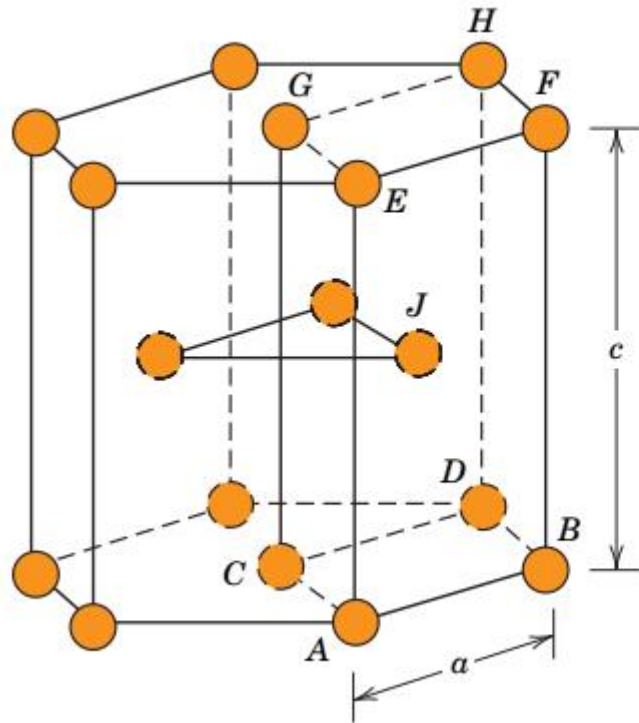
YMK birim hücrede: $N = (6 \text{ yüzey atomu})/2 + (8 \text{ köşe atomu})/8 = 4$

Kristal Yapılar

Birim hücre başına düşen atom sayısı

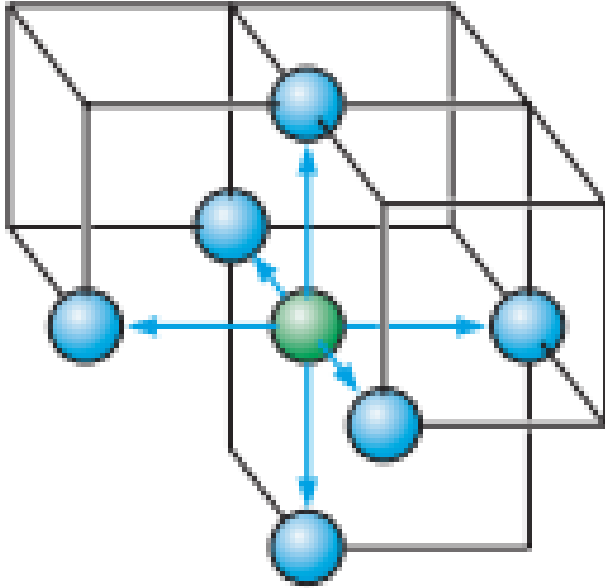
$$N = N_i + \frac{N_f}{2} + \frac{N_c}{6}$$

$$N = 3 + \frac{2}{2} + \frac{12}{6} = 6$$



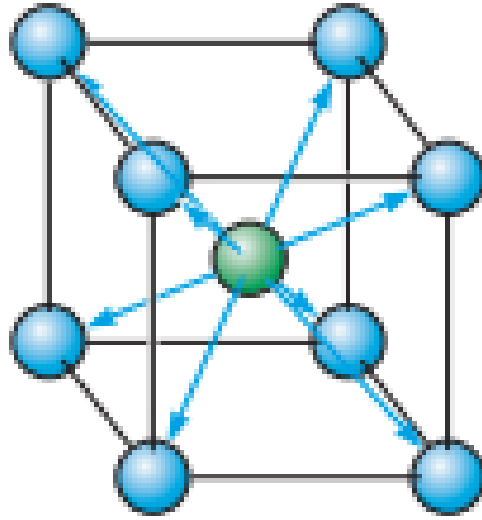
Kristal Yapılar

Koordinasyon sayısı: Herhangi bir atoma dokunan ya da en yakınında konumlanmış atomların sayısına koordinasyon sayısı denir. Kristal yapının ne kadar sıkı paketlenmiş olduğunun bir göstergesidir.



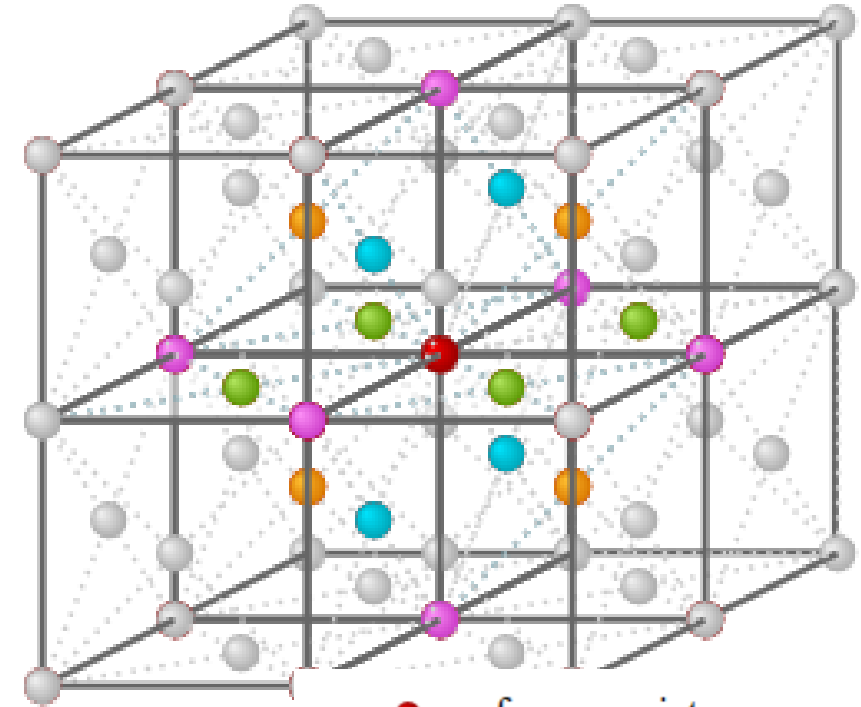
(a)

Basit kübik: 6



(b)

HMK: 8



● reference point

● ● ● 12 nearest neighbours

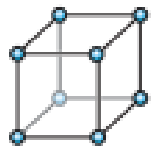
● 6 next-nearest neighbours

YMK: 12

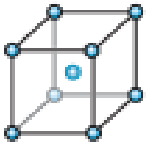
Kristal Yapılar

Atomik dolgu faktörü:

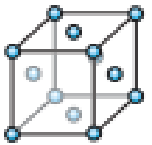
$$\text{ADF} = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom hacmi}}{\text{Birim hücrenin hacmi}} = \frac{\text{Birim hücredeki atomların toplam hacmi}}{\text{Birim hücrenin hacmi}}$$



$$\text{ADF} = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom hacmi}}{\text{Birim hücrenin hacmi}} = \frac{1 * \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\frac{4}{3}\pi}{8} = 0,52$$



$$\text{ADF} = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom hacmi}}{\text{Birim hücrenin hacmi}} = \frac{2 * \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{8}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{8\pi}{3} \cdot \frac{3\sqrt{3}}{64} = 0,68$$



$$\text{ADF} = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom hacmi}}{\text{Birim hücrenin hacmi}} = \frac{4 * \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{16}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{16\pi}{3} \cdot \frac{2\sqrt{2}}{64} = 0,74$$

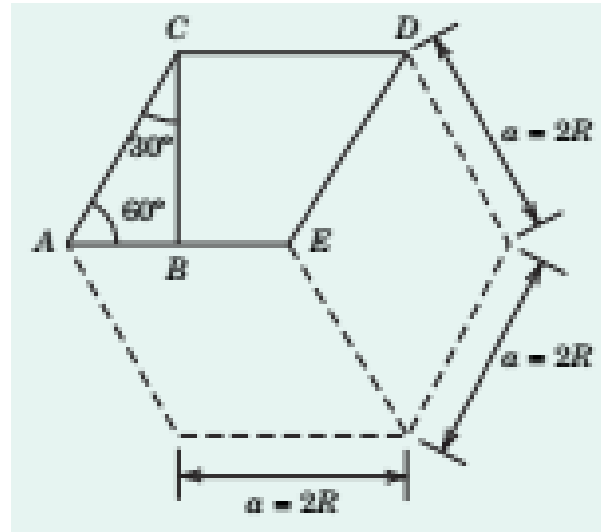
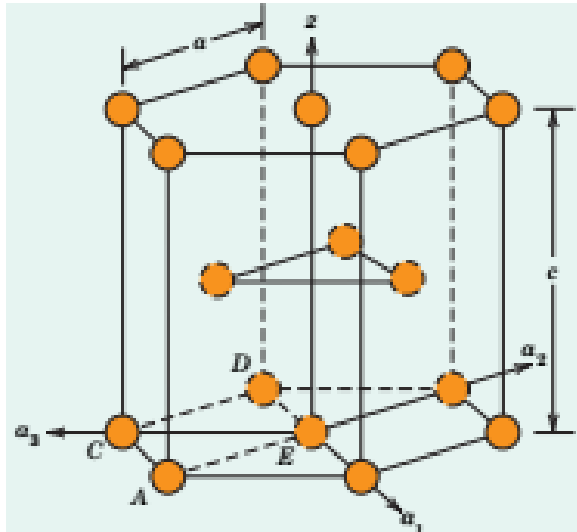
$$a_0 = 2r$$

$$a_0 = \frac{4r}{\sqrt{3}}$$

$$a_0 = \frac{4r}{\sqrt{2}}$$

Kristal Yapılar

Hekzagonal sıkı paket hücrenin hacmi:

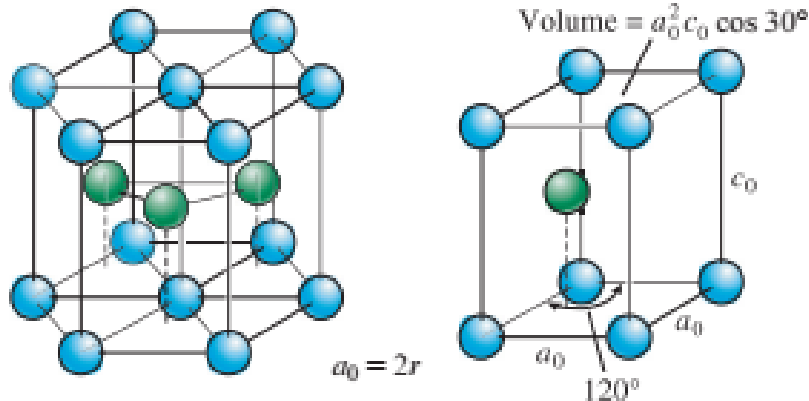


$$\overline{BC} = a \cos(30^\circ) = \frac{a\sqrt{3}}{2}$$

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(a)\left(\frac{a\sqrt{3}}{2}\right) = \frac{3a^2\sqrt{3}}{2}$$

$$\begin{aligned} V_c &= \text{AREA}(c) \\ &= \left(\frac{3a^2\sqrt{3}}{2}\right)(c) \\ &= \frac{3a^2c\sqrt{3}}{2} \end{aligned}$$

$\frac{c}{a} = 1,633$ ise *HSP' de ADF:*



$$\text{ADF} = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom hacmi}}{\text{Birim hücrenin hacmi}} = \frac{6 * \frac{4}{3}\pi r^3}{\frac{3a^2c\sqrt{3}}{2}}$$

$$\text{ADF} = \frac{6 * \frac{4}{3}\pi r^3}{\frac{3a^2c\sqrt{3}}{2}} = \frac{16\pi r^3}{3(2r)^2(1,633 * 2r)\sqrt{3}} = \frac{16\pi r^3}{3(2r)^2(1,633 * 2r)\sqrt{3}}$$

$$\text{ADF} = \frac{16\pi}{67,88} = 0,74$$

Kristal Yapılar

Teorik yoğunluk hesabı:

$$\text{Yoğunluk } (\rho) = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom ağırlığı}}{\text{Birim hücrenin hacmi} * \text{Avogadro sayısı}}$$

$$\rho = \frac{nA}{V_c N_A}$$

HMK Fe'nin yoğunluğu: $a = 0,2866 \text{ nm} = 2,866 \times 10^{-8} \text{ cm}$, Atom ağırlığı = 55,847 g/mol

$$\rho = \frac{(2)(55,847)}{(23,54 \times 10^{-24})(6,022 \times 10^{23})} = 7,879 \text{ g/cm}^3$$

Fe'in ölçülen yoğunluğu : 7,87 g/cm³

Kristal Yapılar

Teorik yoğunluk hesabı:

YMK yapıya sahip bakırın atomik yarıçapı 0,128 nm ve atom ağırlığı 63,5 g/mol'dür. Bakırın teorik yoğunluğunu hesaplayınız.

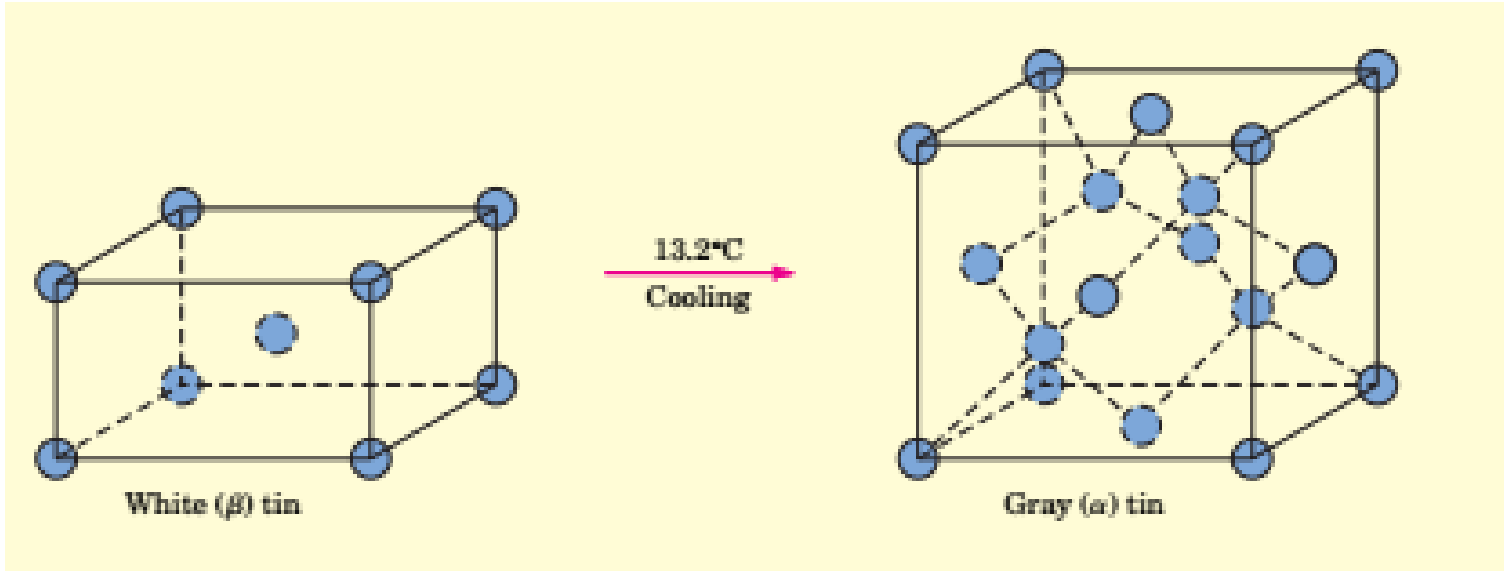
$$\text{Yoğunluk } (\rho) = \frac{\text{Birim hücredeki atom sayısı} * \text{Atom ağırlığı}}{\text{Birim hücrenin hacmi} * \text{Avogadro sayısı}}$$

$$\rho = \frac{(4)(63,5)}{(16\sqrt{2}(1,28 \times 10^{-8})^3)(6,022 \times 10^{23})} = 8,89 \text{ g/cm}^3$$

Cu için ölçülen yoğunluğu : 8,94 g/cm³

Kristal Yapılar

Polimorfizm / Allotropi: Malzemelerin birden fazla kristal formda bulunabilme haline allotropi denir.

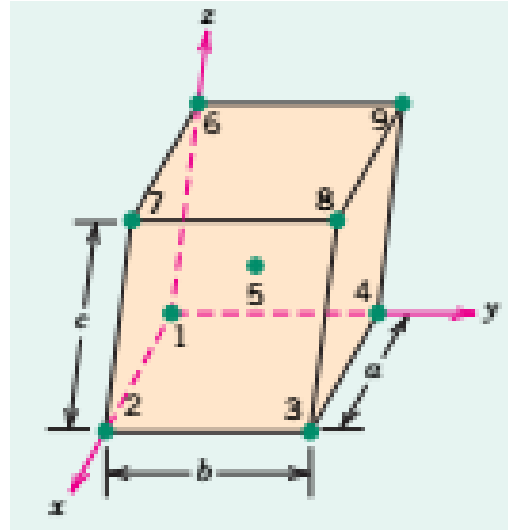
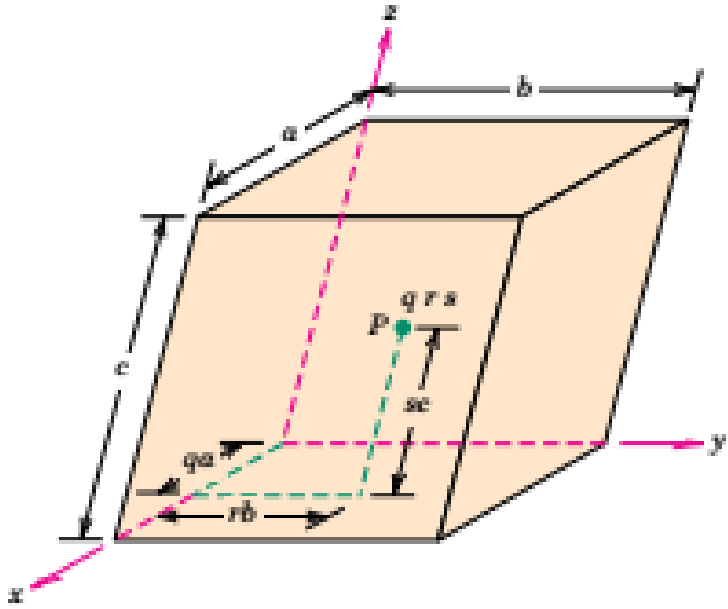


7,3 g/cm³ olan beyaz kalayın yoğunluğu 5,77 g/cm³' e düşer.

