X-ray photon spectroscopy Calculations (lesson 2)

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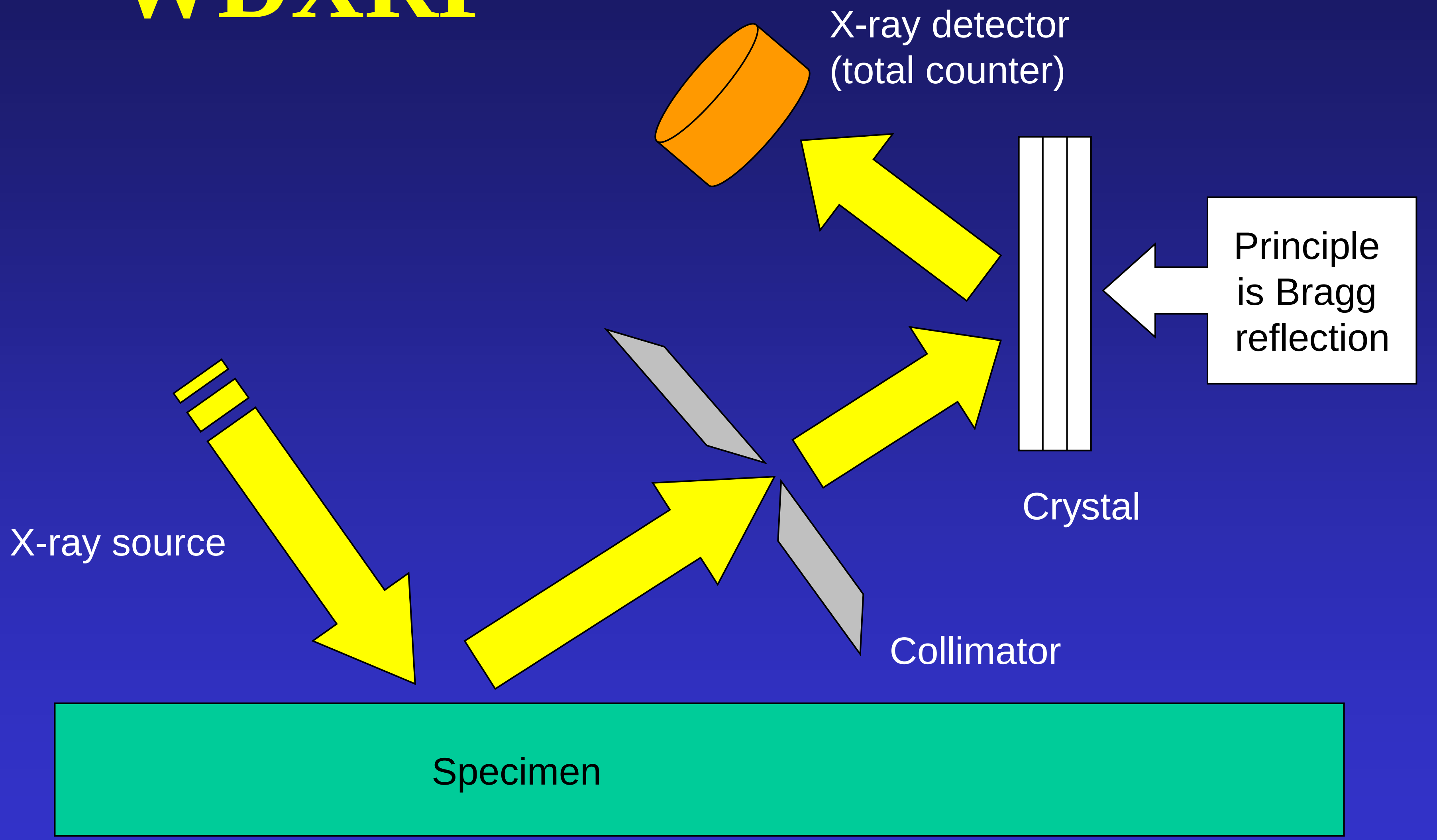
X-Ray Fluorescence

- Wavelength Dispersive XRF (WDXRF)
- Energy Dispersive XRF (EDXRF)

WDXRF


X-ray detector
(total counter)
Principle
is Bragg
reflection
Crystal
X-ray source
Collimator
Specimen

Bragg law (reflection of x-rays)

$$n\lambda = 2a\sin\vartheta$$

where:

a: distance between crystalline planes
n: reflection order (n=1 corresponds to the higher order)
2 ϑ : angle between the incident and the reflected beams

Angular shift (Bragg)

For n=1 we have

$$\Delta\lambda = 2a\,\Delta(\sin\vartheta)$$
$$= 2a\cos\vartheta\,\Delta\vartheta$$

Example:

LiF Crystal (a=0.4028 10^{-9} m = 4.028 A)

