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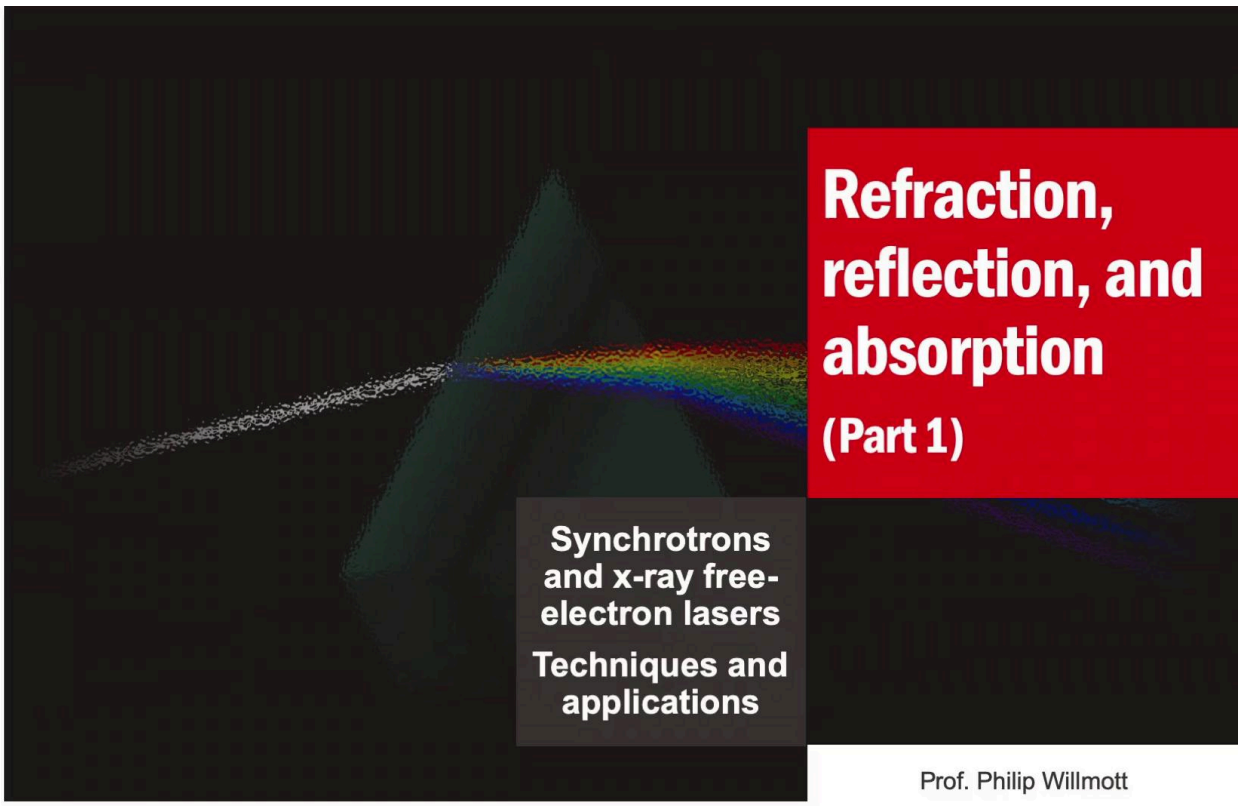