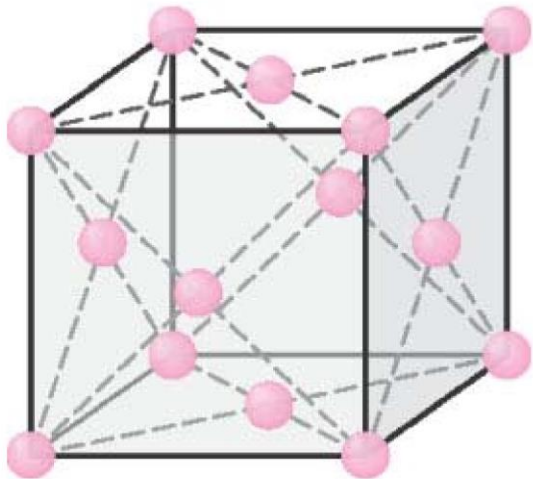
Kristal Yapılar

Örnek: 2 mm çapında ve 100 mm uzunluğunda bir Fe tel, oda sıcaklığından 950 °C'ye ısıtılıyor. 911 °C'de gerçekleşen hmk'dan ymk'ya dönüşüm sırasında telin çapının değişmediği varsayılırsa, son uzunluğu ne olur? (hmk demirin kafes parametresi $a = 0,2866$ nm)

Nokta Koordinatları

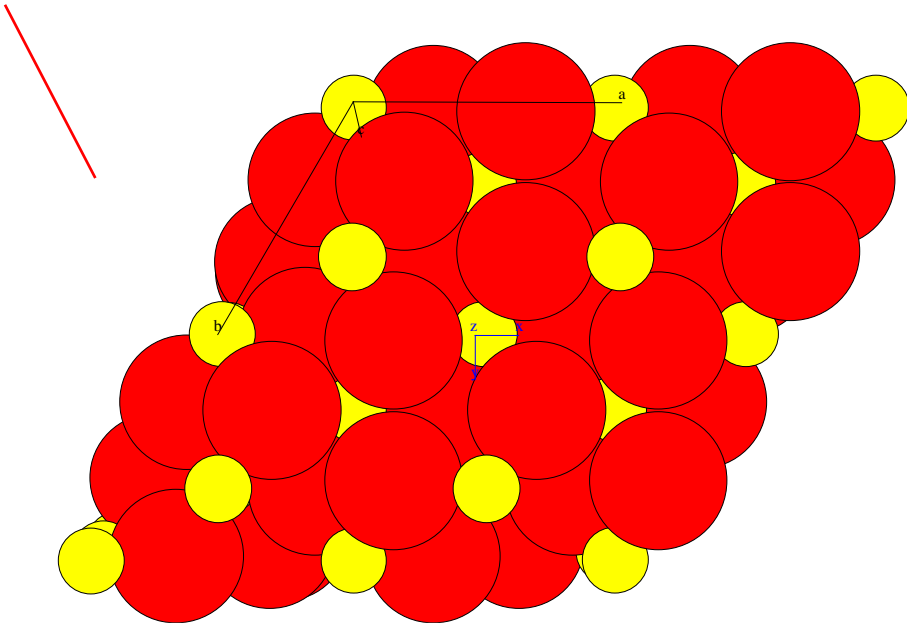


<i>Point Number</i>	<i>q</i>	<i>r</i>	<i>s</i>
1	0	0	0
2	1	0	0
3	1	1	0
4	0	1	0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
6	0	0	1
7	1	0	1
8	1	1	1
9	0	1	1



YMK için nokta koordinatları

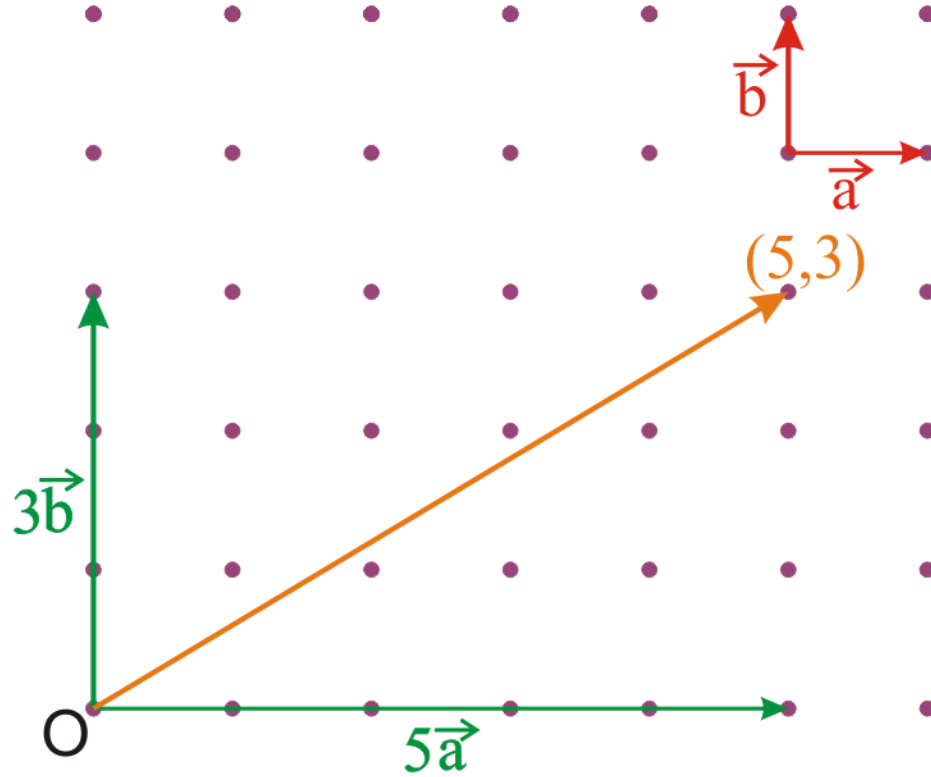
Nokta Koordinatları



Trigonal yapıya sahip Fe_2O_3

Atom	X	Y	Z	R	Occ
Fe 3+	0	0	0.35529	0.64	1.00
O 2-	0.30609	0	1/4	1.32	1.00
Fe 3+	0	0	0.64471	0.64	1.00
O 2-	0.69391	0	3/4	1.32	1.00
Fe 3+	0	0	0.85529	0.64	1.00
O 2-	0	0.30609	1/4	1.32	1.00
O 2-	0.69391	0.69391	1/4	1.32	1.00
O 2-	0	0.69391	3/4	1.32	1.00
O 2-	0.30609	0.30609	3/4	1.32	1.00
Fe 3+	0	0	0.14471	0.64	1.00
Fe 3+	1/3	2/3	0.02196	0.64	1.00
Fe 3+	1/3	2/3	0.52196	0.64	1.00
O 2-	0.63942	2/3	11/12	1.32	1.00
O 2-	1/3	0.97276	11/12	1.32	1.00
O 2-	0.02724	0.36058	11/12	1.32	1.00
O 2-	1/3	0.36058	5/12	1.32	1.00
O 2-	0.02724	2/3	5/12	1.32	1.00
O 2-	0.63942	0.97276	5/12	1.32	1.00
Fe 3+	1/3	2/3	0.31138	0.64	1.00
Fe 3+	1/3	2/3	0.81138	0.64	1.00
Fe 3+	2/3	1/3	0.68862	0.64	1.00
Fe 3+	2/3	1/3	0.18862	0.64	1.00
O 2-	0.97276	1/3	7/12	1.32	1.00
O 2-	2/3	0.63942	7/12	1.32	1.00
O 2-	0.36058	0.02724	7/12	1.32	1.00
O 2-	2/3	0.02724	1/12	1.32	1.00
O 2-	0.36058	1/3	1/12	1.32	1.00
O 2-	0.97276	0.63942	1/12	1.32	1.00
Fe 3+	2/3	1/3	0.97804	0.64	1.00
Fe 3+	2/3	1/3	0.47804	0.64	1.00

Miller İndisleri – Yönler



1- Bitiş ve başlangıç noktasının koordinatlarını belirle.

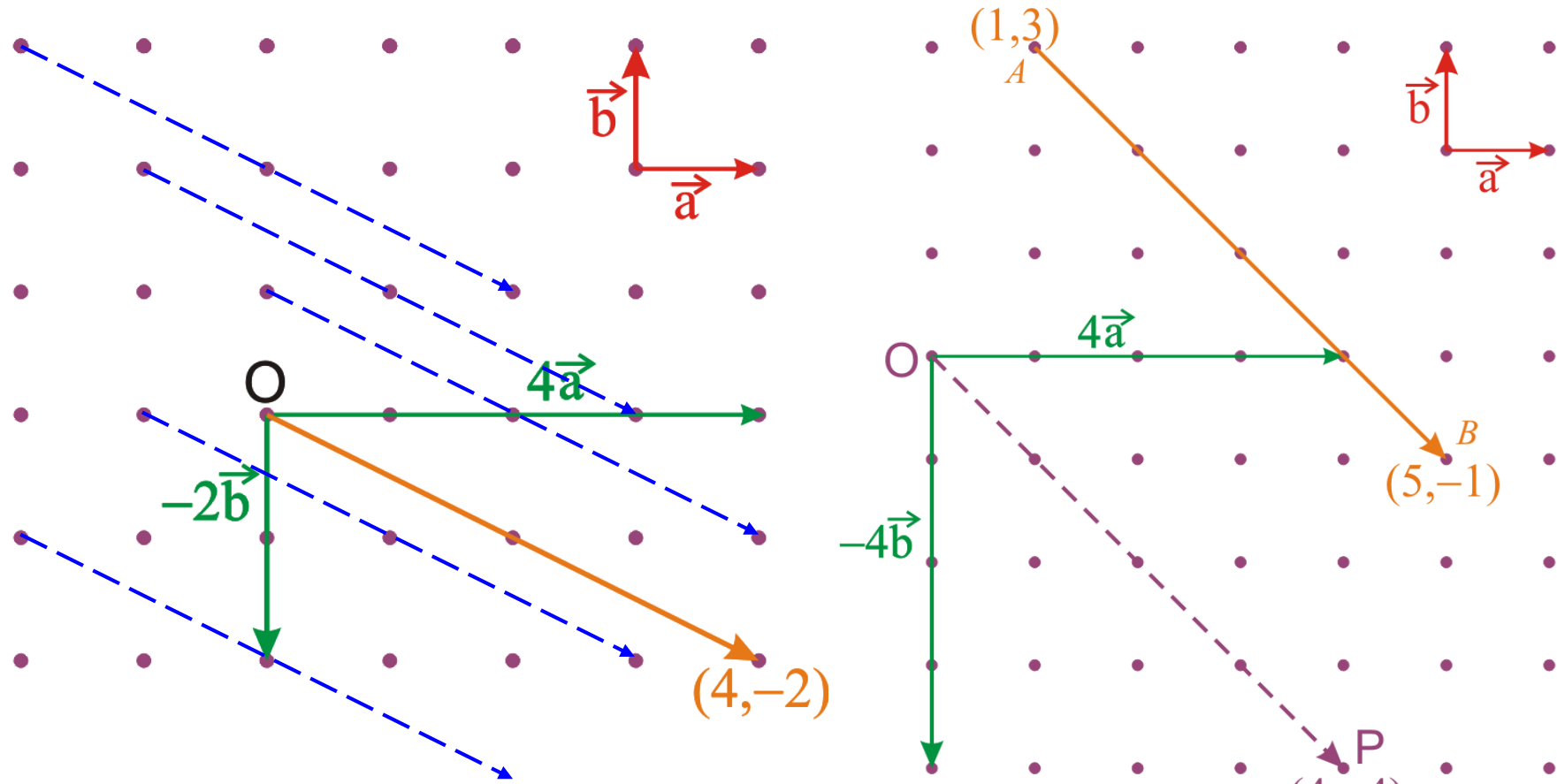
2- Bitiş noktasından başlangıç noktasını çıkar.

3- Paydalardan kurtul ya da sadeleştir.

4- Köşeli parantez içinde göster.

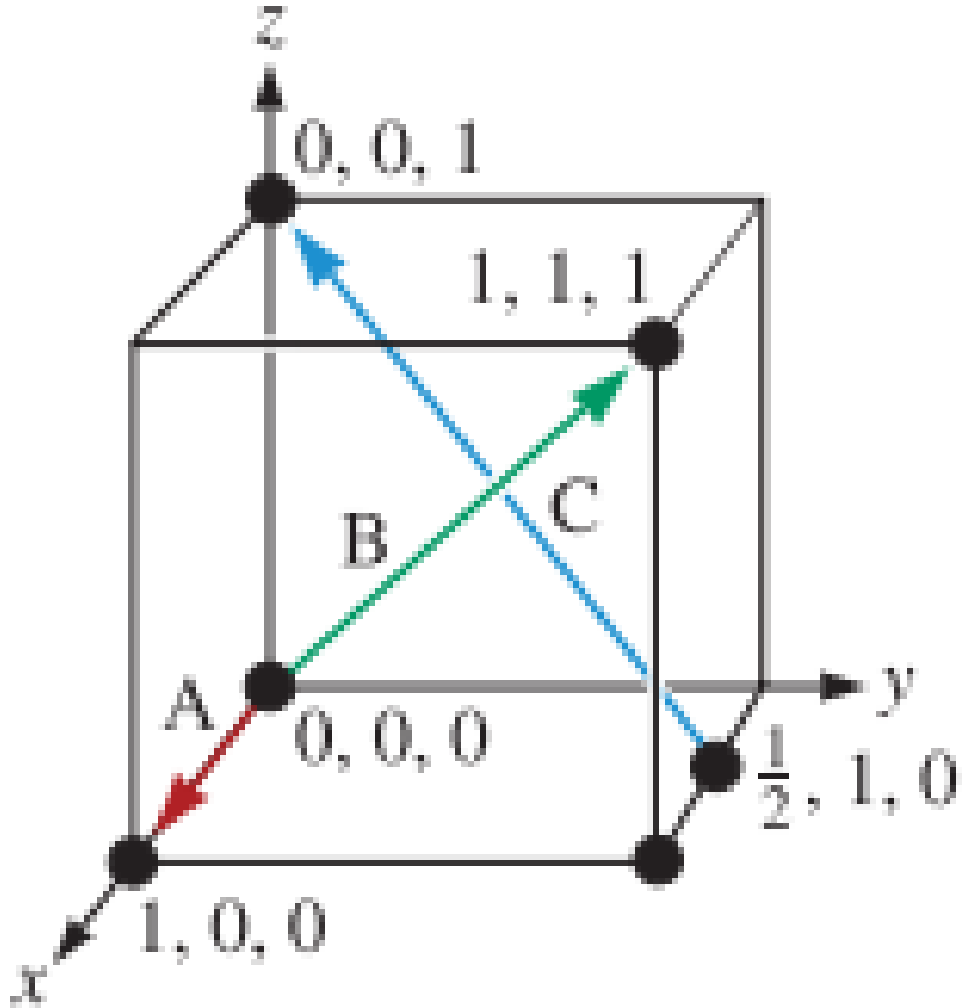
Miller indisi $\rightarrow [53]$

Miller İndisleri – Yönler



Miller indisi $\rightarrow [4\bar{2}]$
 $\rightarrow 2[2\bar{1}]$
 $\rightarrow [2\bar{1}]$

Miller İndisleri – Yönler



A yönü:

- 1- Nokta koordinatları: 1,0,0 ve 0,0,0.
- 2- $1,0,0 - 0,0,0 = 1,0,0$.
- 3- Payda eşitlemeye gerek yok.
- 4- **[100]**

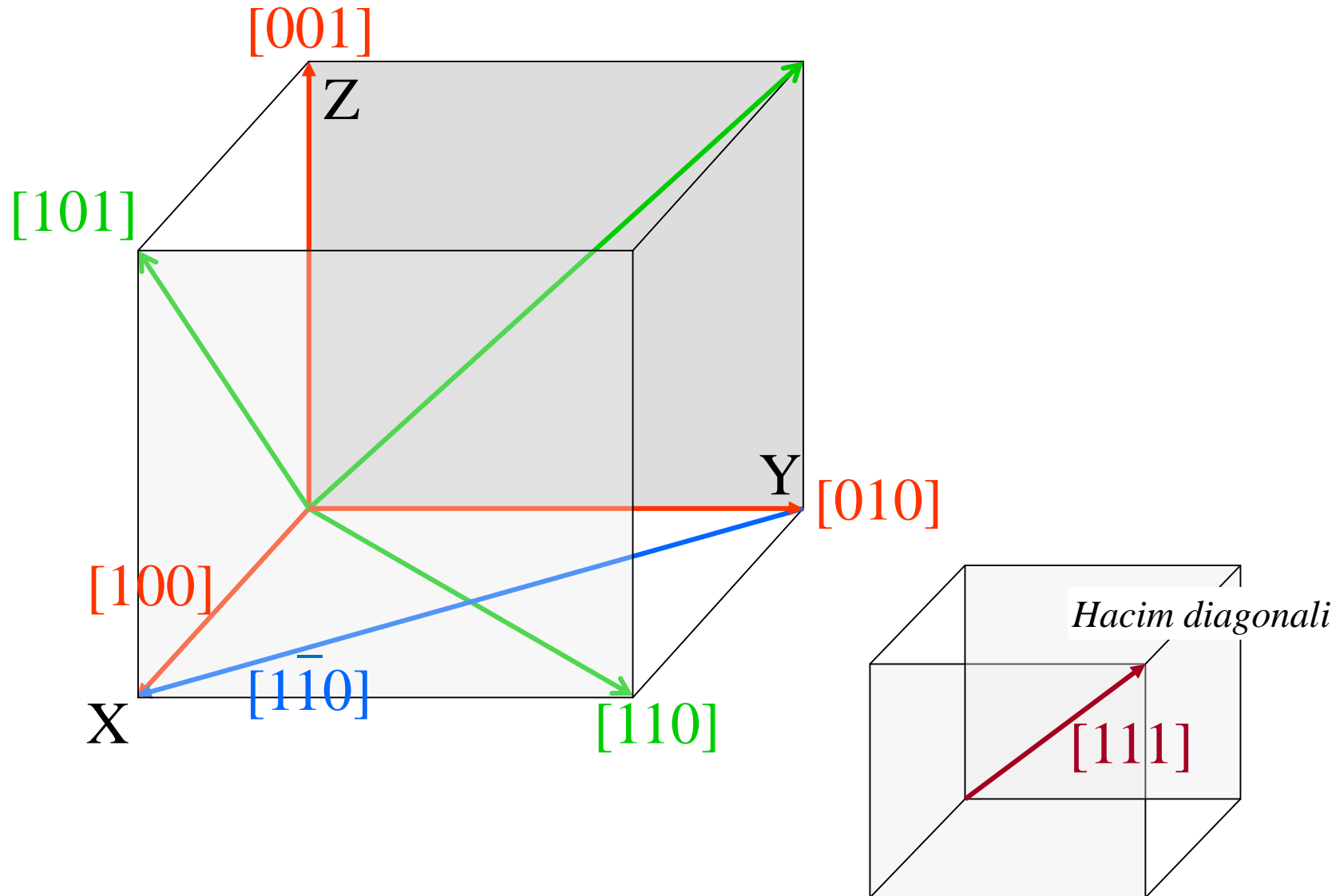
B yönü:

- 1- Nokta koordinatları: 1,1,1 ve 0,0,0.
- 2- $1,1,1 - 0,0,0 = 1,1,1$.
- 3- Payda eşitlemeye gerek yok.
- 4- **[111]**

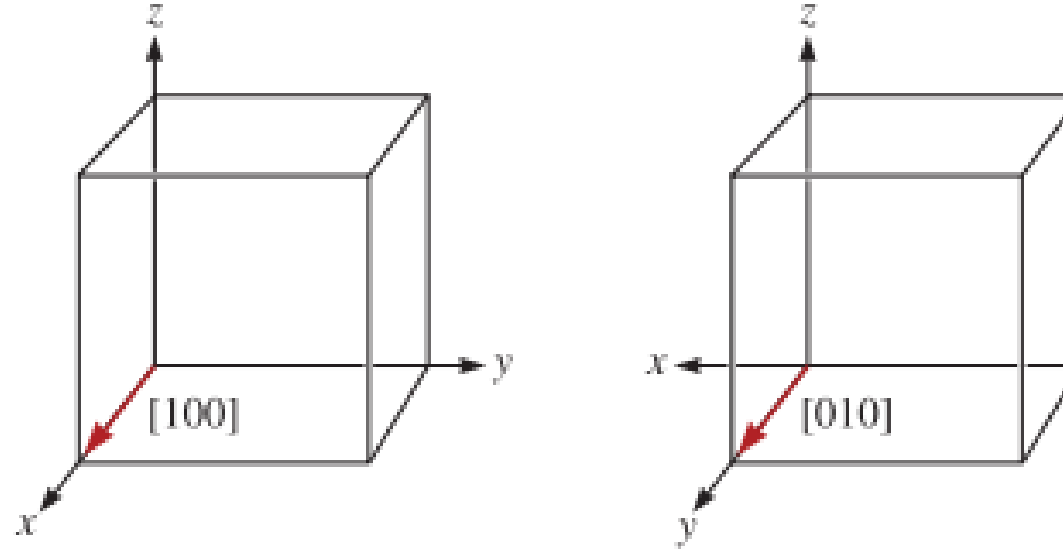
C yönü:

- 1- Nokta koordinatları: 0,0,1 ve $1/2, 1, 0$.
- 2- $0,0,1 - 1/2, 1, 0 = -1/2, -1, 1$.
- 3- $2(-1/2, -1, 1) = -1, -2, 2$.
- 4- **[-1-22]**

Miller İndisleri – Yönler



Miller İndisleri – Yönler



İndeks	Kübik Latis İçin Yön Ailesi Üyeleri	Sayı
$\langle 100 \rangle$	$[100], [\bar{1}00], [010], [0\bar{1}0], [001], [00\bar{1}]$	$3 \times 2 = 6$
$\langle 110 \rangle$	$[110], [\bar{1}10], [1\bar{1}0], [\bar{1}\bar{1}0], [101], [\bar{1}01], [10\bar{1}], [\bar{1}0\bar{1}], [011], [0\bar{1}1], [01\bar{1}], [0\bar{1}\bar{1}]$	$6 \times 2 = 12$
$\langle 111 \rangle$	$[111], [\bar{1}11], [1\bar{1}1], [11\bar{1}], [\bar{1}\bar{1}1], [\bar{1}1\bar{1}], [1\bar{1}\bar{1}], [\bar{1}\bar{1}\bar{1}]$	$4 \times 2 = 8$

Miller İndisleri – Yönler

Table 3.4

**Modulus of Elasticity
Values for Several
Metals at Various
Crystallographic
Orientations**

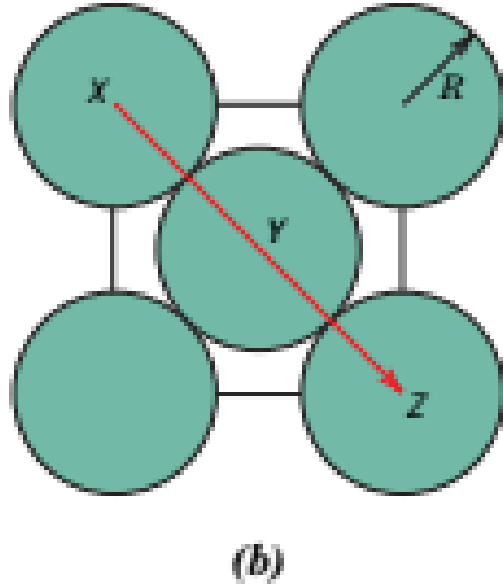
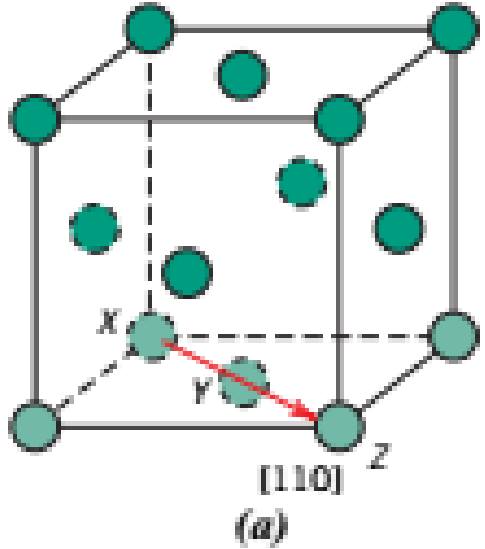
<i>Metal</i>	<i>Modulus of Elasticity (GPa)</i>		
	<i>[100]</i>	<i>[110]</i>	<i>[111]</i>
Aluminum	63.7	72.6	76.1
Copper	66.7	130.3	191.1
Iron	125.0	210.5	272.7
Tungsten	384.6	384.6	384.6

Source: R. W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd edition. Copyright © 1989 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.

Miller İndisleri – Yönler

Lineer (doğrusal) yoğunluk:

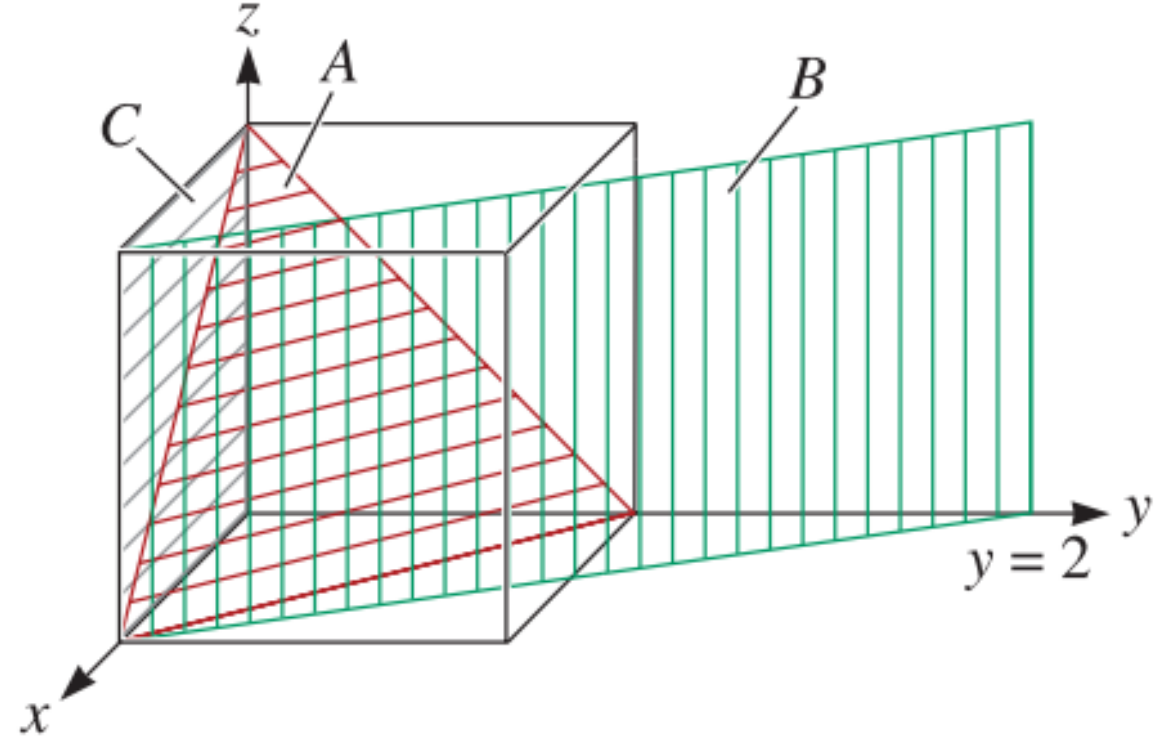
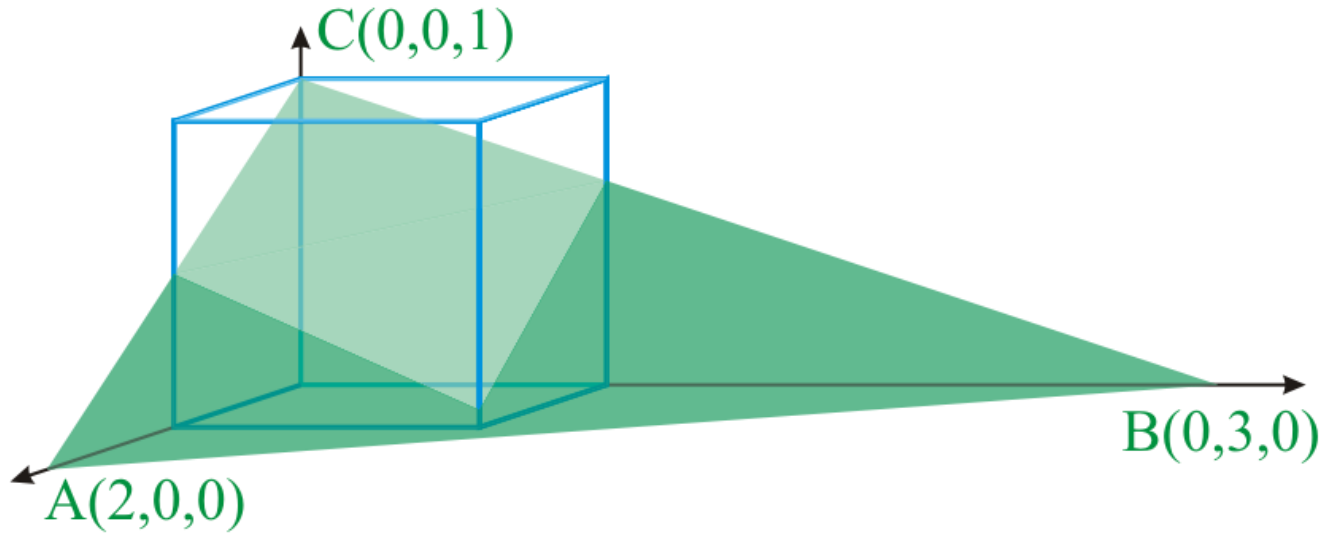
$$\text{Lineer Yoğunluk (LY)} = \frac{\text{Doğrultu vektörü boyunca atom sayısı}}{\text{Doğrultu vektörünün uzunluğu}}$$



$$LY_{110} = \frac{2 \text{ atom}}{4r} = \frac{1}{2r} (\text{atom. nm}^{-1})$$

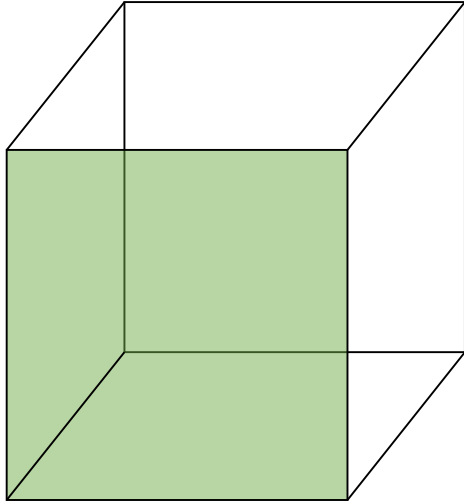
Atomik yarıçapı $r = 0,143$ nm olan ymk alüminyum için $[110]$ doğrultusunda lineer yoğunluğu atom/cm olarak hesaplayınız.

Miller İndisleri – Düzlemler

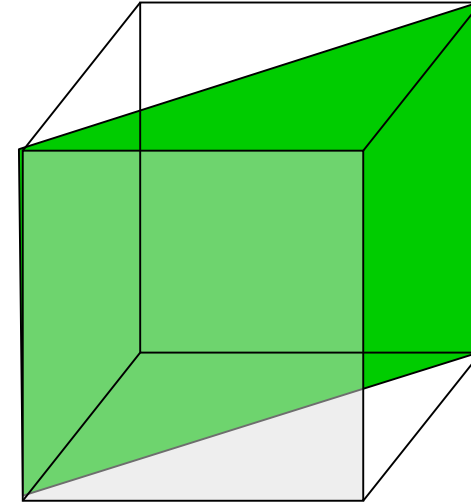
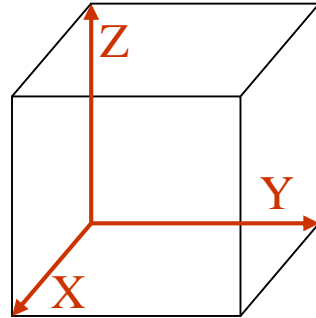


- 1- Eksenler boyunca kestiği noktaları bul $\rightarrow 2 \ 3 \ 1$
- 2- Tersini al $\rightarrow 1/2 \ 1/3 \ 1$
- 3- En küçük tamsayıya göre çarp (Payda eşitle) $\rightarrow 3 \ 2 \ 6$
- 4- Paranteze al $\rightarrow (326)$

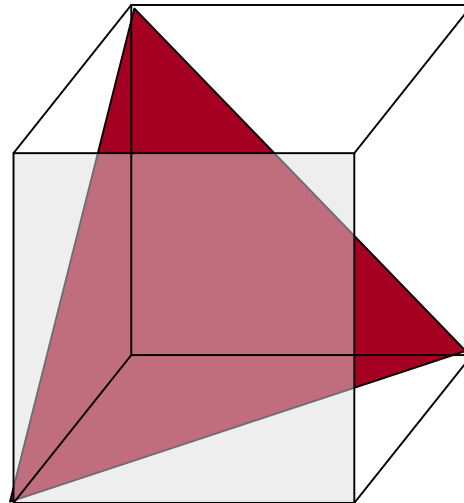
Miller İndisleri – Düzlemler



Kesişim $\rightarrow 1 \infty \infty$
Düzlem $\rightarrow (100)$

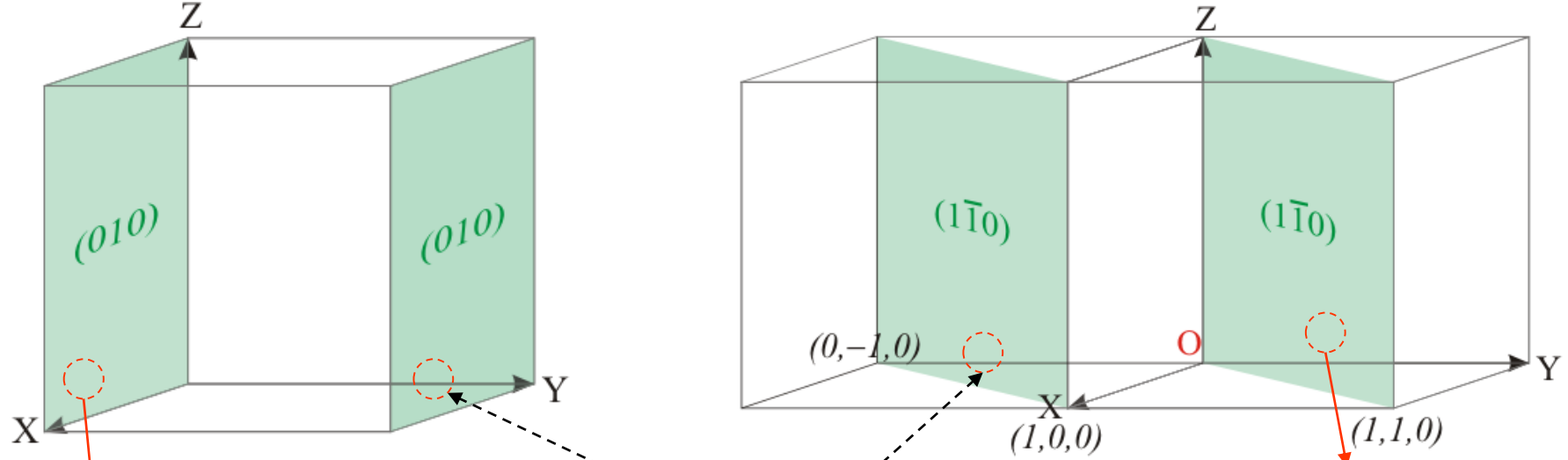


Kesişim $\rightarrow 1 1 \infty$
Düzlem $\rightarrow (110)$



Kesişim $\rightarrow 1 1 1$
Düzlem $\rightarrow (111)$

Miller İndisleri – Düzlemler



X düzlemi orijin noktasından geçiyor!

Orijin noktasından geçen düzlem

Kesişim $\rightarrow \infty 0 \infty$
Düzlem $\rightarrow (0 \infty 0)$

Bu düzlemleri kullan!

Kesişim $\rightarrow 0 0 \infty$
Düzlem $\rightarrow (\infty \infty 0)$

**Miller indislerinde sonsuz ifadelerinden kaçınıyoruz!
Bu gibi durumlarda, ilgili düzlemi 0 olmayan eksenleri boyunca bir
birim uzaklığa taşıyoruz ve Miller indisini hesaplıyoruz.**

Miller İndisleri – Düzlemler

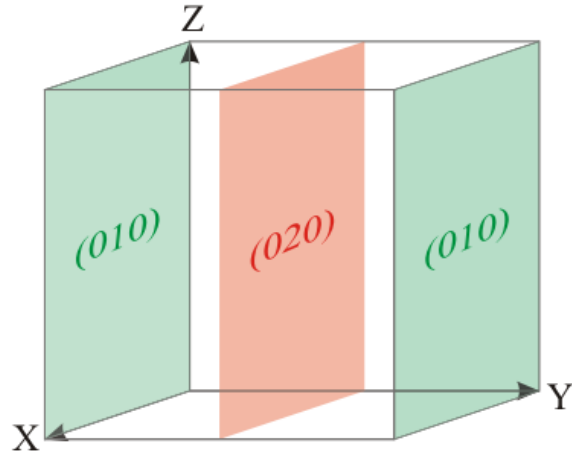
Düzlem ve yönler ile ilgili bazı önemli noktalar:

- ❑ Bilinmeyen yön $\rightarrow [uvw]$
- ❑ Bilinmeyen düzlem $\rightarrow (hkl)$
- ❑ 2 basamaklı indisler virgül ile ayrılabilir $\rightarrow (12,22,3)$
ya da $(12\ 22\ 3)$
- ❑ Kübik latis/kristallerde $[hkl] \perp (hkl)$

$$d_{hkl}^{cubic\ lattice} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

h, k, l, arttıkça d azalır.

Miller İndisleri – Düzlemler



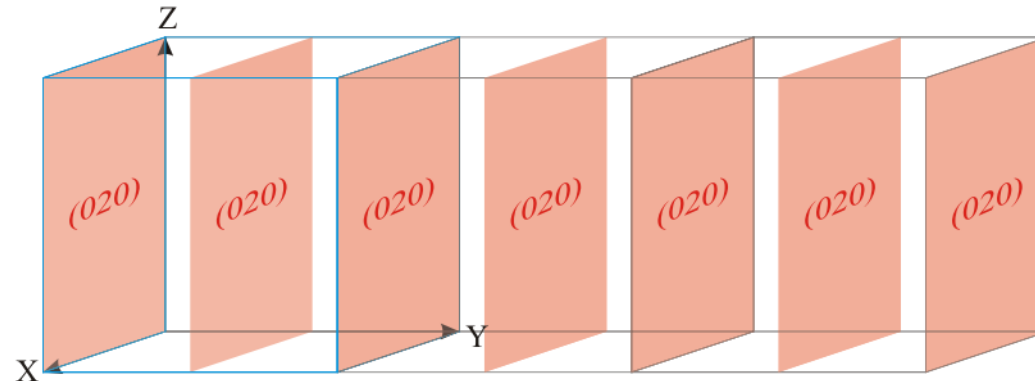
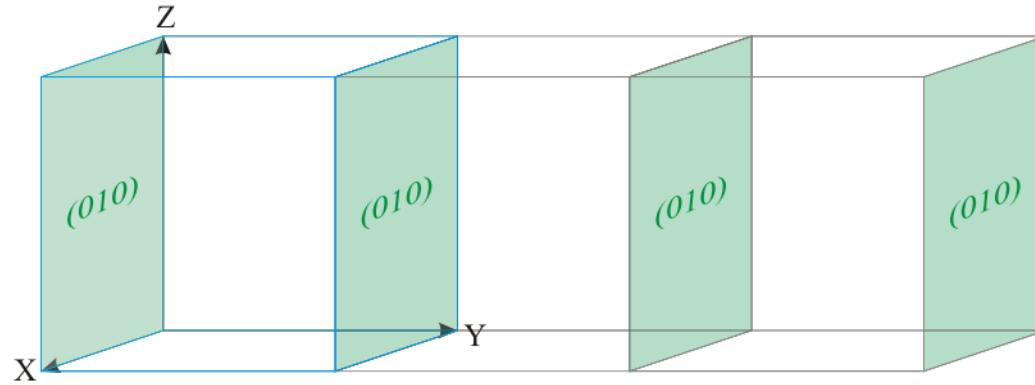
$$d_{010}^{\text{cubic lattice}} = \frac{a}{\sqrt{0^2 + 1^2 + 0^2}} = a$$

$$d_{020}^{\text{cubic lattice}} = \frac{a}{\sqrt{0^2 + 2^2 + 0^2}} = \frac{a}{2}$$

$$d_{020} = \frac{d_{010}}{2}$$

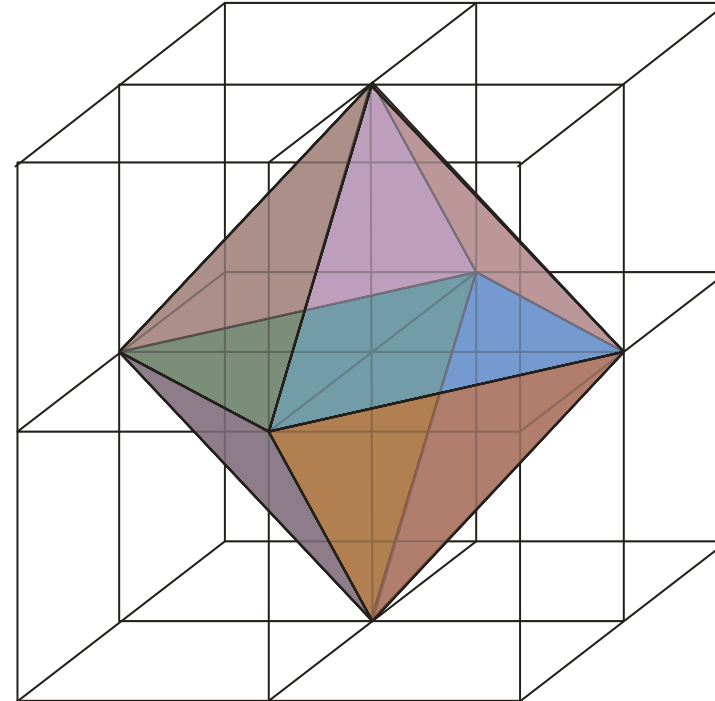
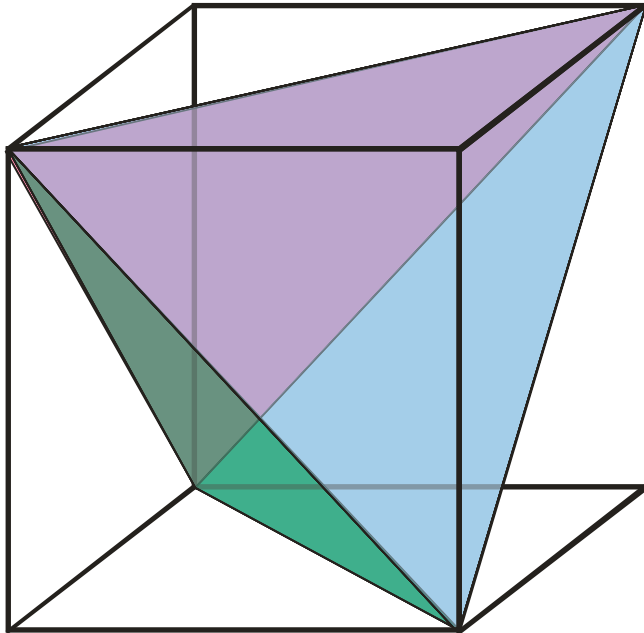
(020), (010) düzleminin yarısı kadar mesafeye sahiptir.

