

BMM 205

Malzeme Biliminin Temelleri

X-Işınları ile Kristal Yapı Analizi



Dr. Ersin Emre Ören

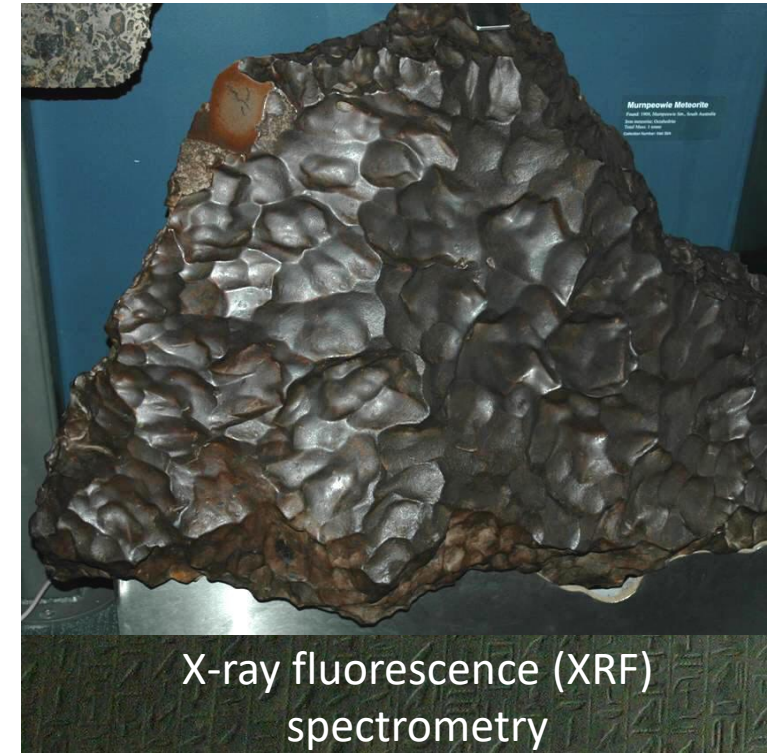
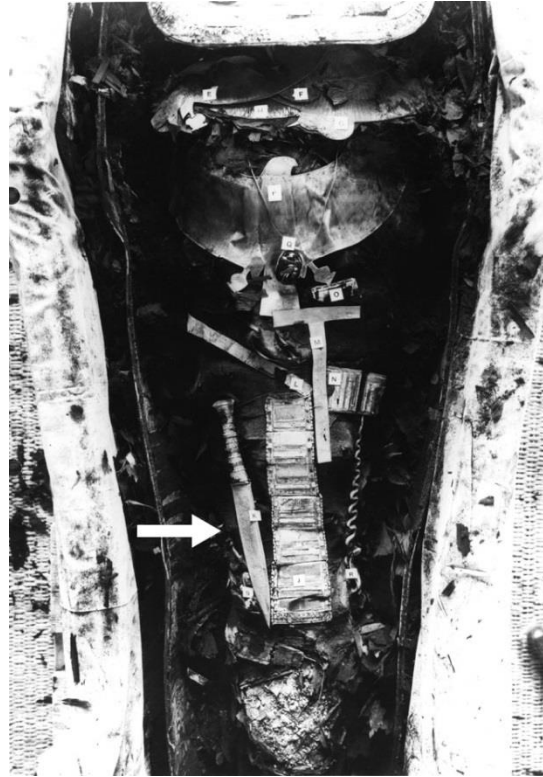
**Biyomedikal Mühendisliği Bölümü
Malzeme Bilimi ve Nanoteknoloji Mühendisliği Bölümü**

**TOBB Ekonomi ve Teknoloji Üniversitesi
Ankara - TÜRKİYE**

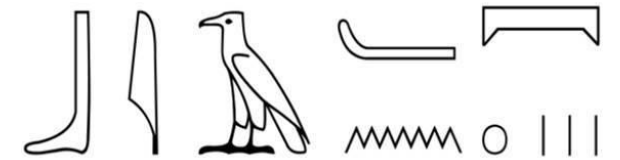
eeoren@etu.edu.tr
<http://eeoren.etu.edu.tr>