Refraction, reflection, and absorption

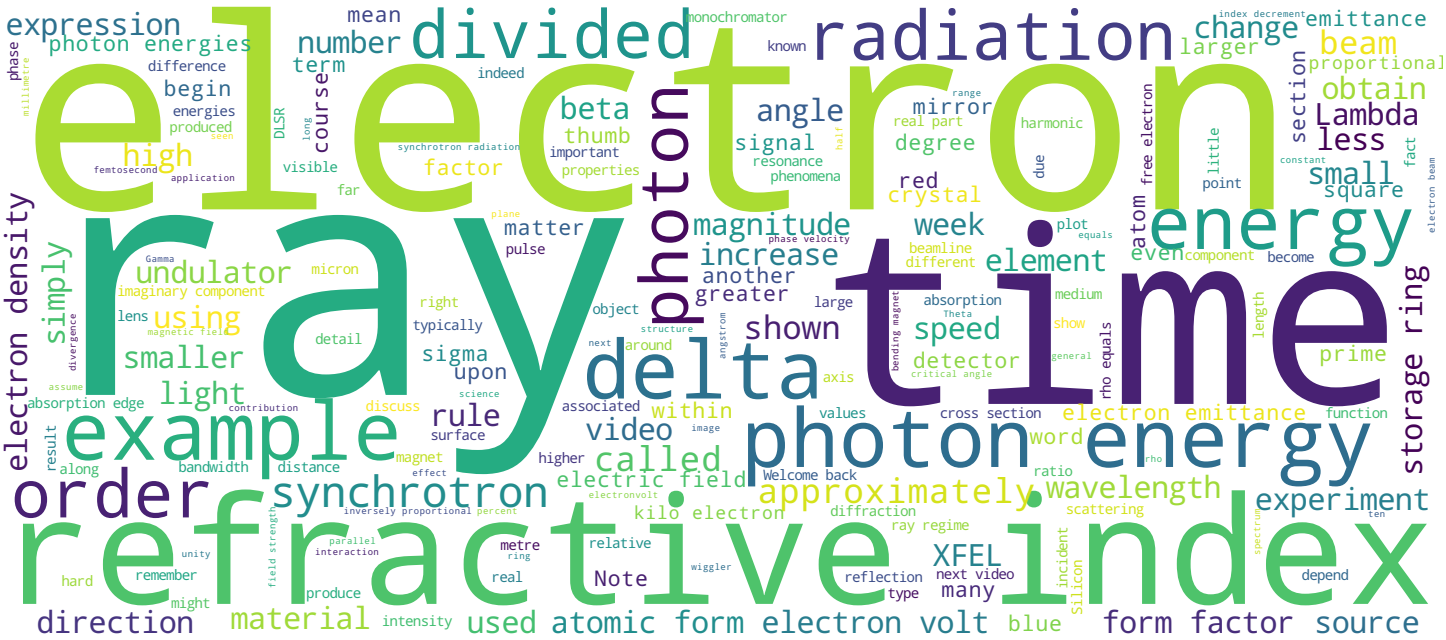
(Part 1)