*Kesişim $\rightarrow \infty \frac{1}{2} \infty$
Düzlem $\rightarrow (0\ 2\ 0)$*



Miller İndisleri – Düzlemler

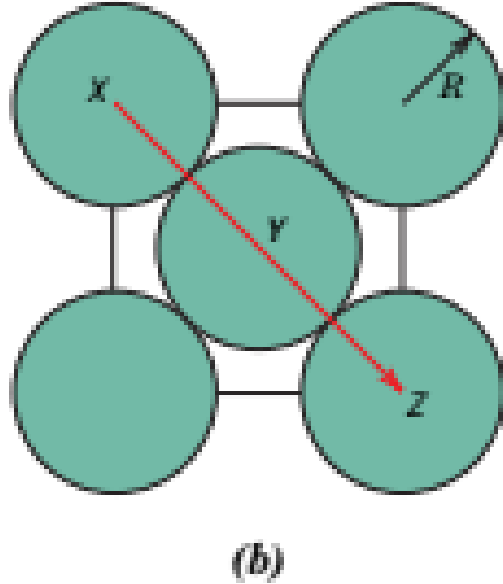
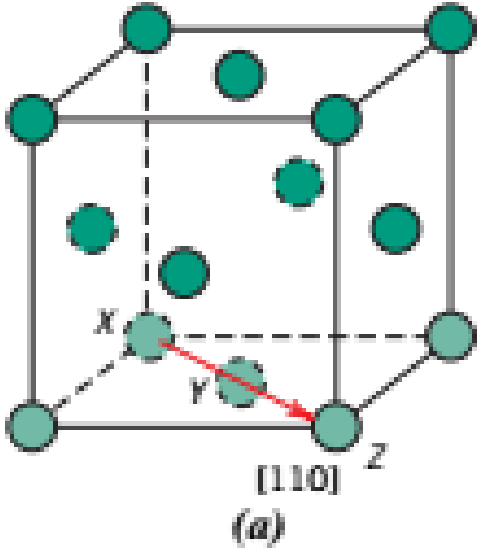
İndeks	Kübik latisdeki üye sayısı	d_{hkl}	
{100}	6	$d_{100} = a$	
{110}	12	$d_{110} = a/\sqrt{2} = a\sqrt{2}/2$	(110) yüzey diagonalini ikiye keser.
{111}	8	$d_{111} = a/\sqrt{3} = a\sqrt{3}/3$	(111) Hacim diagonalini üçe keser.



Miller İndisleri – Yönler

Düzlemsel yoğunluk:

$$\text{Düzlemsel yoğunluk}(DY) = \frac{\text{Düzlemdeki atomların sayısı}}{\text{Düzlemin alanı}}$$



$$DY_{100} = \frac{2 \text{ atom}}{\left(\frac{4r}{\sqrt{2}}\right)^2} = \text{atom}/\text{nm}^2$$

$$DDF_{100} = \frac{2 \text{ atom} * \pi r^2}{\left(\frac{4r}{\sqrt{2}}\right)^2} = 0.7854$$

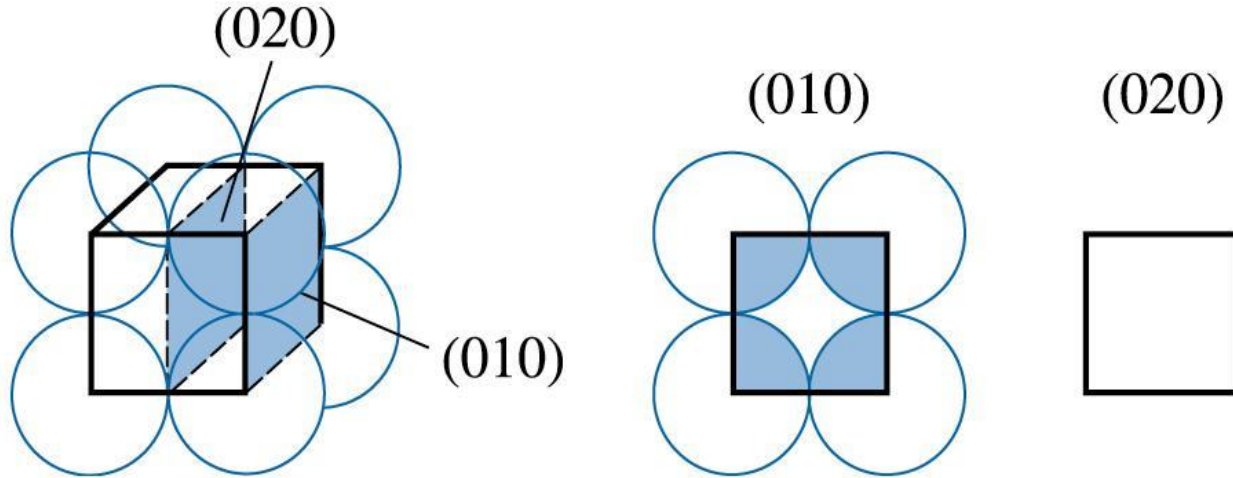
$$\text{Düzlemsel dolgu faktörü}(DDF) = \frac{\text{Düzlemdeki atomların alanı}}{\text{Düzlemin alanı}}$$

Miller İndisleri – Yönler

Düzlemsel yoğunluk:

$$\text{Düzlemsel dolgu faktörü}(DDF) = \frac{\text{Düzlemdeki atomların alanı}}{\text{Düzlemin alanı}}$$

Basit kübik yapıya sahip Polonyum (Po) metalinin (010) ve (020) düzlemlerinin düzlemsel dolgu faktörünü hesaplayınız. ($a = 0.336$ nm)



$$DDF_{100} = \frac{1 \text{ atom} * \pi r^2}{(2r)^2} = 0.7854$$

(c) 2003 Brooks/Cole Publishing /
Thomson Learning™

Miller İndisleri – Düzlemler

	Sembol		Alternatif Sembol		
Yön	[]	[uvw]		→	Belirli bir yön
	< >	<uvw>	[[]]	→	Yön ailesi
Düzlem	()	(hkl)		→	Belirli bir düzlem
	{ }	{hkl}	(())	→	Düzlem ailesi
Nokta	..	.xyz.	[[]]	→	Belirli bir nokta
	::	:xyz:		→	Nokta ailesi

Miller İndisleri – Düzlemler

Drag each index to the box below the correct plane

$(\bar{1}\bar{1}\bar{1})$ $(1\bar{1}3)$
 $(\bar{2}10)$ $(1\bar{1}2)$
 $(\bar{1}1\bar{2})$ (310)

Clear and see new set

Score: Score

Reset these indices

www.doitpoms.ac.uk

Drag each index to the box below the correct plane

$(1\bar{3}2)$ $(\bar{2}00)$
 (300) $(2\bar{2}3)$
 (110) $(\bar{1}20)$

Clear and see new set

Score: Score

Reset these indices

www.doitpoms.ac.uk

Miller İndisleri – Düzlemler

Drag each index to the box below the correct plane

$(3\ 1\ 0)$
 $(\bar{1}\ \bar{1}\ 0)$

$(2\ 2\ \bar{3})$
 $(0\ \bar{1}\ \bar{1})$

$(\bar{1}\ \bar{1}\ 2)$
 $(\bar{2}\ 2\ \bar{2})$

Clear and see new set

Score: Score

Reset these indices

www.doitpoms.ac.uk

Drag each index to the box below the correct plane

$(0\ 1\ 0)$
 $(1\ 2\ 0)$

$(1\ 1\ 1)$
 $(\bar{2}\ 2\ \bar{1})$

$(0\ 1\ \bar{1})$
 $(\bar{1}\ 3\ \bar{1})$

Clear and see new set

Score: Score

Reset these indices

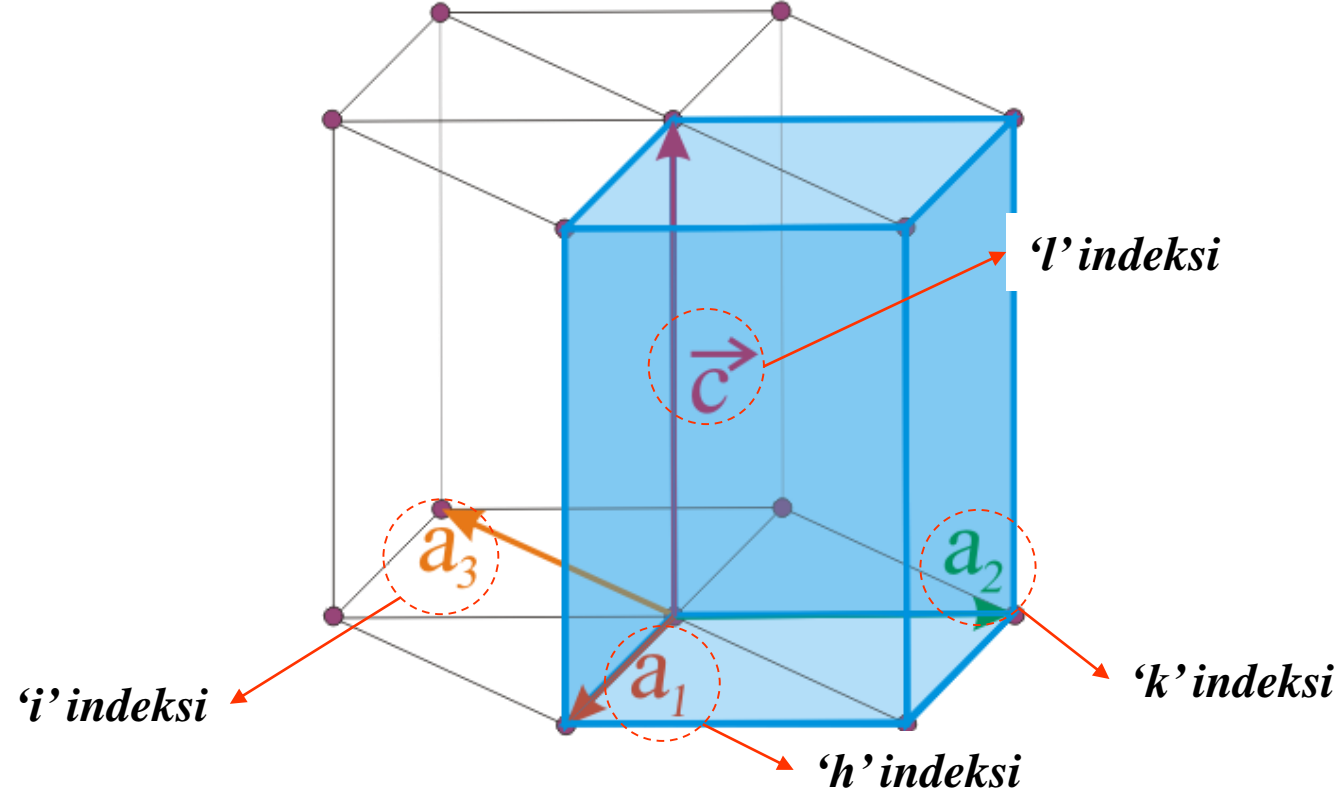
www.doitpoms.ac.uk

Miller-Bravais İndisleri – Düzlemler

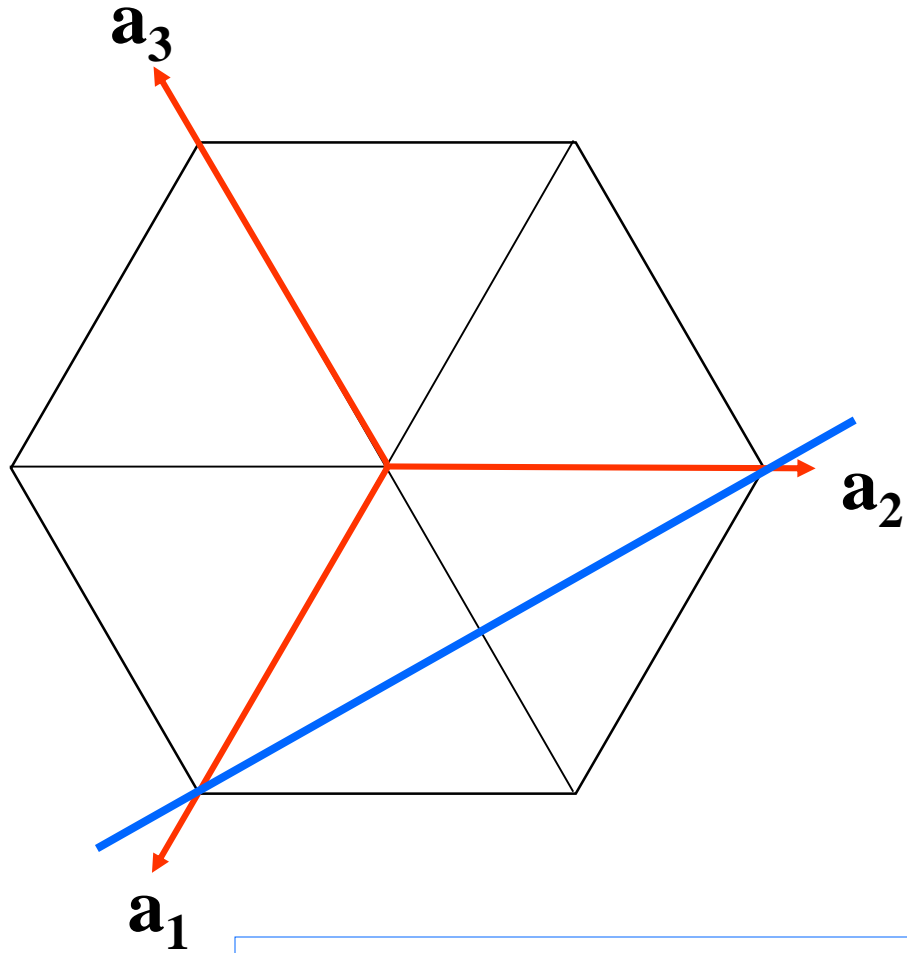
Hekzagonal latisler ve kristaller Miller-Bravais İndisleri olarak adlandırılan dörtlü indeksleme ile gösterilir. (h,k,i,l)

Bu dört indeksten;

- İlk üçü taban düzlemine ait simetrik indekslerdir.
- Üçüncü indeks gereksiz olabilir çünkü ilk iki indeksten çıkarılabilir. $h + k = -i$ (Yalnızca yön ve düzlemlerin aynı sayıda indekse sahip olması için verilmektedir.)
- Dördüncü indeks 'c' eksenini temsil eder.