Tutankhamun
1341–1323 BC
Bronze Age

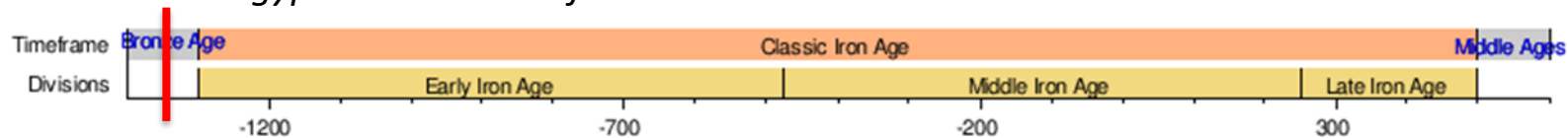


Egyptian Museum of Cairo

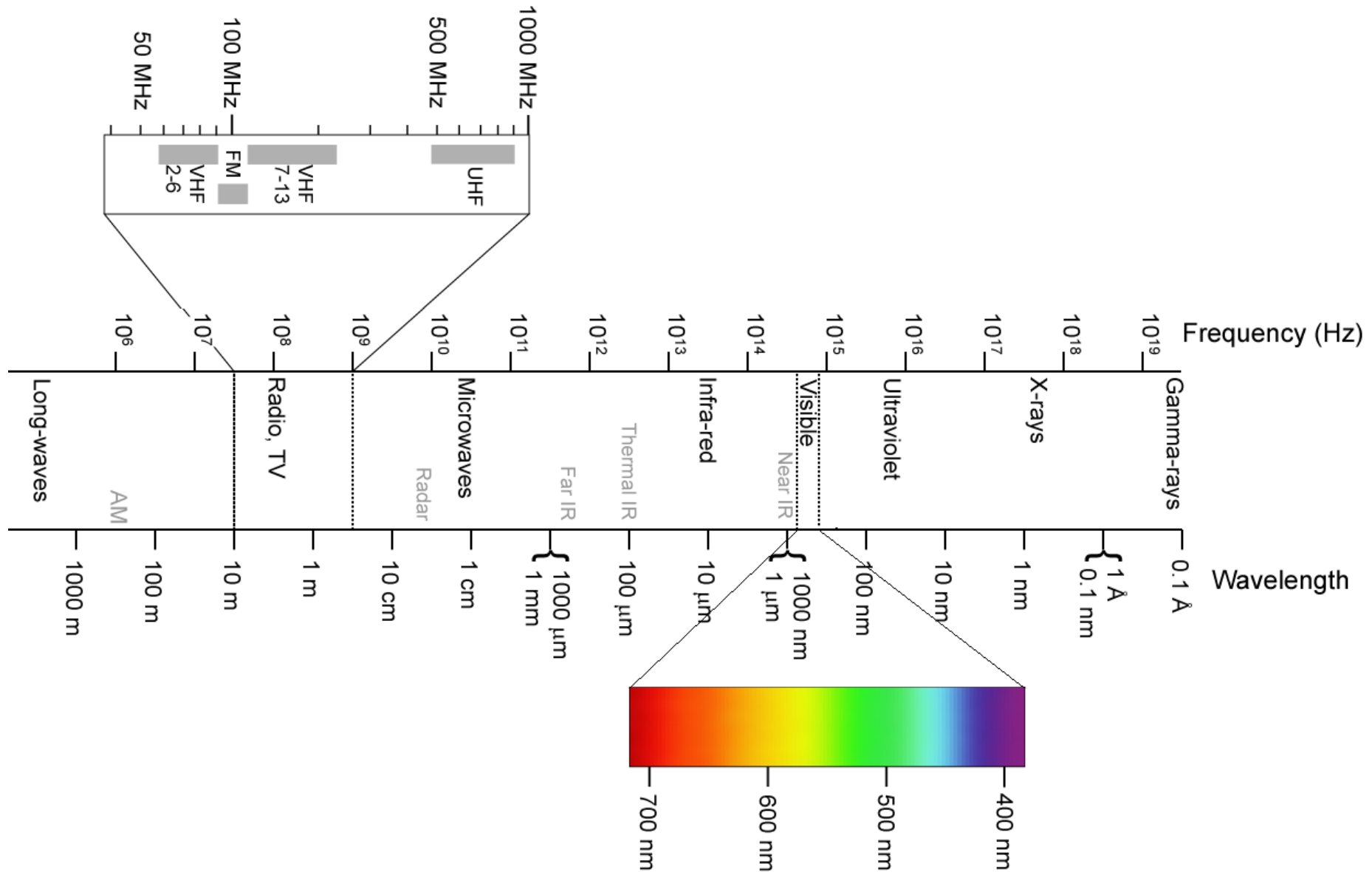


bi3 n pt

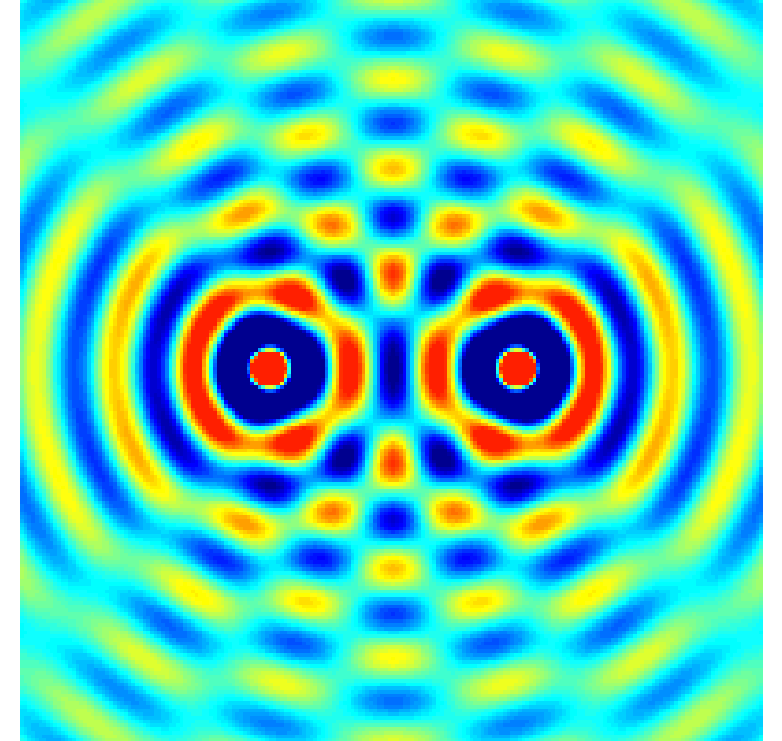
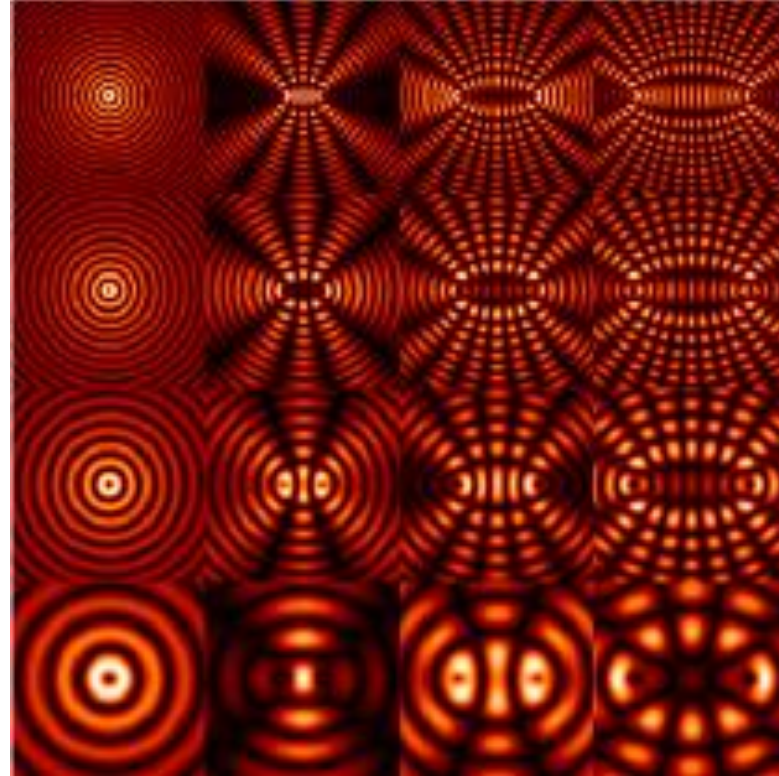
“sword of the heaven/sky”