Synchrotrons and x-ray free-electron lasers

Techniques and applications

Prof. Philip Willmott

École polytechnique fédérale de Lausanne



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Video

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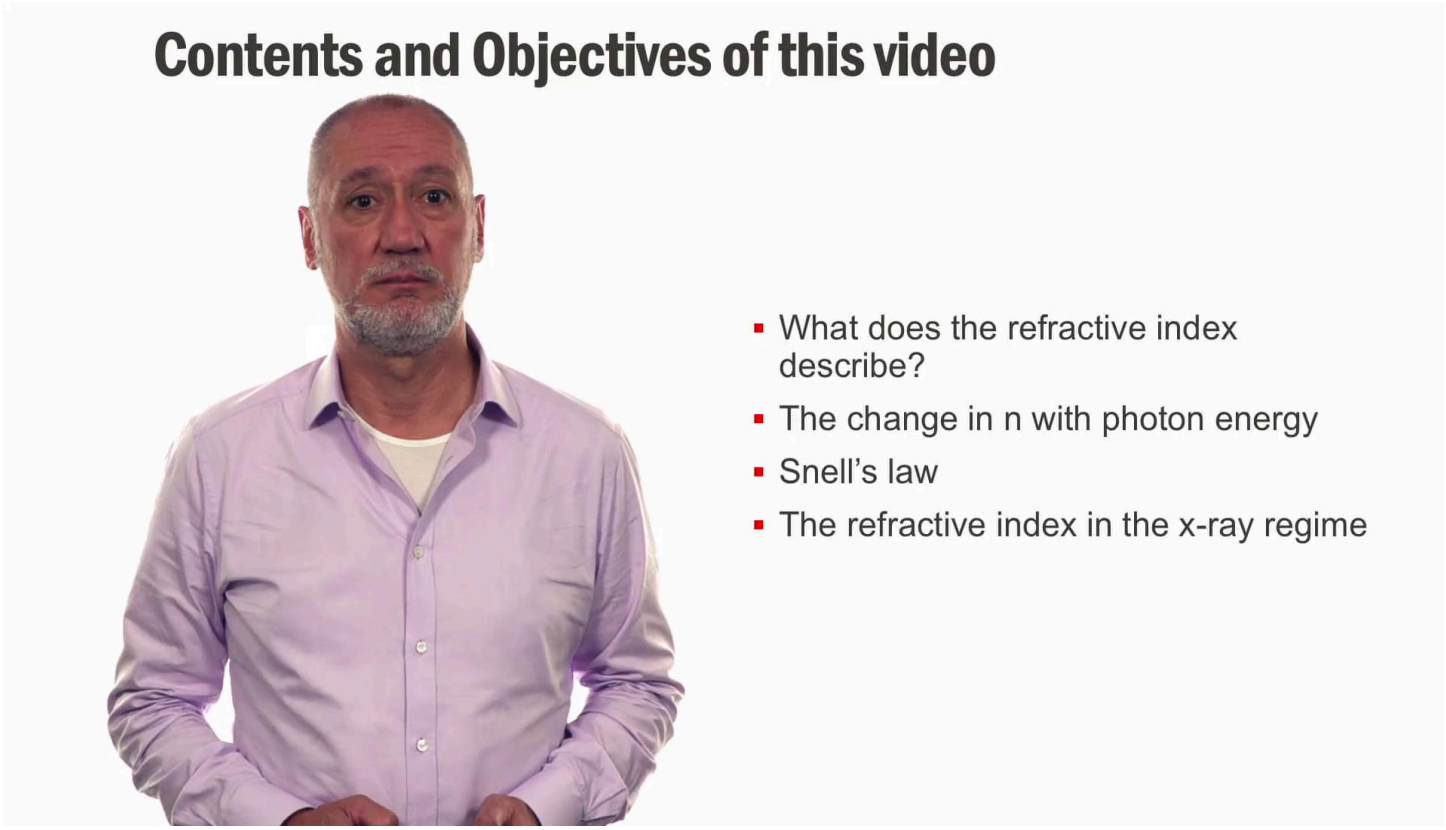


Hello and welcome back to the third section of week two of this course, Synchrotrons and X-ray Free-Electron Lasers. Techniques and Applications. In this section, we will discuss the phenomena of refraction, reflection and absorption in the X-ray regime. In this first video of this section, we consider what the refractive index describes, how it changes with photon energy, and how Snell's law determines refraction within the X-ray regime.

Notes

Summary

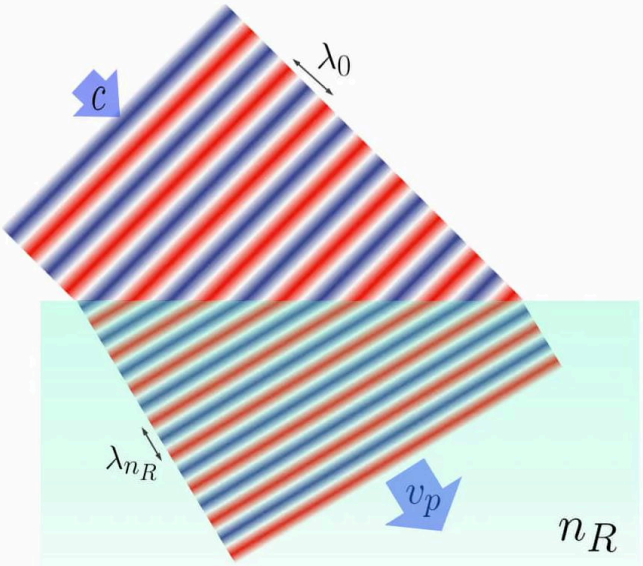
0m 05s

What does n exactly describe?