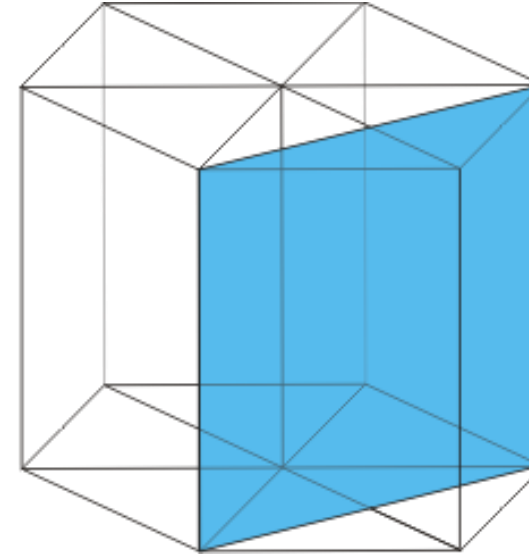


Miller-Bravais İndisleri – Düzlemler



Kesişim $\rightarrow 1 \ 1 \ -\frac{1}{2} \ \infty$

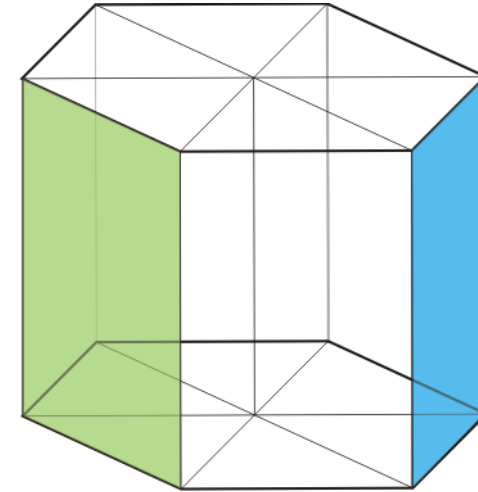
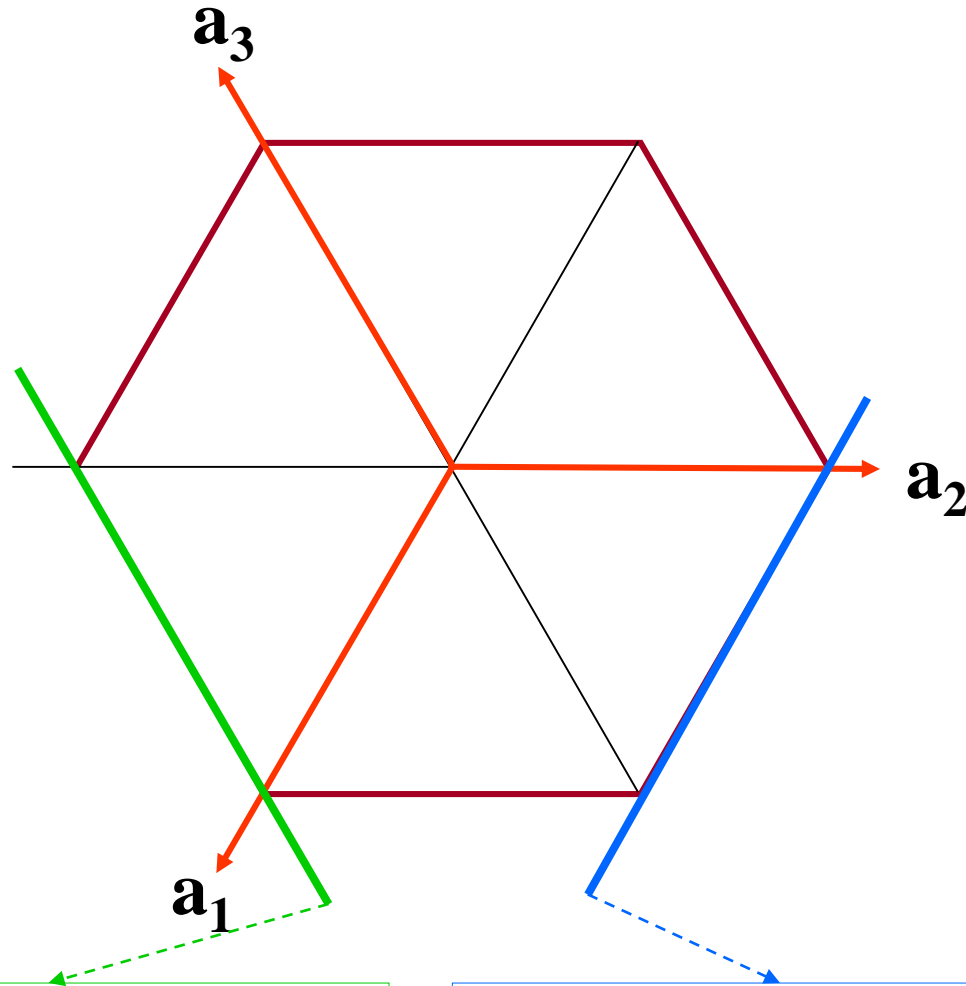
Düzlem $\rightarrow (1 \ 1 \ \bar{2} \ 0)$



$(h \ k \ i \ l)$

$i = -(h + k)$

Miller-Bravais İndisleri – Düzlemler



Kesişim $\rightarrow 1 -1 \infty \infty$

Miller $\rightarrow (1 \bar{1} 0)$

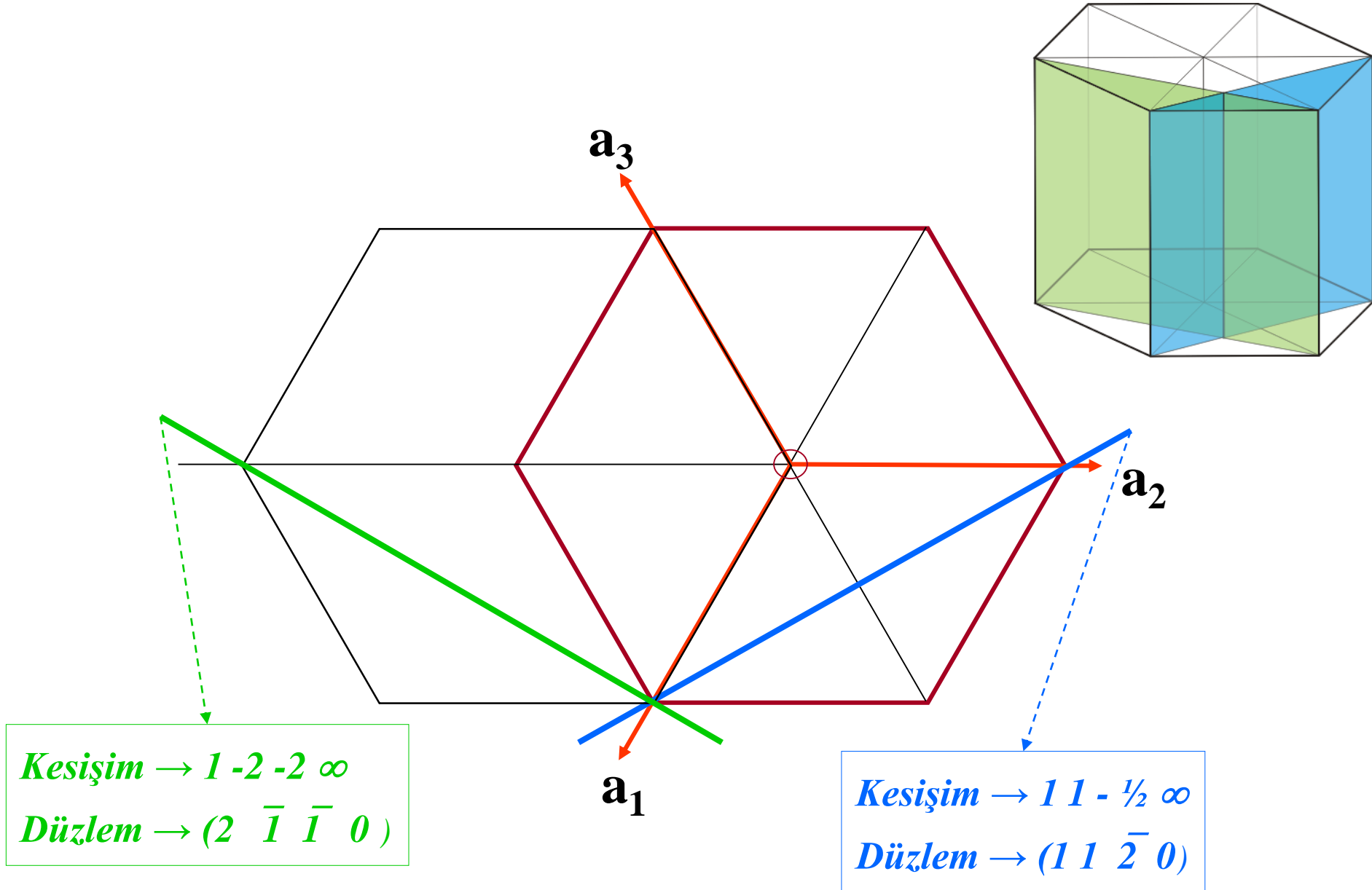
Miller-Bravais $\rightarrow (1 \bar{1} 0 0)$

Kesişim $\rightarrow \infty 1 -1 \infty$

Miller $\rightarrow (0 1 0)$

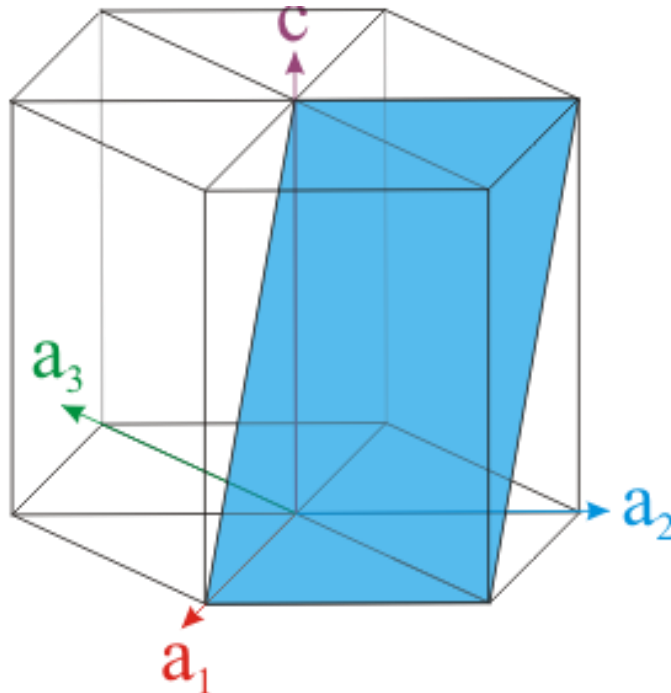
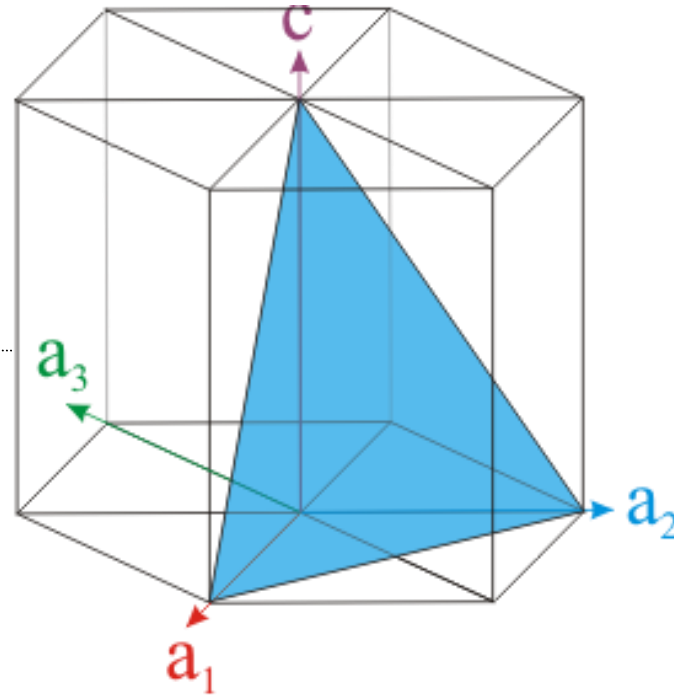
Miller-Bravais $\rightarrow (0 1 \bar{1} 0)$

Miller-Bravais İndisleri – Düzlemler



Miller-Bravais İndisleri – Düzlemler

Kesişim $\rightarrow 1\ 1\ -\frac{1}{2}\ 1$
Düzlem $\rightarrow (1\ 1\ \bar{2}\ 1)$



Kesişim $\rightarrow 1\ \infty\ -1\ 1$
Düzlem $\rightarrow (1\ 0\ \bar{1}\ 1)$

Miller-Bravais İndisleri – Yönler

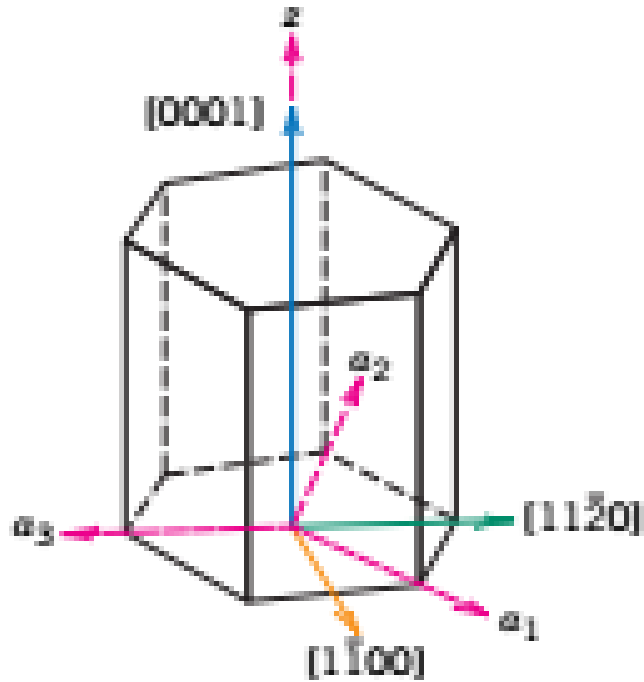


Figure 3.9 For the hexagonal crystal system, the $[0001]$, $[1\bar{1}00]$, and $[11\bar{2}0]$ directions.

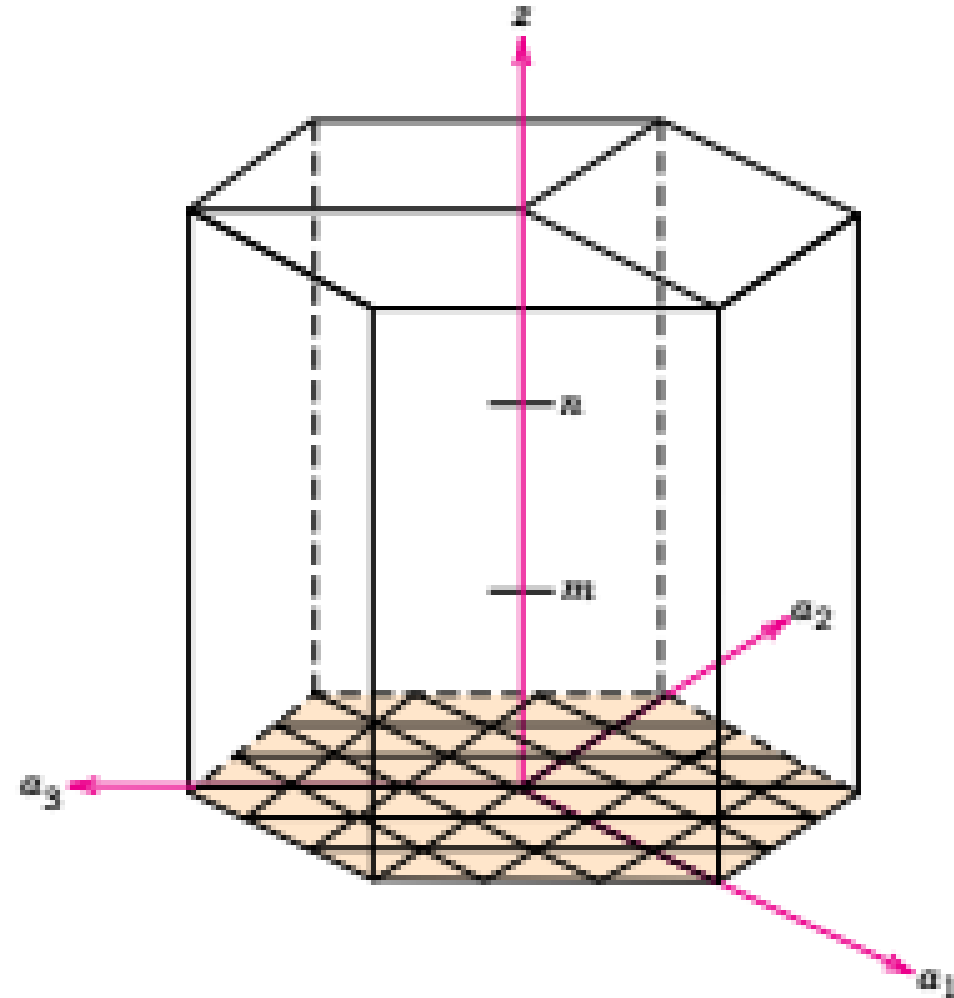
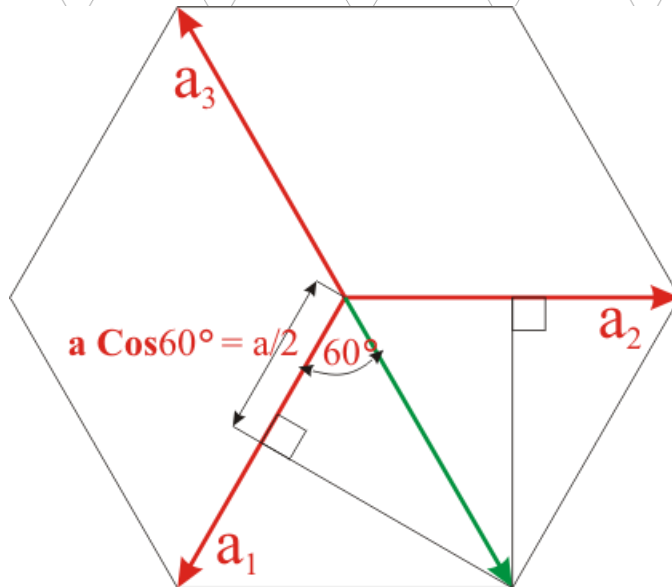
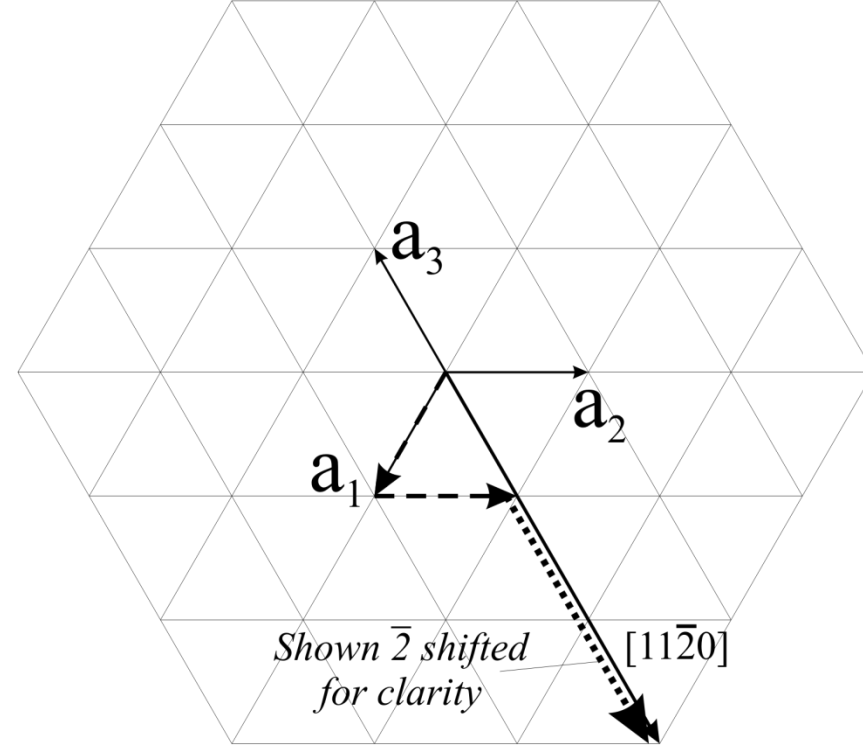
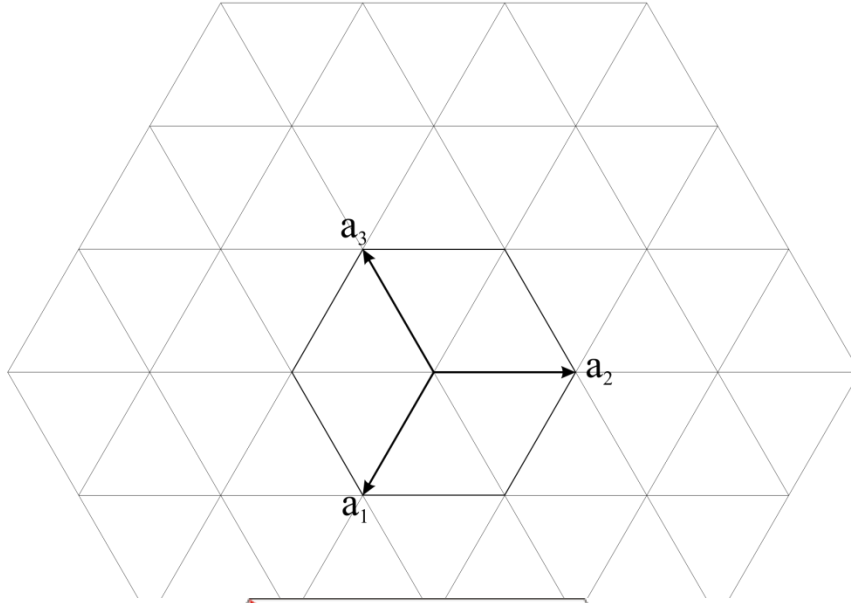


Figure 3.10 Ruled-net coordinate axis system for hexagonal unit cells that may be used to plot crystallographic directions.