Elektromanyetik spektrum



X-Işınımı Kırınımı





Tarihçe: **29 NOBEL ÖDÜLÜ**

1901 Nobel Fizik



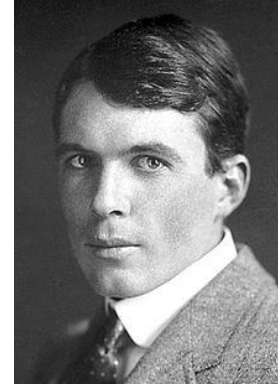
Wilhelm Conrad Röntgen

1914 Nobel Fizik

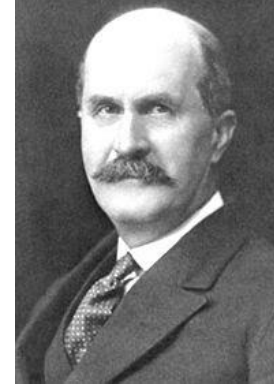


Max von Laue

1915 Nobel Fizik



William Lawrence Bragg



Sir William Henry Bragg

1917 Nobel Fizik



Charles Barkla

$$n\lambda = 2d \sin \theta$$

1962 Nobel Tıp



Francis Crick



James Watson

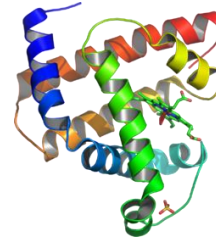


Maurice Wilkins

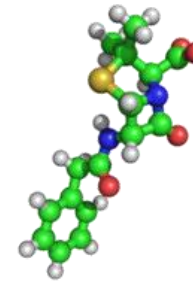
1962 Nobel Kimya



John Cowdery Kendrew



Myoglobin



Penisilin

1964 Nobel Kimya



Dorothy Hodgkin

Protein Data Bank



<http://www.rcsb.org/>



Structural Biology and Nobel Prizes **64**
Method-related Nobel Prizes **11**
Total: **75**

A Resource for Studying Biological Macromolecules

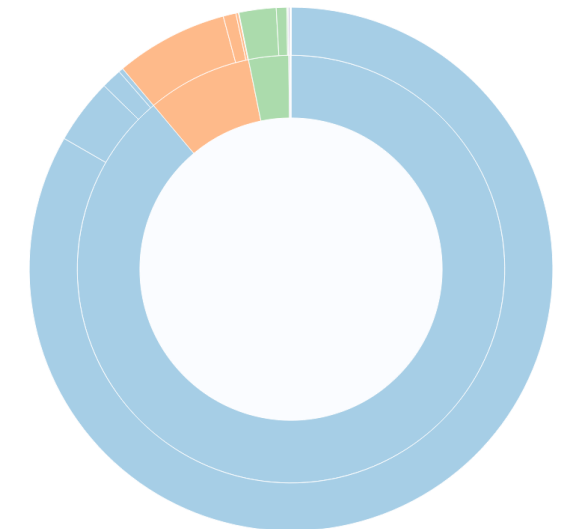
The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies

Protein Structure Prediction

Experimental

As of Tuesday May 12, 2020, there are 163362 Structures...

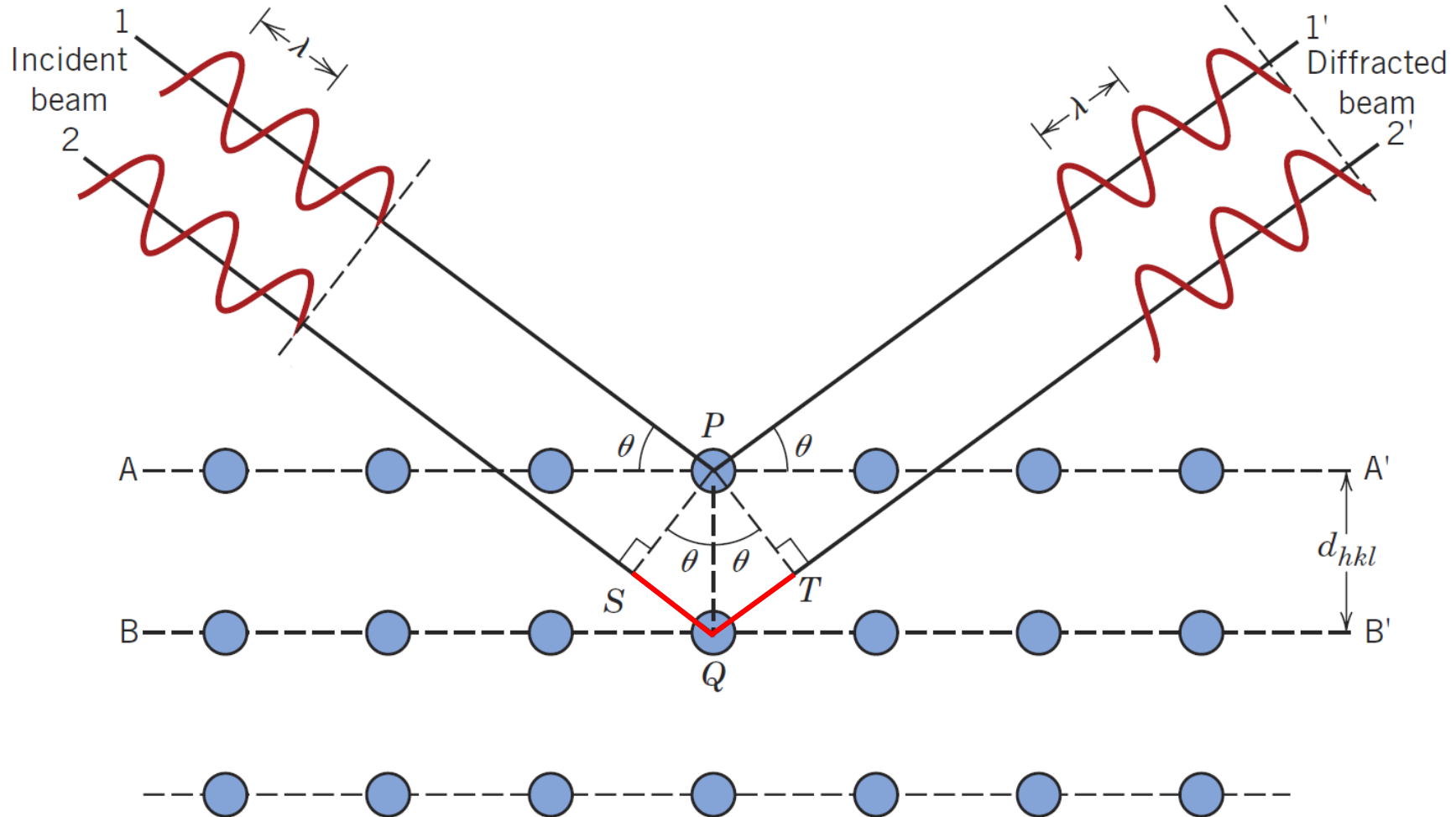
X-ray Crystallography	% 88.90	145437
Nuclear Magnetic Resonance	% 7.93	12973
Electron Microscopy	% 3.17	4952