ϑ = 45°

$$\lambda = 2a_{LiF}\sin 45^{o} = 5.6\text{A}$$

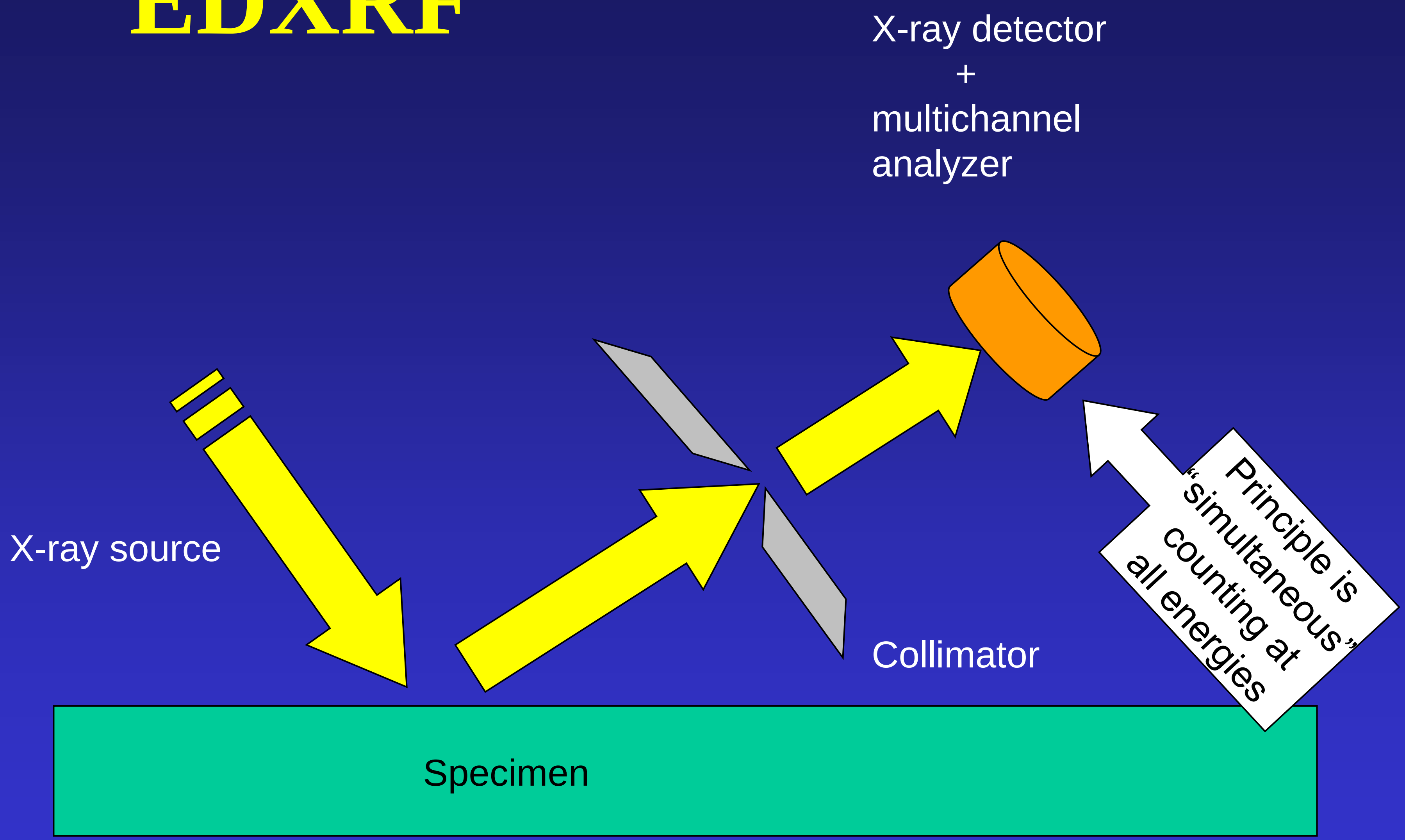
Useful data on crystals

Table 4.1 *Analysing crystals (Jenkins and de Vries, 1970)**

Crystal	Reflection Plane	2*d* Spacing (nm) 10^{-9} m	Lowest Atomic Number Detectable: K Series	Lowest Atomic Number Detectable: L Series	Reflection Efficiency
Topaz	(303)	0.2712	V(23)	Ce (58)	Average
Lithium Fluoride	(220)	0.2848	V (23)	Ce (58)	High
Lithium Fluoride	(200)	0.4028	K (19)	In (49)	Intense
Sodium Chloride	(200)	0.5639	S (16)	Ru (44)	High
Quartz	(10$\bar{1}$1)	0.6686	P (15)	Zr (40)	High
Quartz	(1010)	0.850	Si (14)	Rb (37)	Average
Penta erythritol	(002)	0.8742	Al (13)	Rb (37)	High
Ethylenediamine Tartrate	(020)	0.8808	Al (13)	Br (35)	Average
Ammonium Dihydrogen Phosphate	(110)	1.065	Mg (12)	As (23)	Low
Gypsum	(020)	1.519	Na (11)	Cu (29)	Average
Mica	(002)	1.98	F (9)	Fe (26)	Low
Potassium Hydrogen Phthalate	(10$\bar{1}$1)	2.64	O (8)	V (23)	Average
Lead Stearate		10.0	B (5)	Ca (20)	Average

* Additions to this list have been given by Jenkins (1972).

EDXRF


X-ray detector
+
multichannel
analyzer
X-ray source
Collimator
“Principle is
“simultaneous”
counting at
all energies
Specimen

WDXRF vs EDXRF

	λ	E
Spectrum measurement	Through angle variation (using Bragg law)	"simultaneous" at all the energies
Influence of source/detector instabilities	Is transferred on the single measurement	Is the same for all the spectrum
Misure on a wide range	May need several detectors and/or crystals	always uses the same detector

Equivalence wavelength-energy

For the conversion, the following relation is used:

$$E[keV] = hc/\lambda[A] = 12.39/\lambda[A]$$

Then, an x-ray spectrum intensity is converted as follows

$$I_\lambda(\lambda)\frac{hc}{E^2} = I_E(E)$$

where

$$\int_0^\infty I_\lambda(\lambda)\,d\lambda = \int_0^\infty I_E(E)\,dE$$