$$n_R = \frac{c}{v_p}$$

$$\lambda_{n_R} = \lambda_0 / n_R$$

$$\omega_{n_R} = \omega_0 \quad (\omega = 2\pi\nu)$$



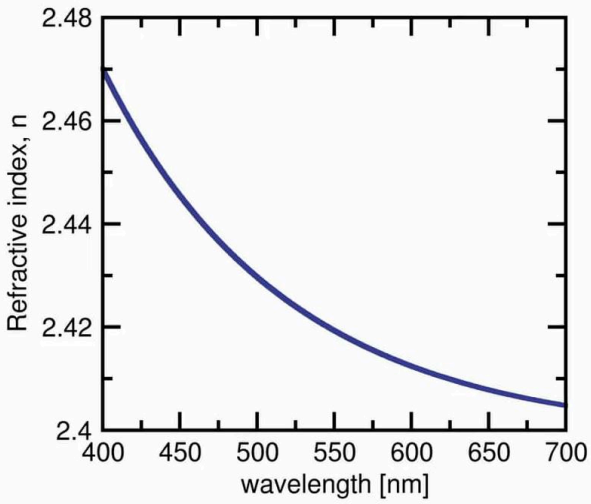
So how do the additional refinements to the atomic form factor affect the properties of X-rays travelling through matter? The phenomena we will be most interested in are refraction, reflection and absorption. We begin with refraction. We're all familiar at some level with refraction in the visual regime. Here, the wavelength of visible light is shortened because velocity is smaller in a transparent medium by a factor N known as the refractive index. And the light beams are bent to steeper angles when entering the medium. Here, we call the refractive index NR, because as we will soon discover, the refractive index has both a real and an imaginary component. NR is the real component of course.

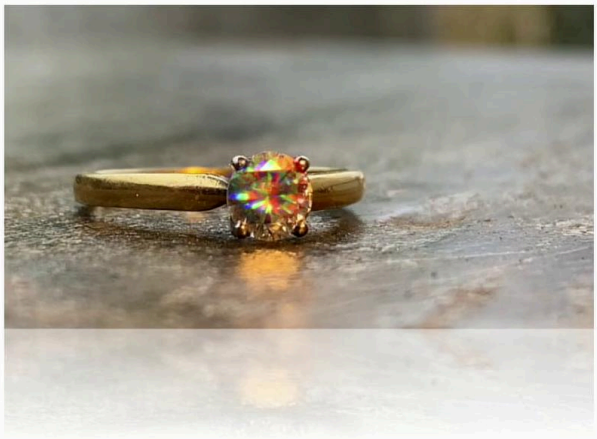
Notes

Summary

0m 35s

Refraction in the visible





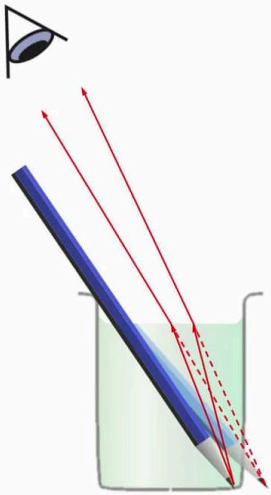
Typical values for N in the visible are, for example, approximately 1.33 for water or approximately 2.4 for diamond. Note also that diamond sparkles in a very characteristic manner due to significant dispersion of the refractive index across the visible from approximately 2.4 in the red to 2.47 in the blue, which causes this rainbow effect.

Notes

Summary

1m 33s

Refraction in the visible



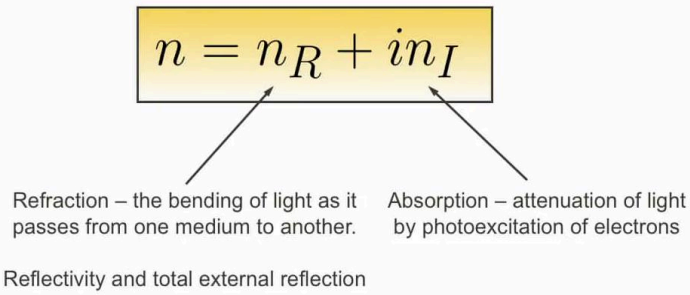
This simple concept explains why, for example, an object partially in water seems to be abruptly bent at the air-water interface. Shown step for step here.