BMM 310 Numerical Methods in Biomedical Engineering

<http://www.rcsb.org/structure/6WOJ>

X-Işınımı Kırınımı

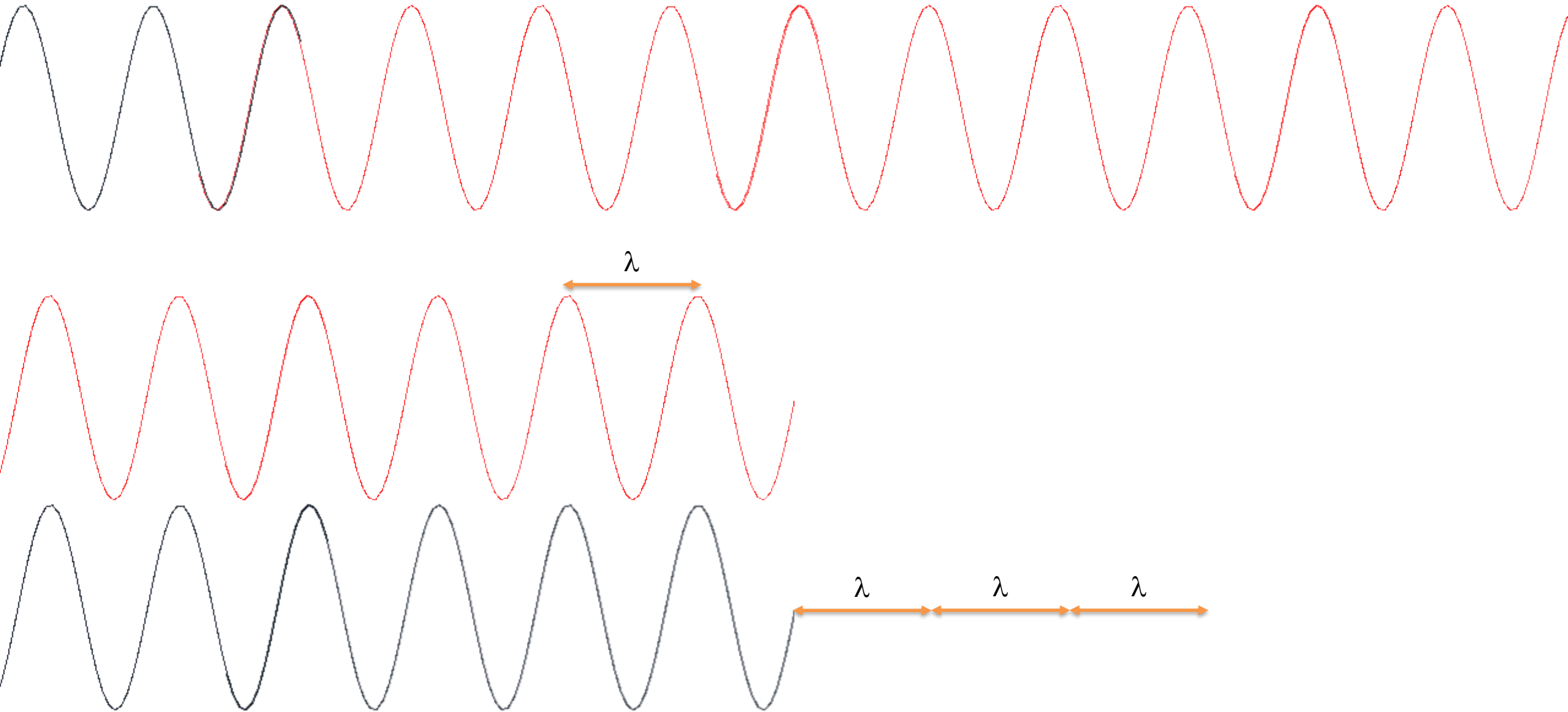


Bragg Kanunu: $n\lambda = 2d_{hkl} \sin \theta$

d_{hkl} : Düzlemler arası uzaklık

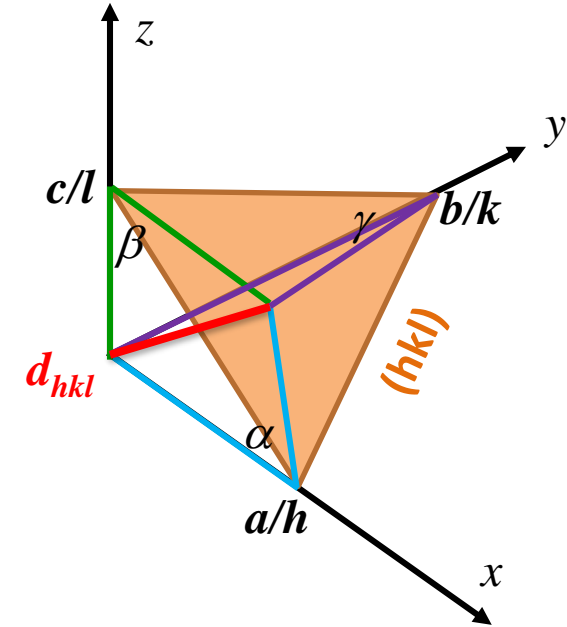
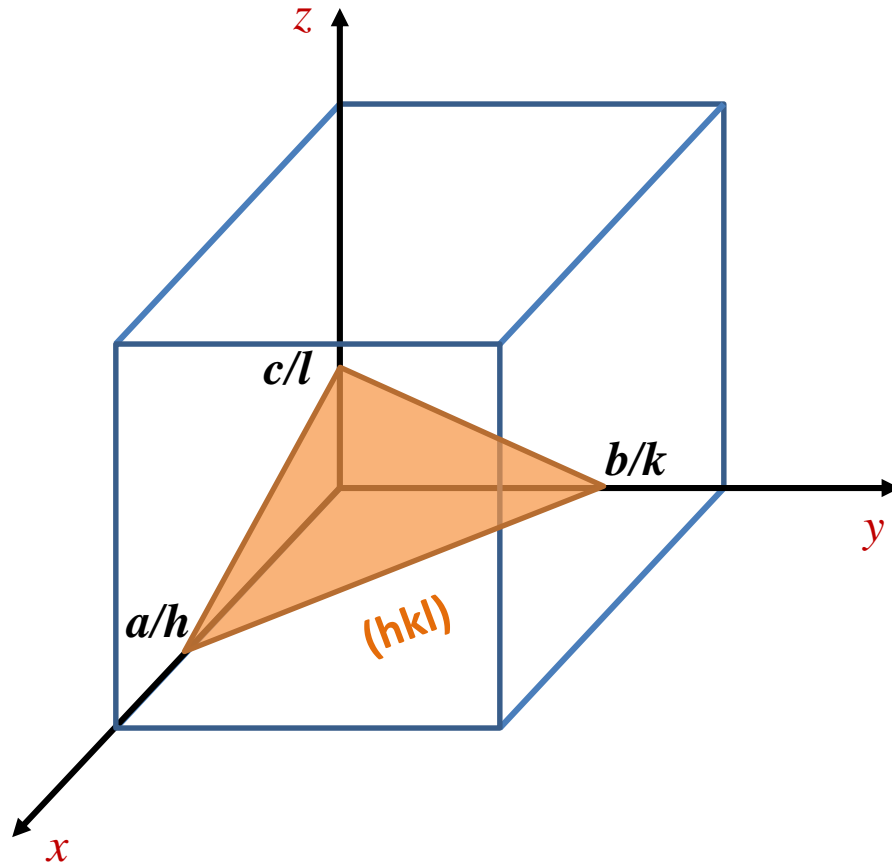
<https://www.youtube.com/watch?v=QHmzFUo0NL8>