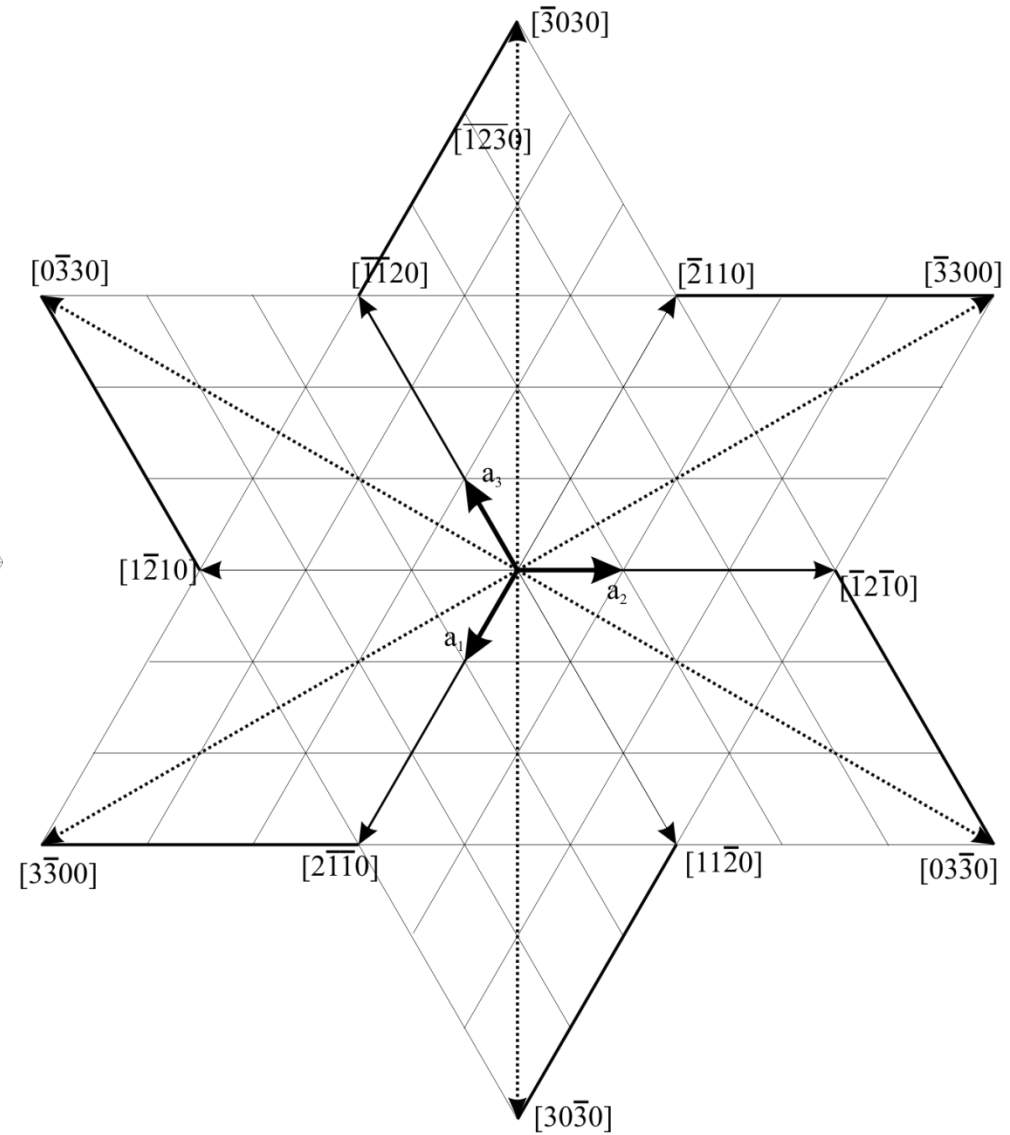
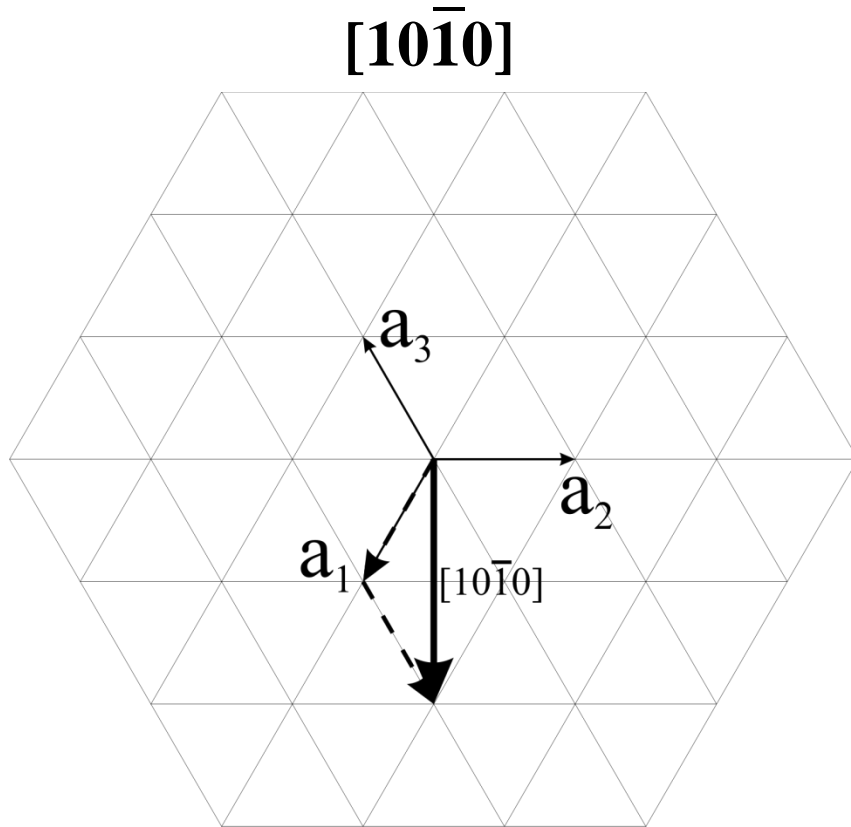
Miller-Bravais İndisleri – Yönler

[11 $\bar{2}$ 0] Yönü



	a_1	a_2	a_3
Projeksiyon	$a/2$	$a/2$	$-a$
Kafes Parametresine Göre Normalizasyon	$1/2$	$1/2$	-1
Çarpan	2	2	-2
İndeks	$[1\ 1\ \bar{2}\ 0]$		

Miller-Bravais İndisleri – Yönler



Miller-Bravais İndisleri – Yönler

Miller \longrightarrow Miller-Bravais dönüşümü

$[UVW] \longrightarrow [uvtw]$

$$u = \frac{1}{3}(2U - V)$$

$$\mathbf{u} = 2\mathbf{U} - \mathbf{V}$$

$$v = \frac{1}{3}(2V - U)$$

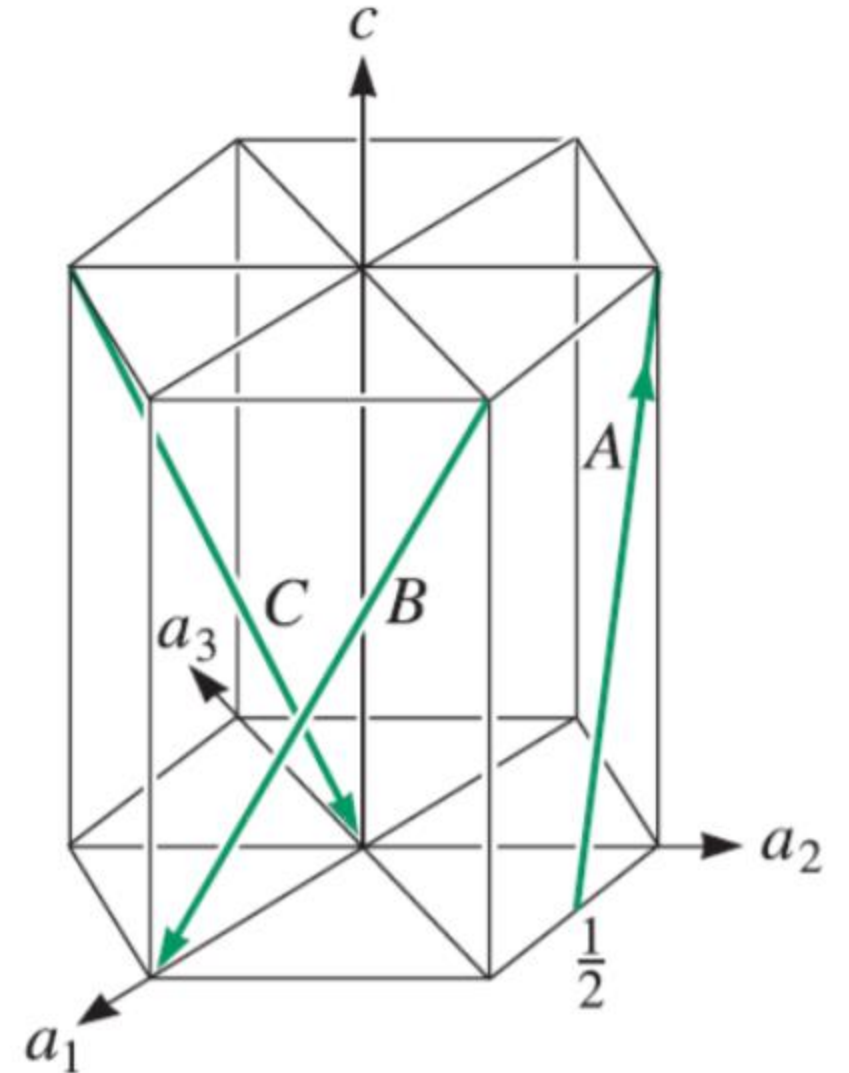
$$\mathbf{v} = 2\mathbf{V} - \mathbf{U}$$

$$t = -(u + v)$$

$$\mathbf{t} = -(\mathbf{u} + \mathbf{v})$$

$$w = W$$

$$\mathbf{w} = 3\mathbf{W}$$



Sıkı paketlenmiş düzlemler ve yönler

TABLE 3-5 ■ *Close-packed planes and directions*

Structure	Directions	Planes
SC	$\langle 100 \rangle$	None
BCC	$\langle 111 \rangle$	None
FCC	$\langle 110 \rangle$	$\{111\}$
HCP	$\langle 100 \rangle$, $\langle 110 \rangle$ or $\langle 11\bar{2}0 \rangle$	(0001) , (0002)

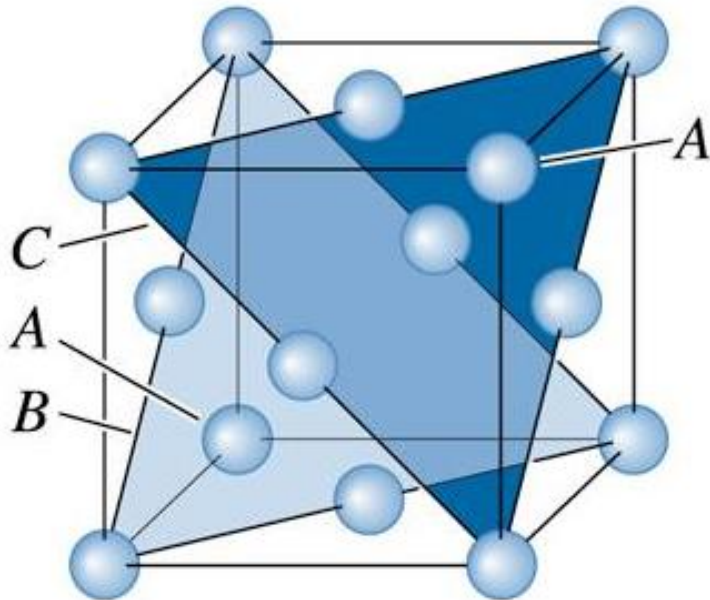
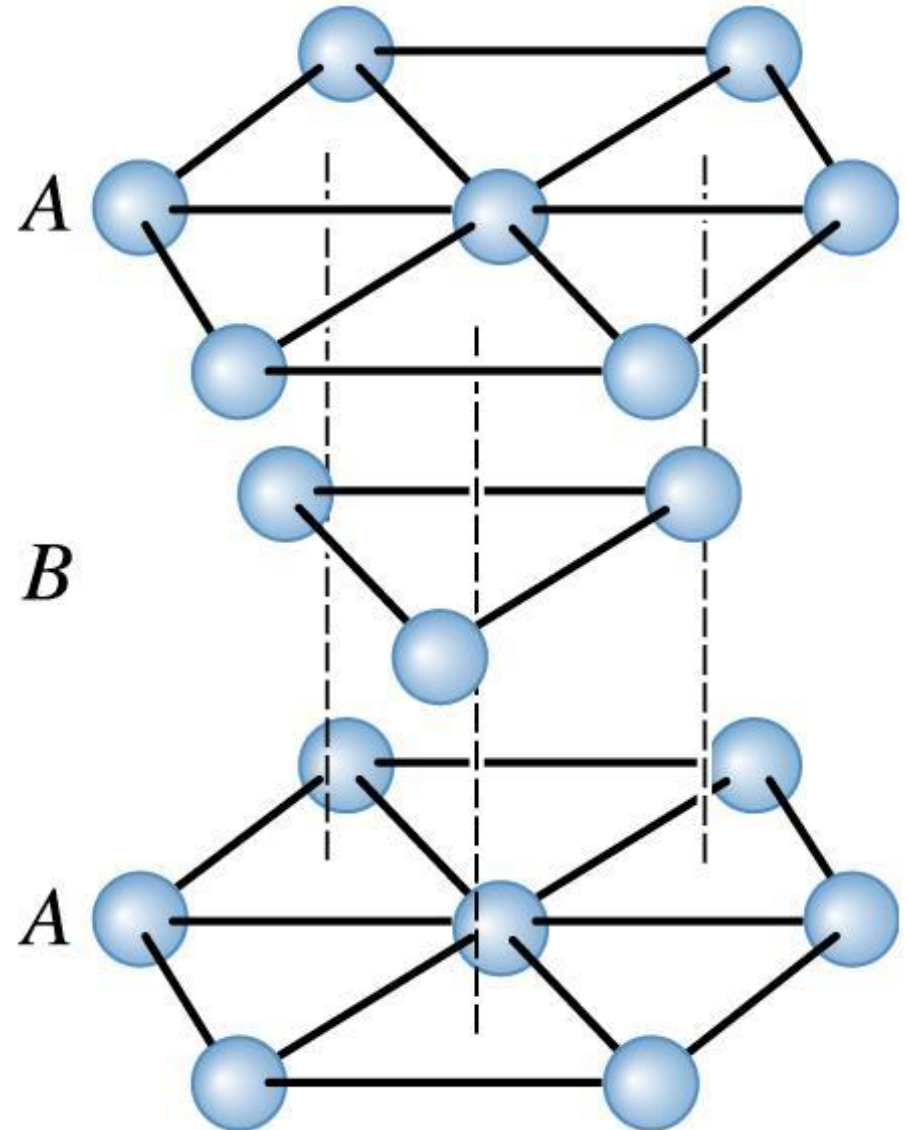


Figure 3.27 The *ABABAB* stacking sequence of close-packed planes produces the HCP structure.



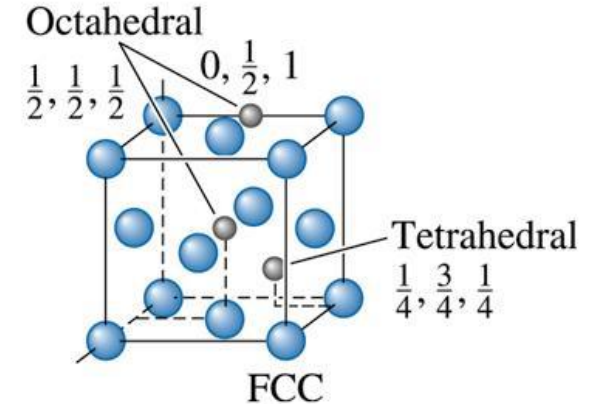
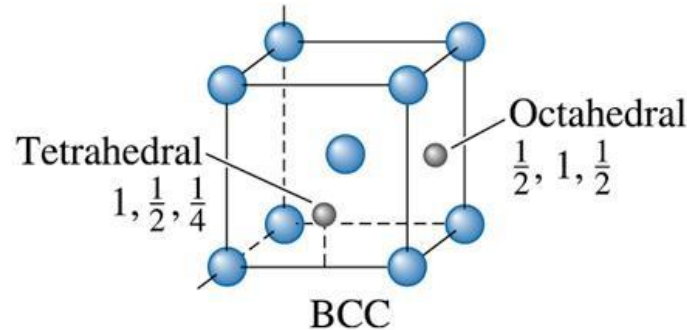
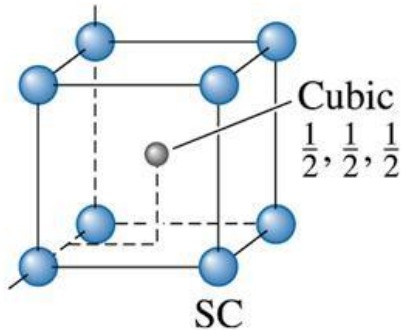
Arayer pozisyonları

Arayer pozisyonları: Kristal yapı içerisinde bulunan atomların/iyonların arasında başka bir atom/iyon yerleştiği pozisyonlara arayer pozisyonları denir. Genel olarak, arayer yerleşimi, yerleşecek atomun/iyonun boyutundan daha küçüktür.

Kübik konum: Koordinasyon sayısı 8 olan arayer pozisyonudur.

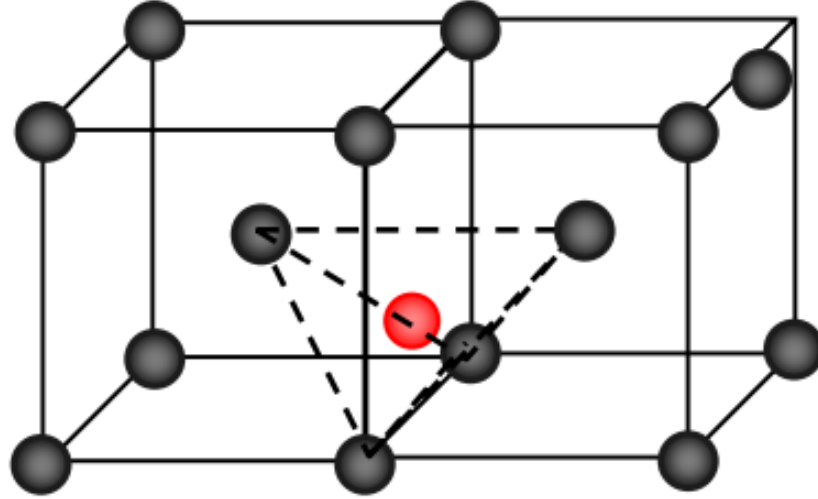
Oktahedral konum: Koordinasyon sayısı 6 olan arayer pozisyonudur.

Tetrahedral konum: Koordinasyon sayısı 4 olan arayer pozisyonudur.