Notes

Summary

1m 59s

What does n exactly describe?



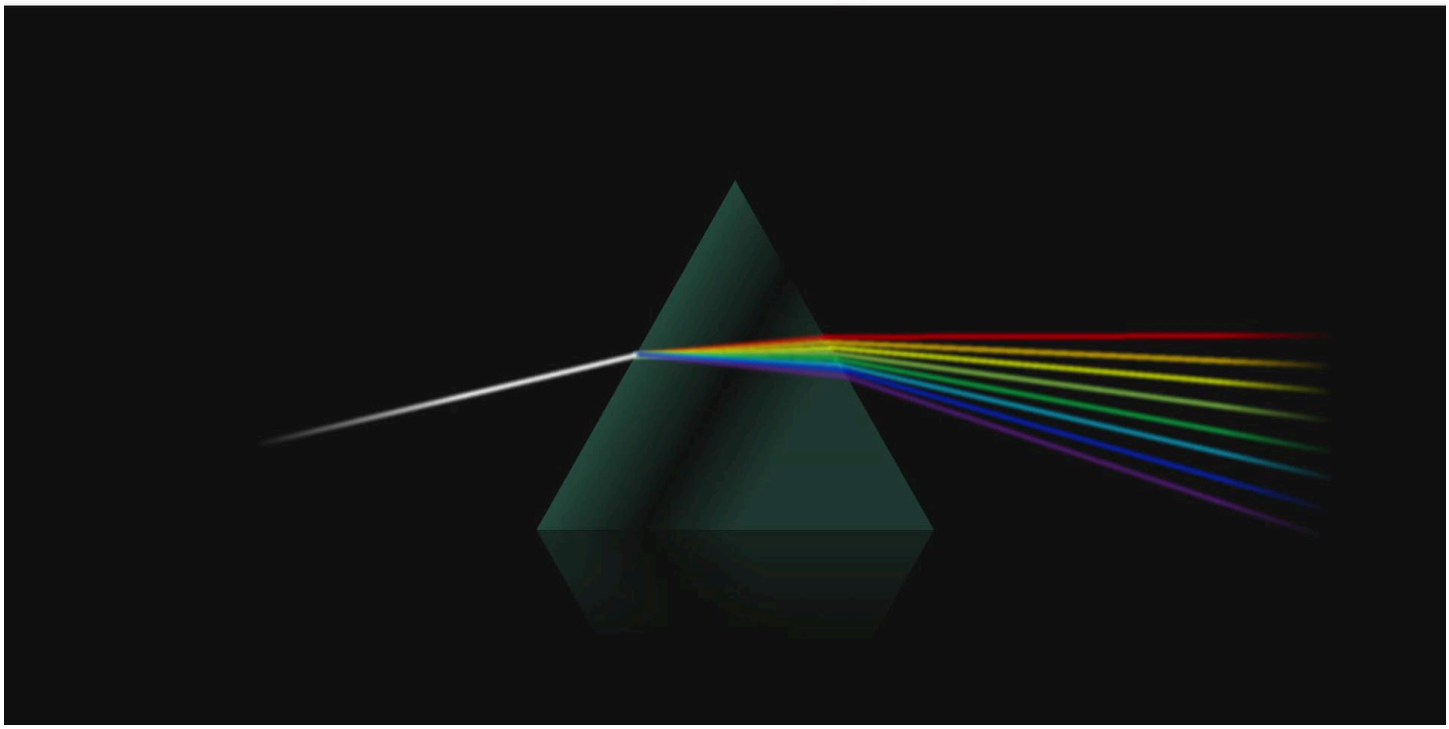
For many of you, you know the refractive index as a single number. I have already said, for example, that the refractive index of water in the visible is about 1.33. This doesn't tell the whole story, however, as this number only describes refraction, the bending of light as it passes from one medium to another and as we shall shortly see also reflection. In fact, the refractive index is a complex number with a real and imaginary component. The real part is a more familiar number describing refraction, while the imaginary part, provides the necessary information to describe absorption.