X-Işınımı Kırınımı



X-IŞINLARI İLE KRİSTAL YAPI ANALİZİ

X-Işınımı Kırınımı d_{hkl} : Düzlemler arası uzaklık



Kesim Noktaları	a/h	b/k	c/l
Tersi	1/h	1/k	1/l
Miller indisleri	h	k	l

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$$

$$\left(\frac{d_{hkl}}{a/h}\right)^2 + \left(\frac{d_{hkl}}{b/k}\right)^2 + \left(\frac{d_{hkl}}{c/l}\right)^2 = 1$$

$$d_{hkl}^2 \left[\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2 \right] = 1$$

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

Kübik Kristallerin X-Işınımı Kırınımı olan Düzlemleri

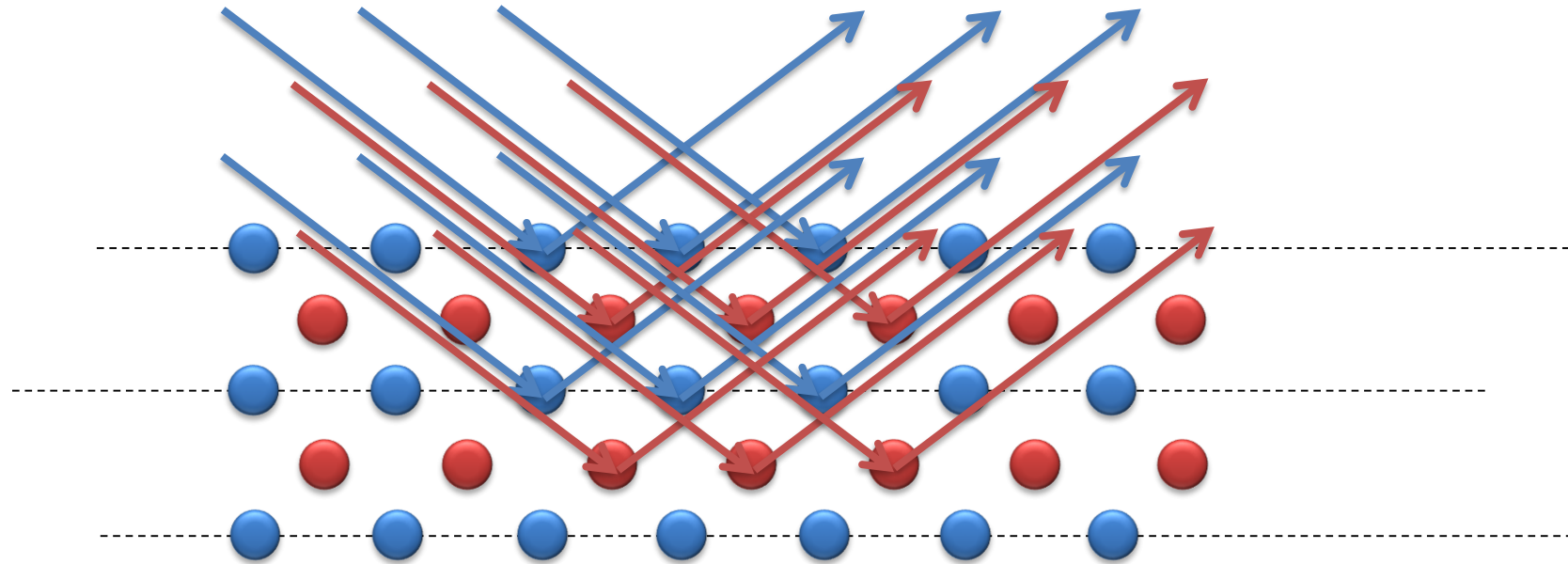
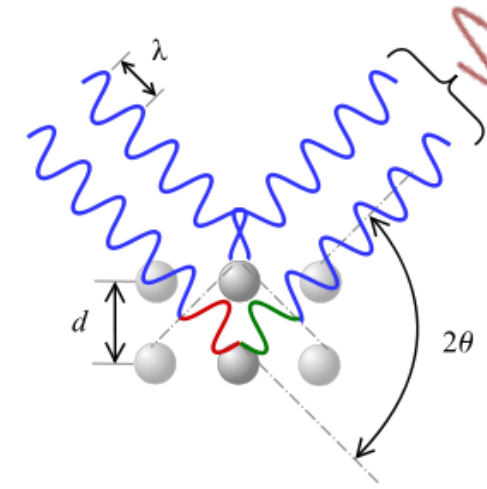
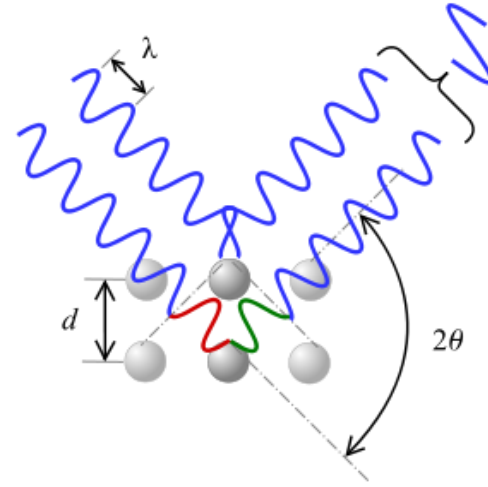
Kübik Kristaller:
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

	Kırınım Olur	Kırınım Olmaz
Basit Kübik (BK) (SC)	Hepsi	-
Hacim Merkezli Kübik (HMK) (BCC)	$(h+k+l)=\text{Çift}$	$(h+k+l)=\text{Tek}$
Yüzey Merkezli Kübik (YMK) (FCC)	$(h,k,l)=$ Hepsi çift veya hepsi tek	$(h,k,l)=$ Tek çift karışık