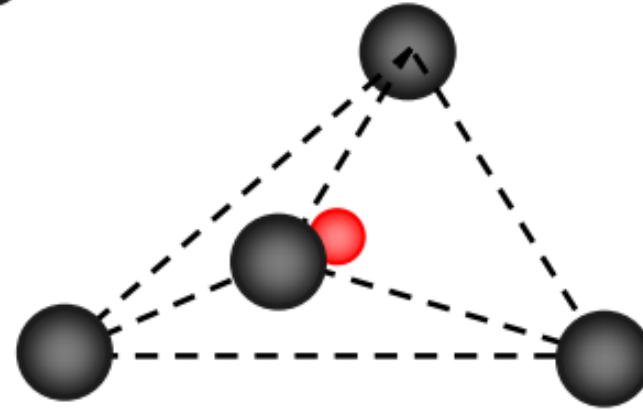


Arayer pozisyonları

Hacim merkezli kübik yapıda tetrahedral boşluk

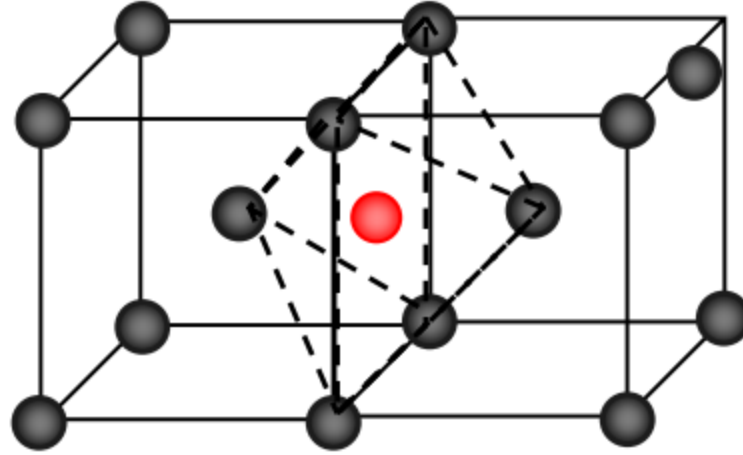


Tetrahedral
 $\frac{1}{2}, 1, \frac{1}{4}$



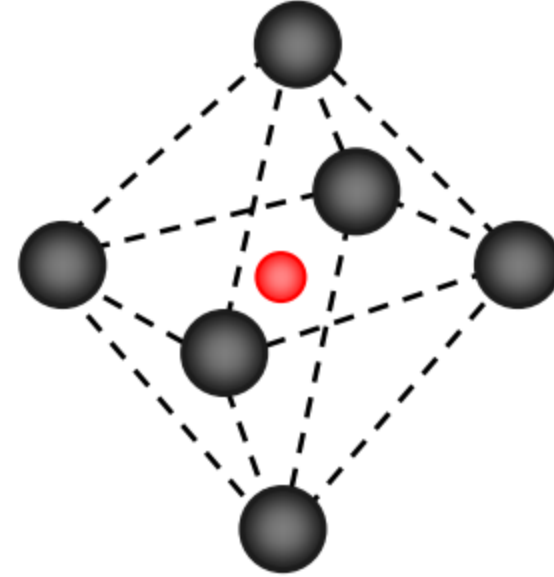
Arayer pozisyonları

Hacim merkezli kübik yapıda oktahedral boşluk

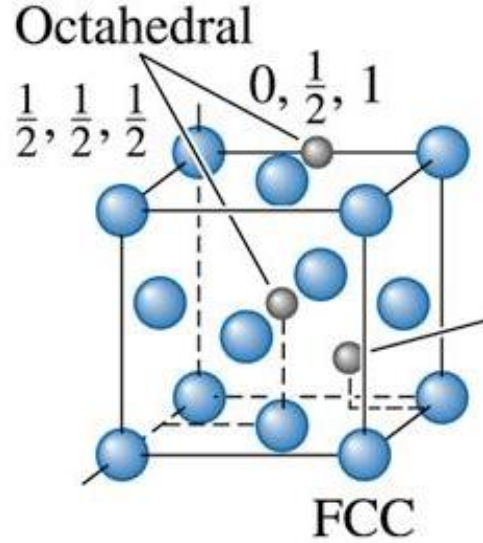


Oktahedral

$\frac{1}{2}, 1, \frac{1}{2}$



Arayer pozisyonları



(c) 2003 Brooks/Cole Publishing / Thomson Learning™


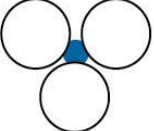
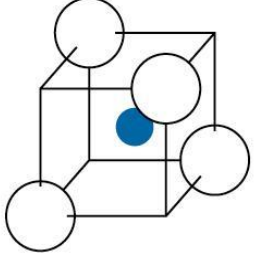
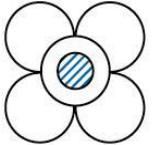
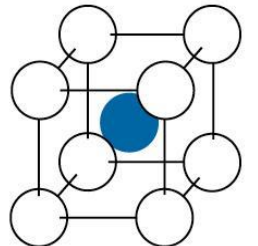
YMK birim hücreye ait olan oktahedral arayer pozisyonlarını belirleyiniz.

$$\begin{array}{cccc} \frac{1}{2}, 0, 0 & \frac{1}{2}, 1, 0 & \frac{1}{2}, 0, 1 & \frac{1}{2}, 1, 1 \\ 0, \frac{1}{2}, 0 & 1, \frac{1}{2}, 0 & 1, \frac{1}{2}, 1 & 0, \frac{1}{2}, 1 \\ 0, 0, \frac{1}{2} & 1, 0, \frac{1}{2} & 1, 1, \frac{1}{2} & 0, 1, \frac{1}{2} \end{array}$$

Ve kübün merkezi, $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

Arayer pozisyonlari

TABLE 3-6 ■ *The coordination number and the radius ratio*

Coordination Location of Number	Interstitial	Radius Ratio	Representation
2	Linear	0–0.155	
3	Center of triangle	0.155–0.225	
4	Center of tetrahedron	0.225–0.414	
6	Center of octahedron	0.414–0.732	
8	Center of cube	0.732–1.000	

İyonik Malzemelerde Kristal Yapılar

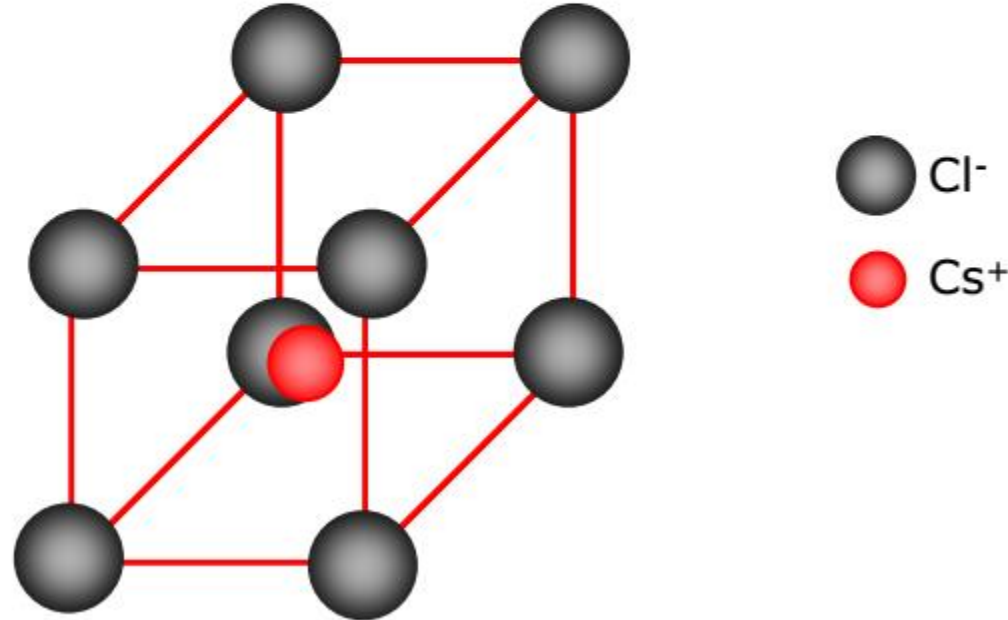
İyonik malzemelerde genellikle anyonlar birim hücrenin kafes noktalarında, katyonlar ise arayer boşluklarda yer alır.

CsCl yapısı

$$r_{\text{Cs}^+} = 0,167 \text{ nm}, r_{\text{Cl}^-} = 0,181 \text{ nm}$$

$$r_{\text{K}} / r_{\text{A}} = 0,167 \text{ nm} / 0,181 \text{ nm} = 0,92 \Rightarrow \text{KS: } 8$$

Basit kübik yapıda kristalleşir, Cl^- iyonları kafes noktalarında, Cs^+ iyonu ise küp merkezinde bulunur



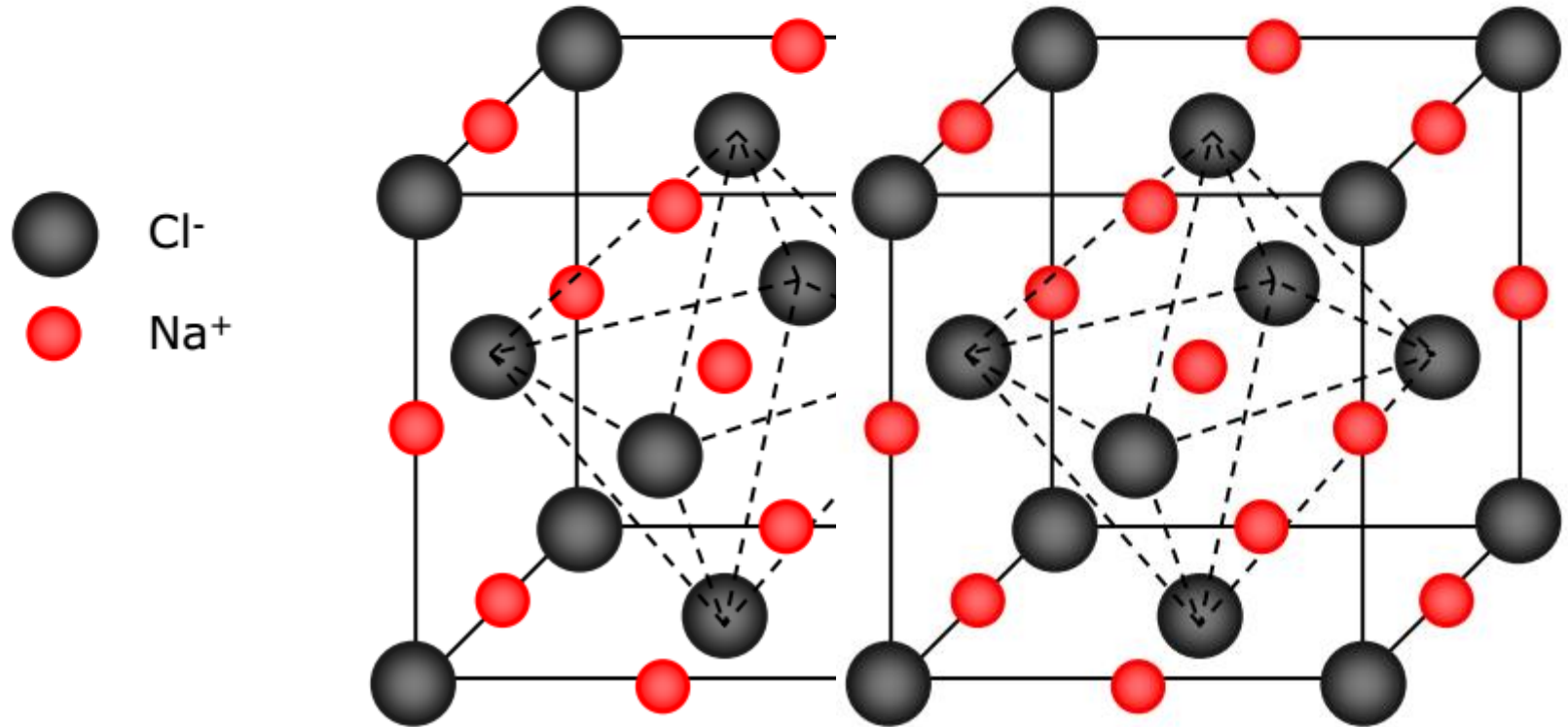
İyonik Malzemelerde Kristal Yapılar

NaCl yapısı

$$r_{\text{Na}^+} = 0,097 \text{ nm}, r_{\text{Cl}^-} = 0,181 \text{ nm}$$

$$r_K / r_A = 0,097 \text{ nm} / 0,181 \text{ nm} = 0,536 \Rightarrow \text{KS: } 6$$

YMK yapıda kristalleşir, Cl^- iyonları kafes noktalarına, Na^+ iyonları ise oktahedral boşluklara yerleşir



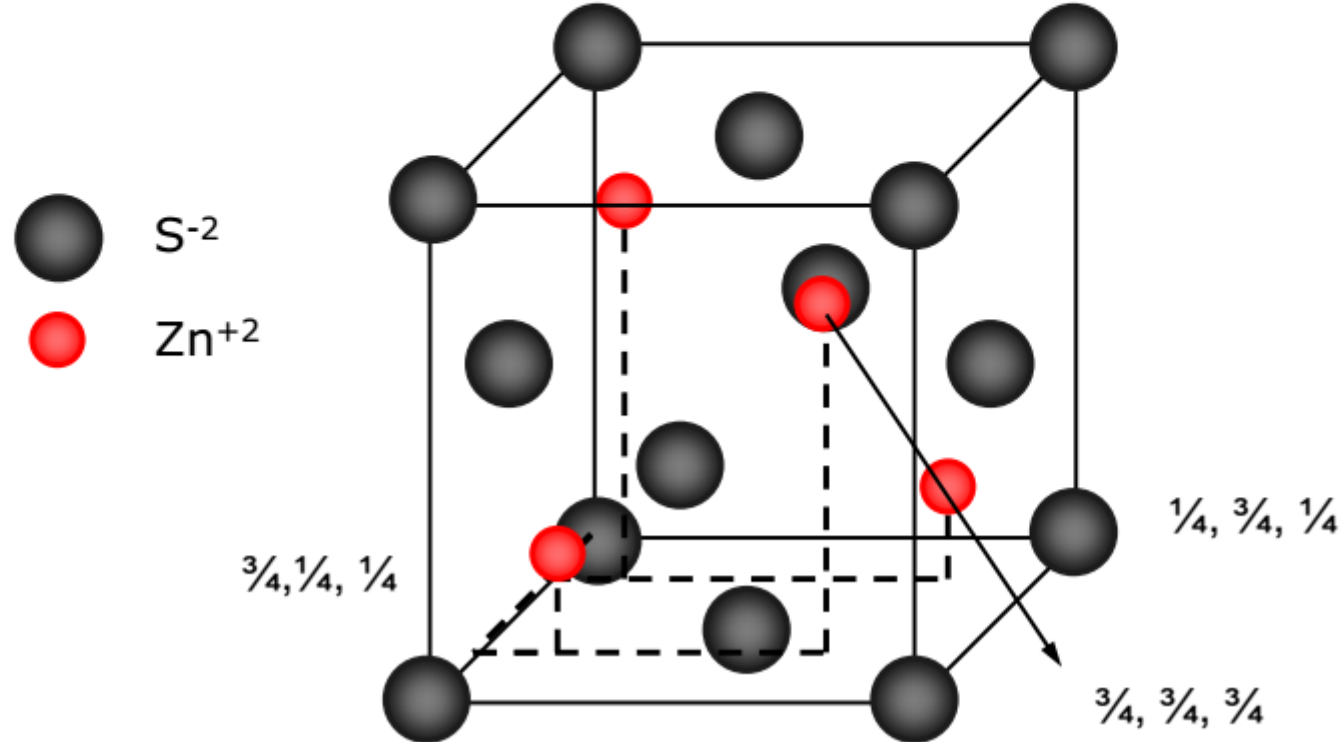
İyonik Malzemelerde Kristal Yapılar

ZnS yapısı

$$r_{\text{Zn}^{+2}} = 0,074 \text{ nm}, r_{\text{S}^{-2}} = 0,184 \text{ nm}$$

$$r_{\text{K}} / r_{\text{A}} = 0,074 \text{ nm} / 0,184 \text{ nm} = 0,402 \Rightarrow \text{KS: } 4$$

YMK yapıda kristalleşir, S^{-2} iyonları kafes noktalarına, Zn^{+2} iyonları ise tetrahedral boşlukların yarısına yerleşir



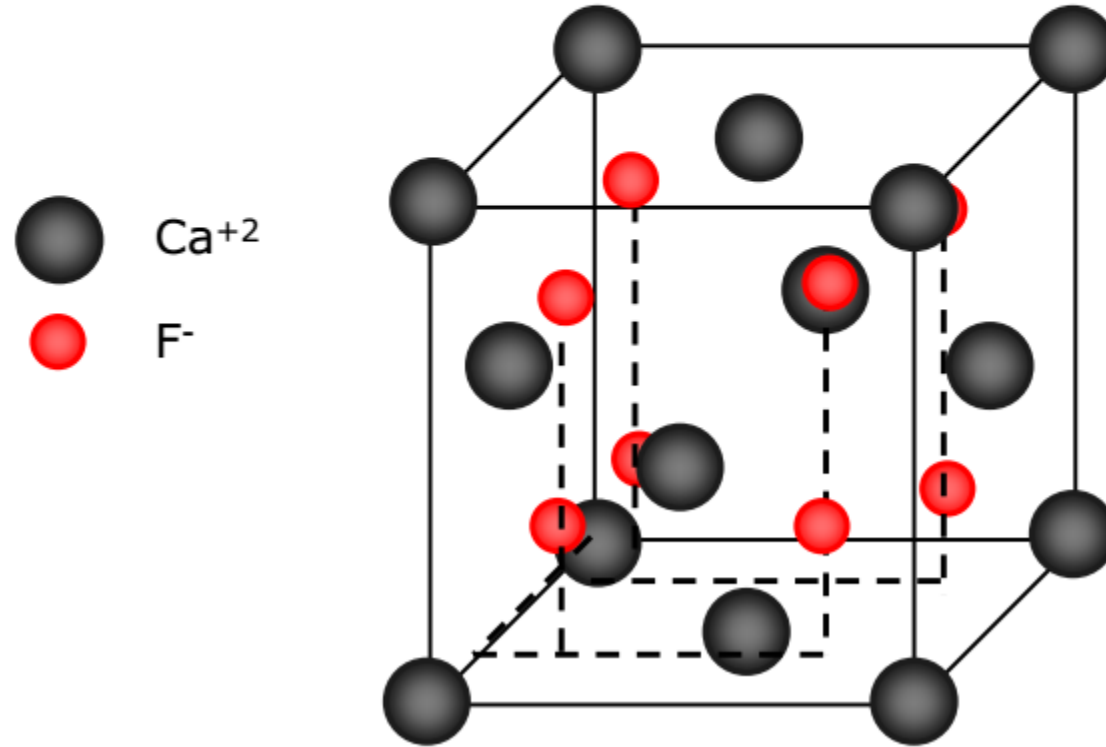
İyonik Malzemelerde Kristal Yapılar

CaF₂ yapısı

$$r_{\text{Ca}^{+2}} = 0,099 \text{ nm}, r_{\text{F}^-} = 0,133 \text{ nm}$$

$$r_{\text{K}} / r_{\text{A}} = 0,099 \text{ nm} / 0,133 \text{ nm} = 0,74 \Rightarrow \text{KS: } 8$$

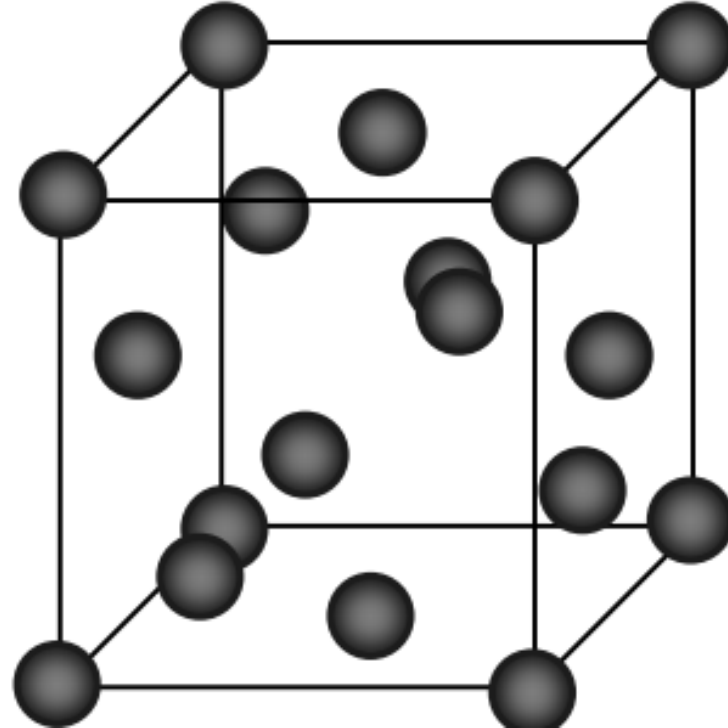
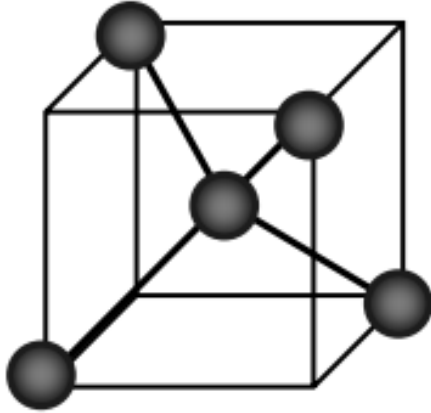
YMK yapıda kristalleşir, Ca⁺² iyonları kafes noktalarına, F⁻ iyonları ise tetrahedral boşluklara yerleşir



Kovalent Malzemelerde Kristal Yapılar

Elmas kübik yapı

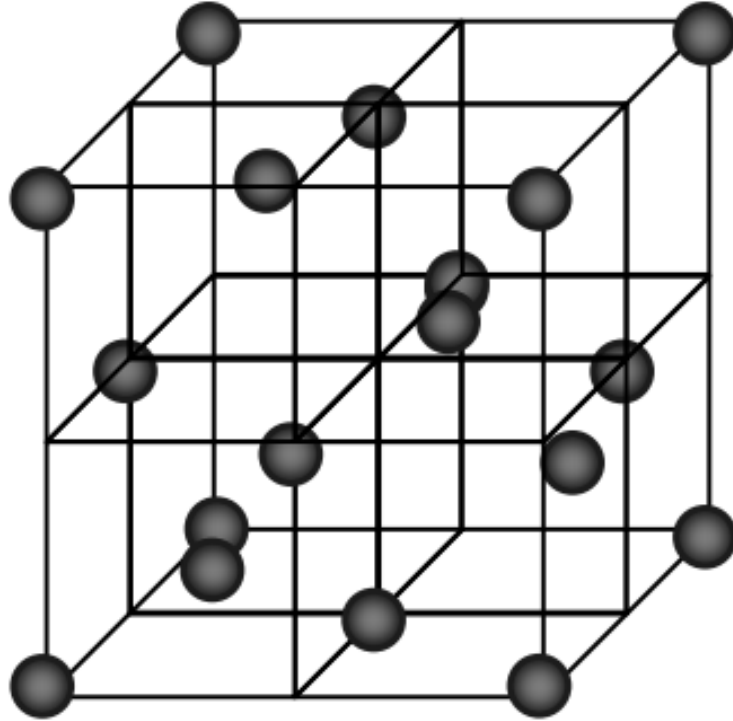
Si, Ge ve C gibi kovalent bağlı elementler tetrahedron oluştururlar. Her bir atomun koordinasyon sayısı dördür.