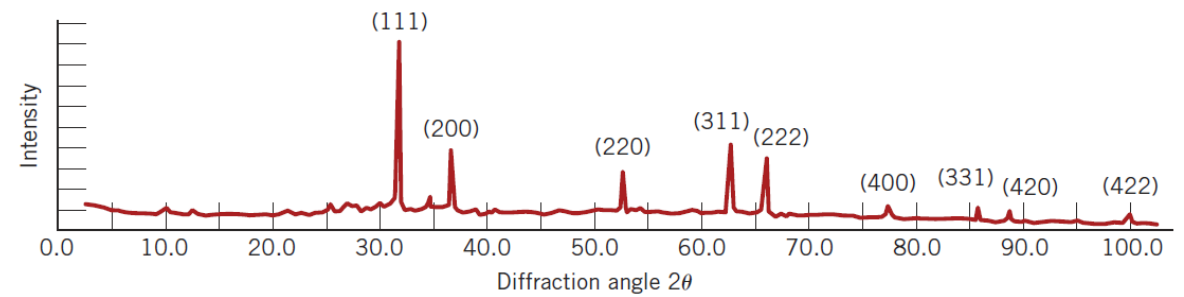
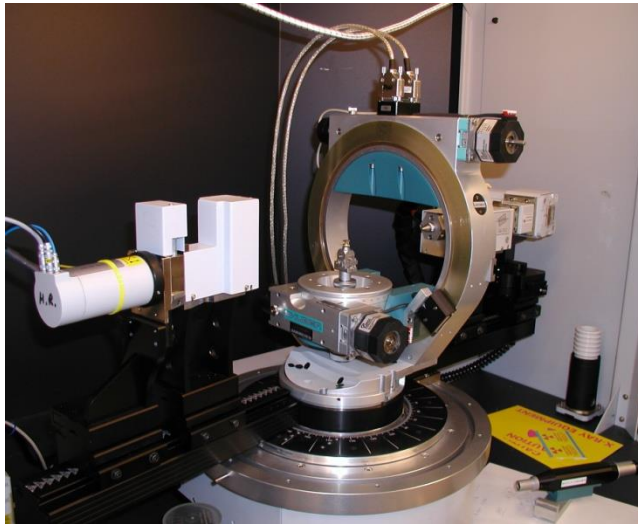
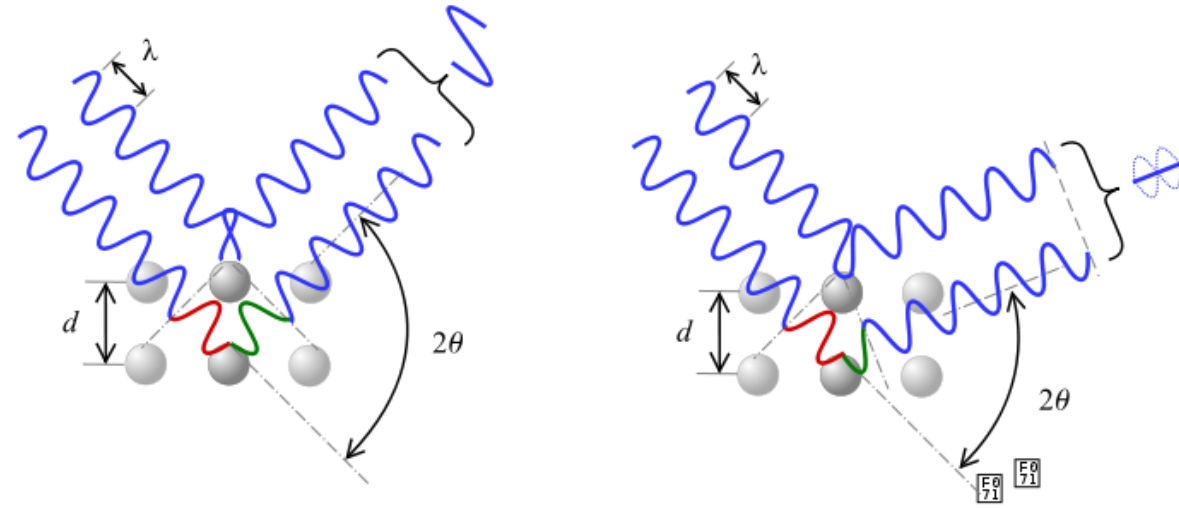
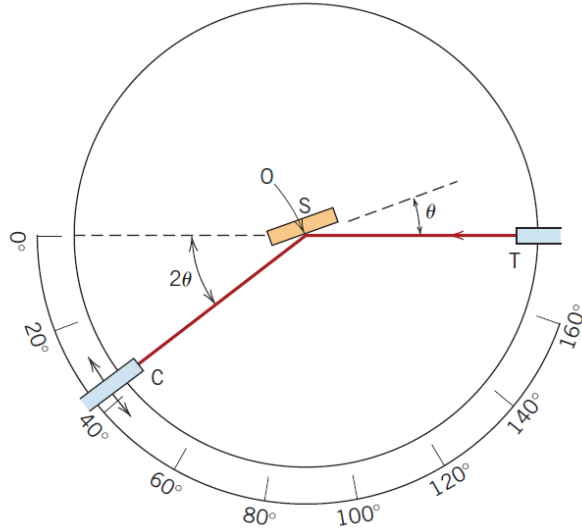
	BK	HMK	YMK
{100}	+	-	-
{110}	+	+	-
{111}	+	-	+

X-Işınımı Kırınımı

HMK {100}



x-ışınları difraktometresi



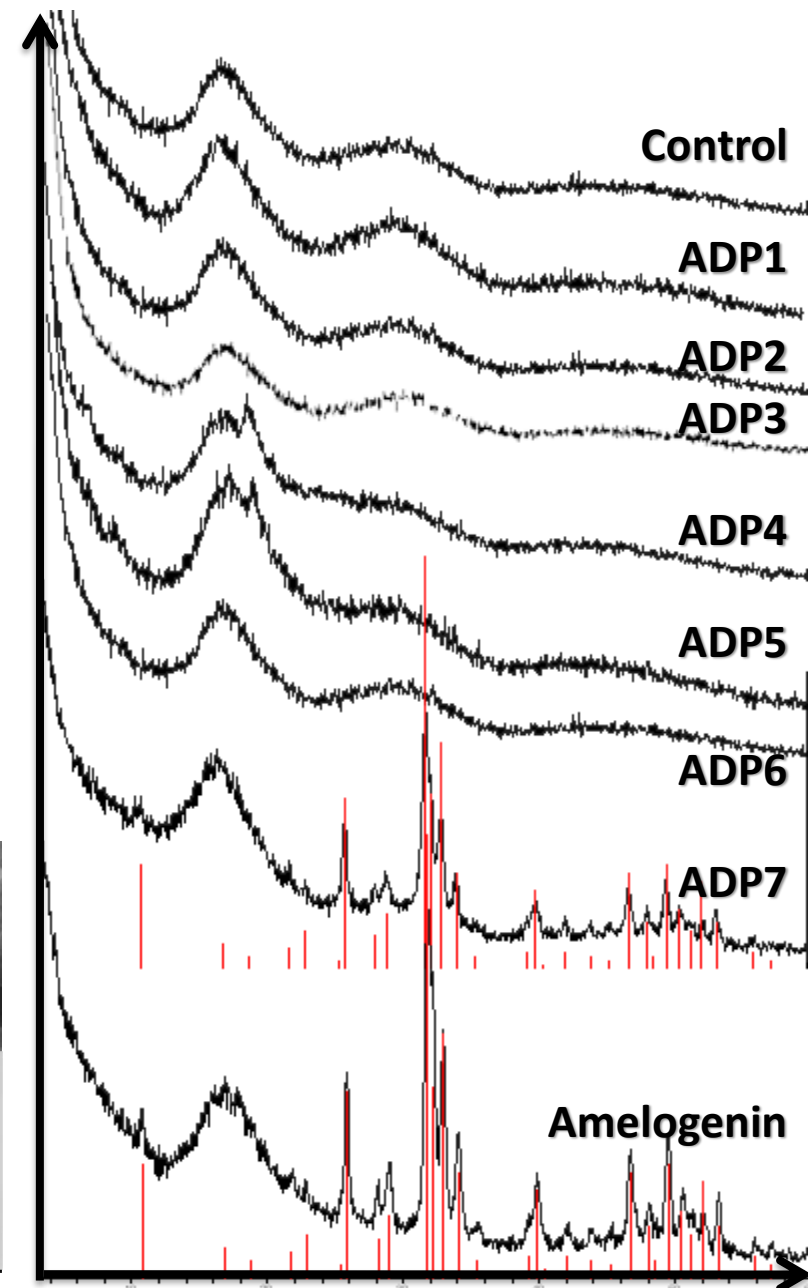
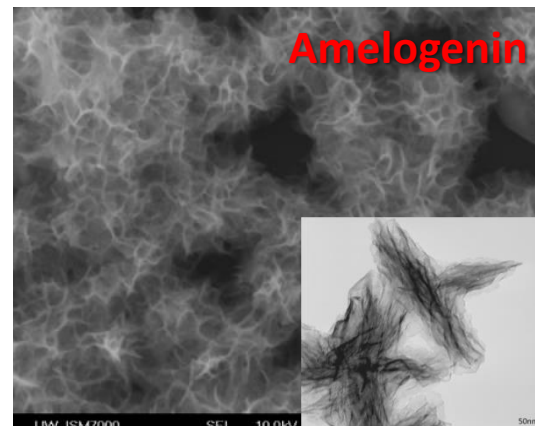
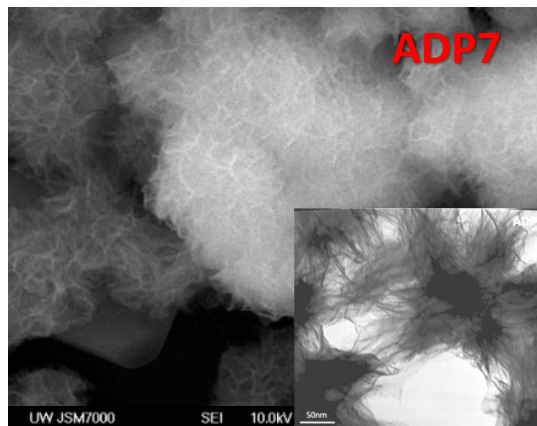
Toz Kurşun

Hangi Kübik Yapı: ?

Biominerallization



Cementomimetics-constructing a cementum-like biomineralized microlayer via amelogenin-derived peptides, *International Journal of Oral Science*, **4**, 69-77 (2012).



Kübik Kristallerin X-Işınımı Kırınımı olan Düzlemleri

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

Bragg Kanunu: $n\lambda = 2d_{hkl} \sin \theta$

$$h^2 + k^2 + l^2 = \frac{4a^2}{n^2 \lambda^2} \sin^2 \theta \quad \sin^2 \theta = \left(h^2 + k^2 + l^2 \right) \frac{n^2 \lambda^2}{4a^2} \quad \frac{\sin^2 \theta_A}{\sin^2 \theta_B} = \frac{\left(h_A^2 + k_A^2 + l_A^2 \right) \frac{n^2 \lambda^2}{4a^2}}{\left(h_B^2 + k_B^2 + l_B^2 \right) \frac{n^2 \lambda^2}{4a^2}}$$

$$\frac{\sin^2 \theta_A}{\sin^2 \theta_B} = \frac{h_A^2 + k_A^2 + l_A^2}{h_B^2 + k_B^2 + l_B^2}$$

	Kırınım Olur	Kırınım Olmaz
Basit Kübik (BK) (SC)	Hepsi	-
Hacim Merkezli Kübik (HMK) (BCC)	$(h+k+l)=\text{Çift}$	$(h+k+l)=\text{Tek}$
Yüzey Merkezli Kübik (YMK) (FCC)	$(h,k,l)=$ Hepsi çift veya hepsi tek	$(h,k,l)=$ Tek çift karışık

Kübik Kristallerin X-Işınımı Kırınımı olan Düzlemleri

Kübik Kristaller:

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

Bragg Kanunu:

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

$$\frac{\sin^2 \theta_A}{\sin^2 \theta_B} = \frac{h_A^2 + k_A^2 + l_A^2}{h_B^2 + k_B^2 + l_B^2}$$

No	Kırınım Düzlemi	BK SC	HMK BCC	YMK FCC	$h^2 + k^2 + l^2$	
1.	{100}	+	-	-	1	←
2. 1.	{110}	+	+	-	2	← ←
3. 1.	{111}	+	-	+	3	←
4. 2. 2.	{200}	+	+	+	4	← ←
5.	{210}	+	-	-	5	
6. 3.	{211}	+	+	-	6	
7. 4. 3.	{220}	+	+	+	8	
8.	{221} {300}	+	-	-	9	
9. 5.	{310}	+	+	-	10	
10. 4.	{311}	+	-	+	11	
11. 6. 5.	{222}	+	+	+	12	
12.	{320}	+	-	-	13	
13. 7.	{321}	+	+	-	14	