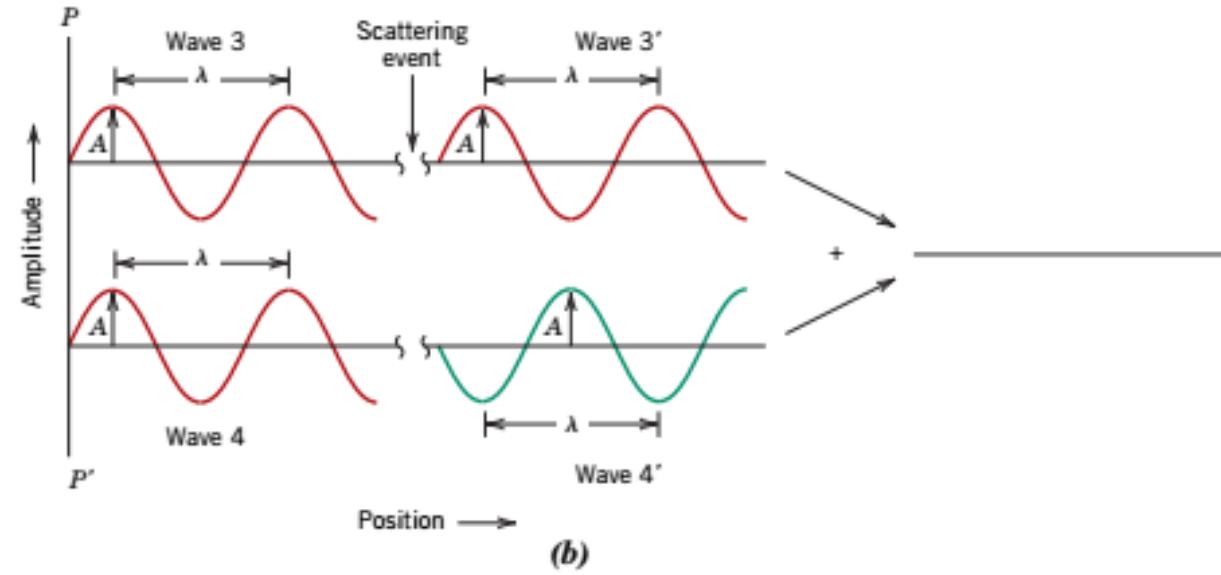
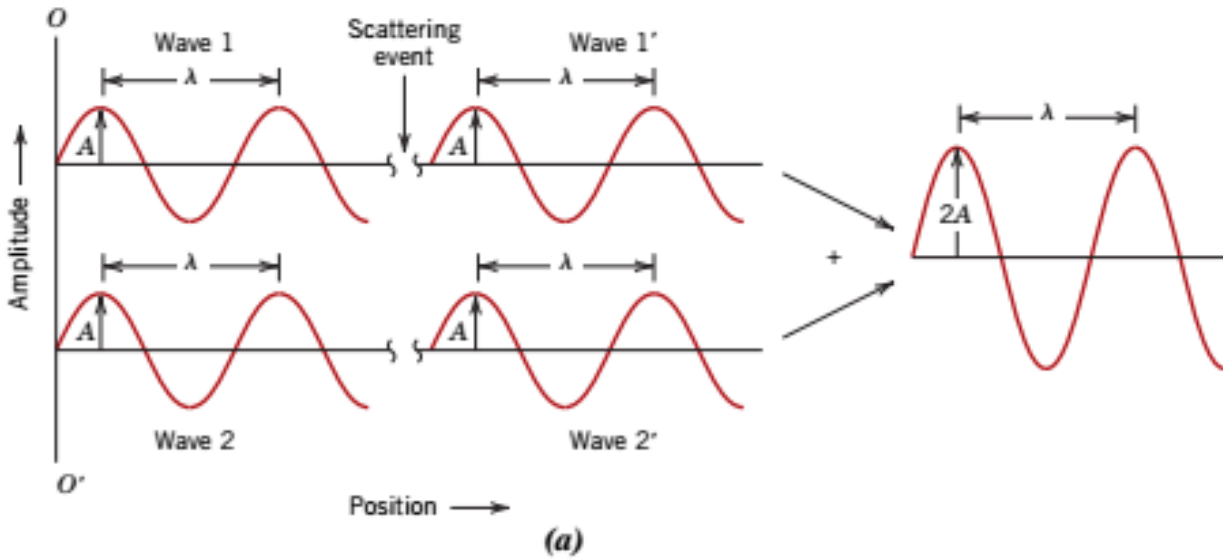
Kovalent Malzemelerde Kristal Yapılar

Elmas kübik yapı

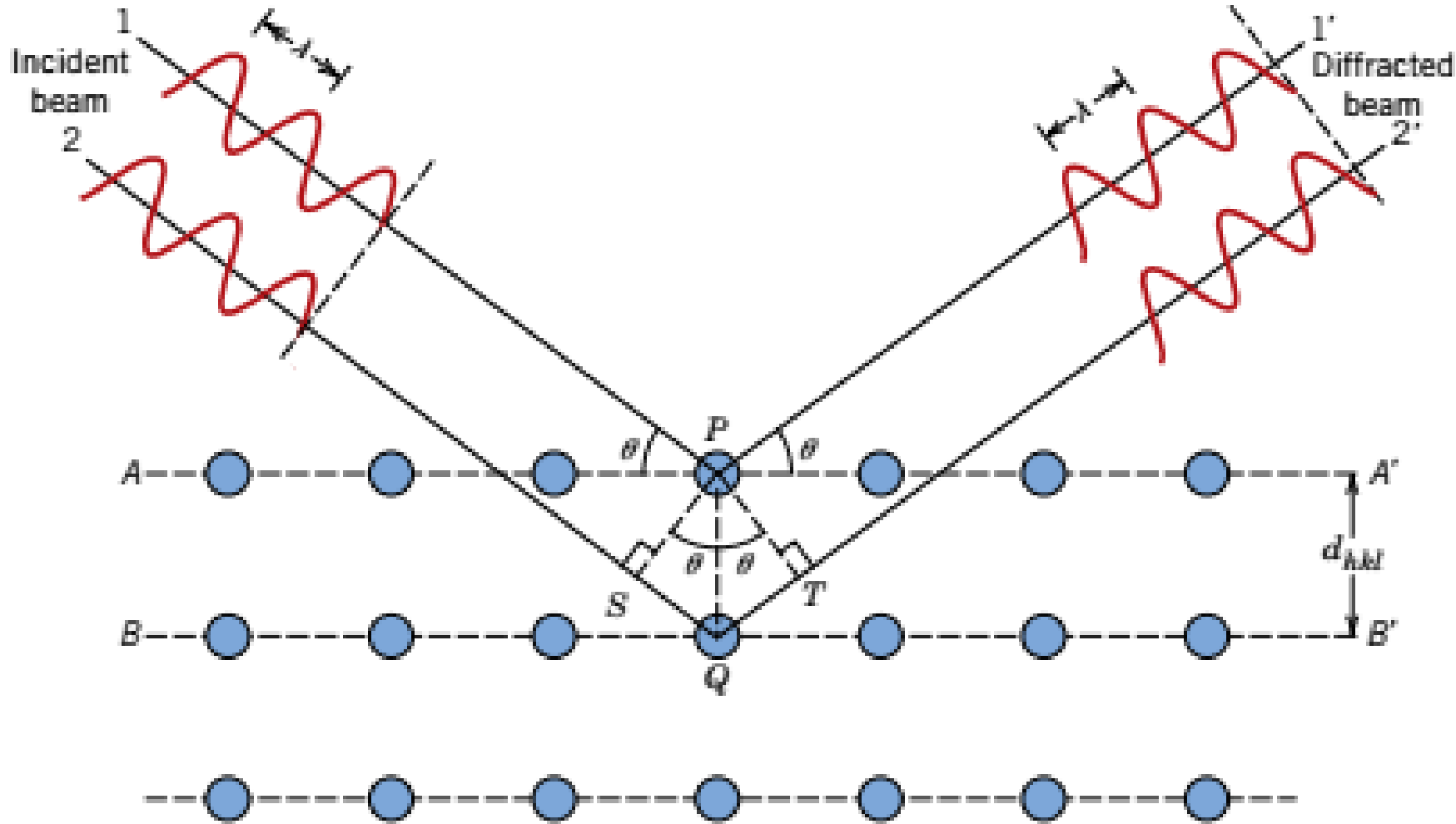
8 tetrahedronun birleşimi ile yüzey merkezli kübik yapı oluşturur, YMK yapıdaki 8 tetrahedral boşluğun yarısı dolu yarısı boştur.



Kristal Yapıların Belirlenmesi: X-Işını Kırınımı (XRD)



X-Işını Kırınımı (XRD): Bragg Kanunu



$$n\lambda = \overline{SQ} + \overline{QT}$$

$$n\lambda = d_{hkl} \sin \theta + d_{hkl} \sin \theta$$

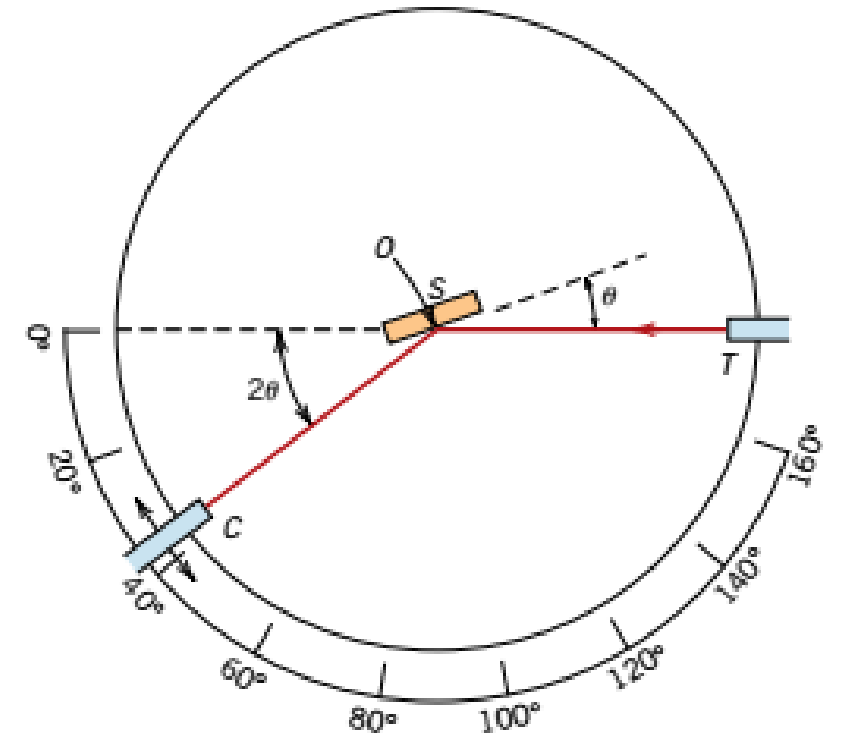
$$= 2d_{hkl} \sin \theta$$

Bragg Kanunu

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

X-Işını Kırınımı (XRD): Bragg Kanunu

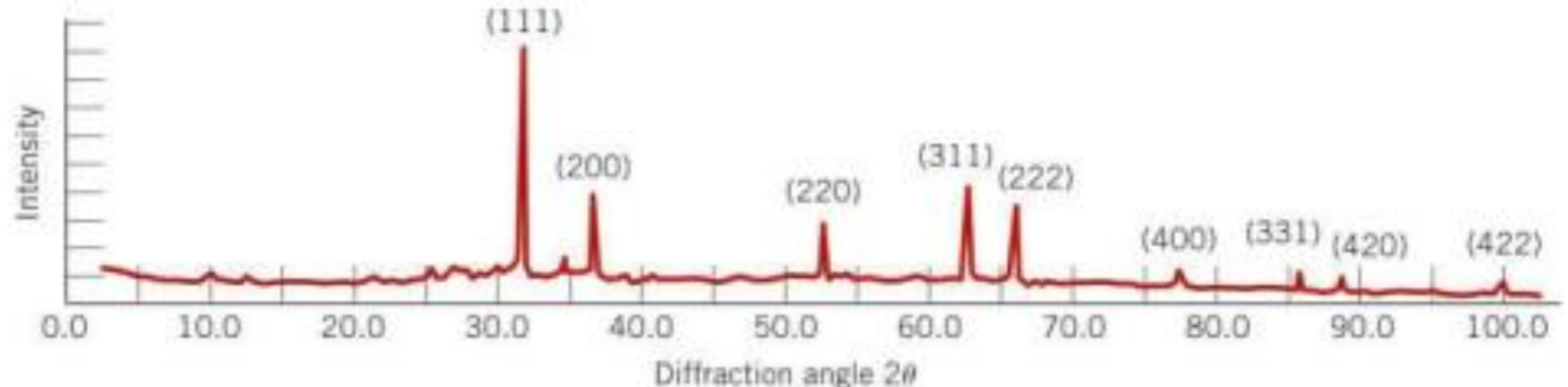
Figure 3.23 Schematic diagram of an x-ray diffractometer; T = x-ray source, S = specimen, C = detector, and O = the axis around which the specimen and detector rotate.



<i>Crystal Structure</i>	<i>Reflections Present</i>	<i>Reflection Indices for First Six Planes</i>
BCC	$(h + k + l)$ even	110, 200, 211, 220, 310, 222
FCC	$h, k,$ and l either all odd or all even	111, 200, 220, 311, 222, 400
Simple cubic	All	100, 110, 111, 200, 210, 211

Figure 3.24

Diffraction pattern for powdered lead. (Courtesy of Wesley L. Holman.)



X-Işını Kırınımı (XRD): Bragg Kanunu

Düzlemler Arası Mesafe ve Kırınım Açısı Hesabı

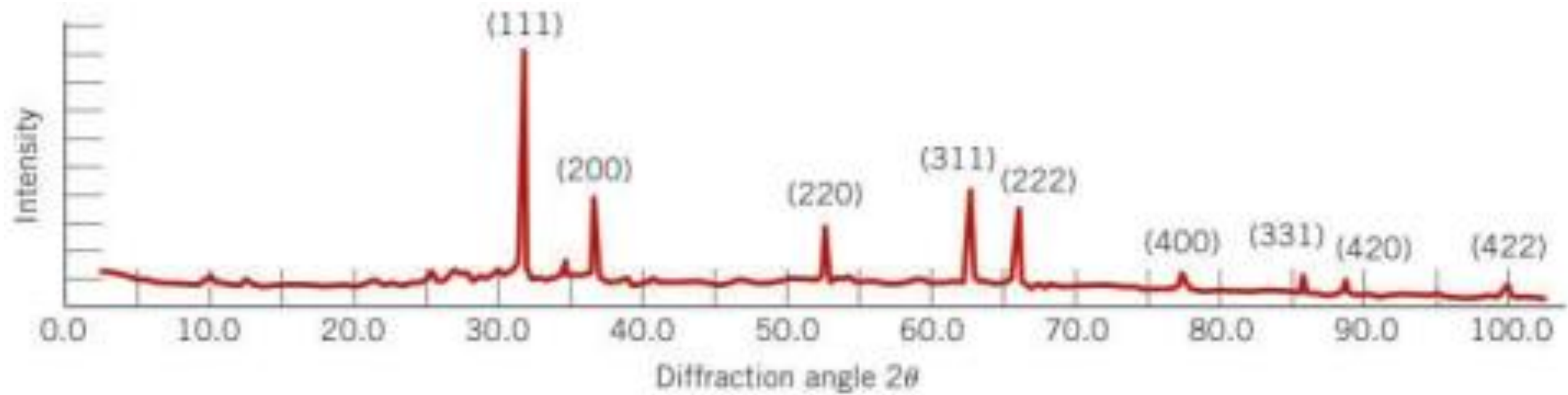
HMK demirden (220) düzlemi için (a) düzlemler arası mesafeyi ve (b) kırınım açısını hesaplayınız. ($a_{\text{Fe}} = 0.2866 \text{ nm}$ ve X-ışını kaynağının dalgaboyu $\lambda = 0.1790 \text{ nm}$, kırınım katsayısı $n = 1$.)

$$\begin{aligned}d_{hkl} &= \frac{a}{\sqrt{h^2 + k^2 + l^2}} \\ &= \frac{0.2866 \text{ nm}}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.1013 \text{ nm}\end{aligned}$$

$$\begin{aligned}\sin \theta &= \frac{n\lambda}{2d_{hkl}} = \frac{(1)(0.1790 \text{ nm})}{(2)(0.1013 \text{ nm})} = 0.884 \\ \theta &= \sin^{-1}(0.884) = 62.13^\circ\end{aligned}$$

$$2\theta = (2)(62.13^\circ) = 124.26^\circ$$

X-Işını Kırınımı (XRD): Bragg Kanunu



$\lambda = 0.1542$ nm olan X-ışını kaynağı ile Pb malzemedeki elde edilmiş XRD paternini kullanarak düzlemler arası mesafe değerlerini ve kafes parametresini hesaplayınız.

$$d_{111} = \frac{n\lambda}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2) \left[\sin \left(\frac{31.3^\circ}{2} \right) \right]} = 0.2858 \text{ nm}$$

$$\begin{aligned} a &= d_{hkl} \sqrt{h^2 + k^2 + l^2} \\ &= d_{111} \sqrt{(1)^2 + (1)^2 + (1)^2} \\ &= (0.2858 \text{ nm}) \sqrt{3} = 0.4950 \text{ nm} \end{aligned}$$