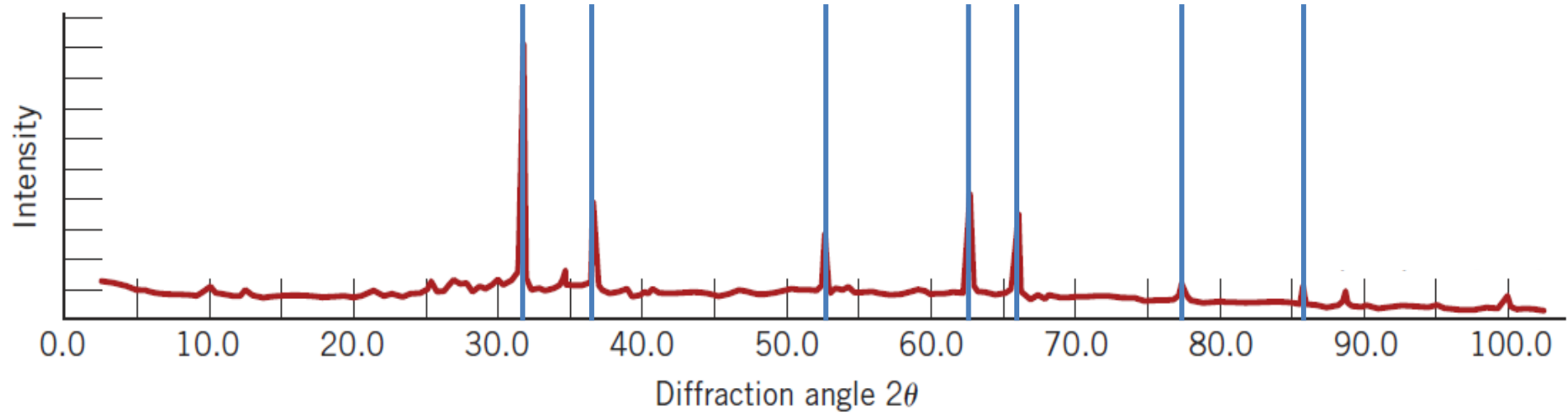


https://www.youtube.com/watch?v=lr_PDXyNu1E



<https://www.youtube.com/watch?v=lcYkOh4nweE>

Mars Exploration Rover Mission 1



$$\lambda = 1.5761 \text{ \AA}$$

Kristal Yapı:

Kafes Parametresi:

Atom Yarıçapı:

Element:

Peak	2θ
1.	31.9
2.	36.8
3.	53.3
4.	63.9
5.	66.0
6.	78.2
7.	86.0



Mars Exploration Rover Mission 1

Peak	2θ	θ	$\sin(\theta)$	$\sin^2(\theta)$	$h^2 + k^2 + l^2$
1.	31.9	15.95	0.275	0.0756	3
2.	36.8	18.40	0.316	0.0999	4
3.	53.3	26.65	0.449	0.2016	8
4.	63.9	31.95	0.529	0.2798	11
5.	66.0	33.00	0.545	0.2970	12
6.	78.2	39.10	0.631	0.3982	16
7.	86.0	43.00	0.682	0.4651	19

- $\frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.0756}{0.0999} = 0.757 \cong 0.75$

Kristal Yapı: YMK

$$\lambda = 1.5761 \text{ \AA}$$

Kristal Yapı:

Yüzey Merkezli Kübik

Kafes Parametresi:

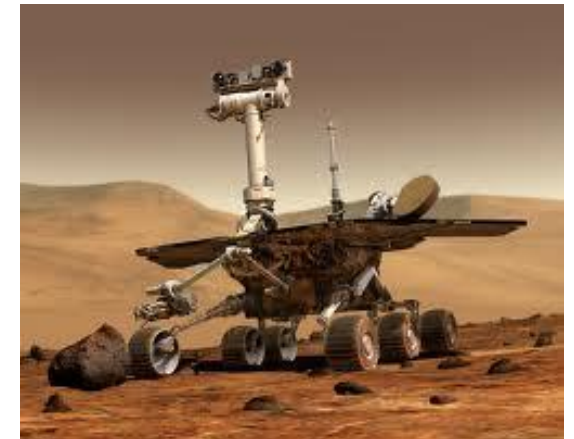
$$a = \sqrt{(h^2 + k^2 + l^2)} \frac{n\lambda}{2\sin\theta} = \sqrt{3} \frac{1.5761}{2 \times 0.275} = 4.963 \text{ \AA}$$

Atom Yarıçapı:

$$a\sqrt{2} = 4r \rightarrow r = \frac{a\sqrt{2}}{4} = 1.755 \text{ \AA}$$

Element:

Kurşun (Pb)



Mars Exploration Rover Mission 2

Peak	2θ	θ	$\sin(\theta)$	$\sin^2(\theta)$	$h^2 + k^2 + l^2$
1.	20.20	10.10	0.175	0.0308 •	2
2.	28.72	14.36	0.248	0.0615 •	4
3.	35.36	17.68	0.304	0.0922	6
4.	41.07	20.54	0.351	0.1230	8
5.	46.19	23.09	0.392	0.1539	10
6.	50.90	25.45	0.430	0.1847	12
7.	55.28	26.64	0.448	0.2152 •	14



- $\frac{\sin^2 \theta_1}{\sin^2 \theta_2} = \frac{0.0308}{0.0615} = 0.501 \cong 0.5$

Kristal Yapı: HMK veya BK

- $\frac{\sin^2 \theta_1}{\sin^2 \theta_7} = \frac{0.0308}{0.2152} = 0.143 \cong \frac{1}{7}$

$$\lambda = 0.7101 \text{ \AA}$$

Kristal Yapı:

Hacim Merkezli Kübik

Kafes Parametresi:

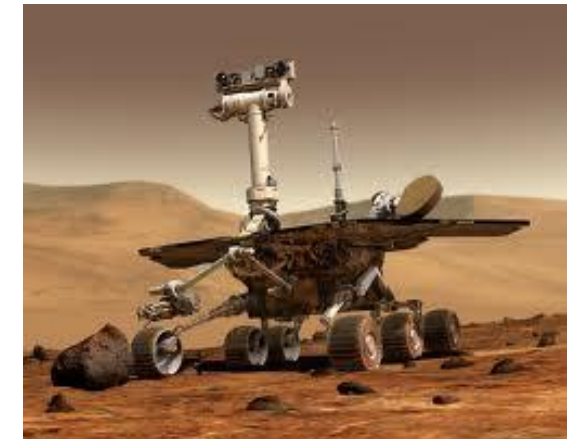
$$a = \sqrt{(h^2 + k^2 + l^2)} \frac{n\lambda}{2 \sin \theta} = \sqrt{2} \frac{0.7101}{2 \times 0.175} = 2.867 \text{ \AA}$$

Atom Yarıçapı:

$$a\sqrt{3} = 4r \rightarrow r = \frac{a\sqrt{3}}{4} = 1.242 \text{ \AA}$$

Element:

Demir (Fe)



Önümüzdeki Ders Saatinde
Ders Kitabımızın 4. Bölümündeki

KRİSTAL KUSURLARI

adlı konuya başlayacağız!