Notes

Summary

2m 17s

Change in n with photon energy



The refractive index changes with photon energy. We are all familiar with the effect of a prism in dispersing white light. The blue and violet end of the spectrum is refracted more strongly than the red end.

Notes

Summary

3m 03s

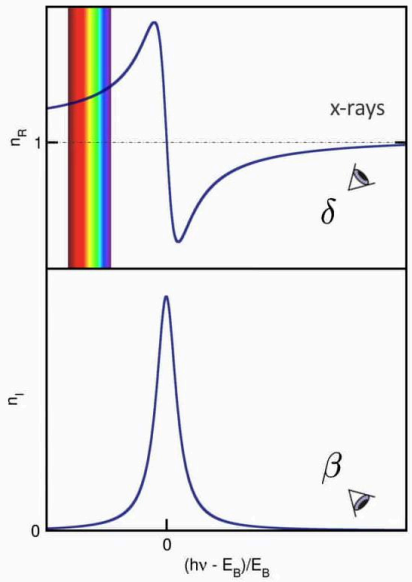
Refractive index in the x-ray regime

$$n^2 = 1 + \left(\frac{e^2\rho}{\epsilon_0 m_e \omega^2}\right) \frac{1}{\left(\frac{\omega_B}{\omega}\right)^2 - 1 - \frac{i\Gamma}{\omega}}$$

$$n = 1 - \delta + i\beta$$

$$n_R = 1 - \delta$$

$$n_I = \beta$$



See also derivation of the equations for n_R and n_I in the supplementary text "The complex refractive index"

Now, the refractive index of a medium described by a model in which the bound electrons are forced into damped oscillations by a driving electromagnetic field, yields the frightening-looking expression, shown upper left here, The plots for the real and imaginary components of N according to this expression, are shown here on the right. Below resonance at EB equals H bar omega B. we are in the visible regime. For photon energies well above resonance, the refractive index can be simplified to N is equal to one minus delta plus I times beta, where both delta and beta are small numbers. Delta is called the refractive index decrement, while beta is the absorption index. Exactly how small these terms are, we shall find out in a moment. Note that below the resonance, the real part of the refractive index is greater than one, while above the resonance it's less than unity. For those of you who would like to understand the physics behind the description of the refractive index more deeply, and how we came to this simple expression from our original equation, a detailed derivation is given in the accompanying supplementary text, The Complex Refractive Index.

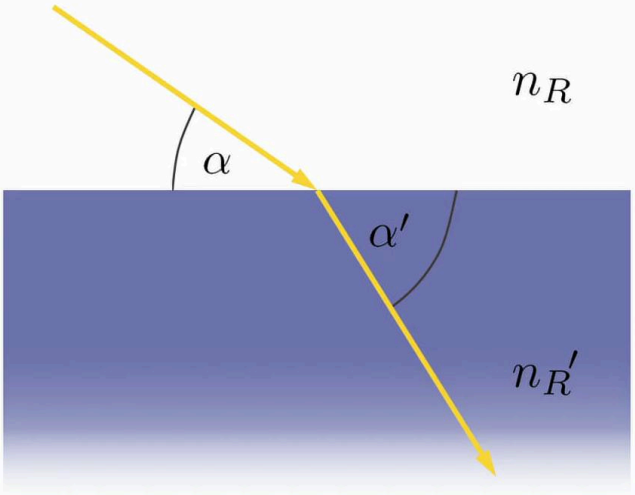
Notes

Summary

3m 18s

Snell's law

$$\frac{\cos\alpha}{\cos\alpha'} = \frac{n_R'}{n_R}$$



The changes in angle of light travelling across a heterogeneous interface is given by Snell's law shown here for a beam of radiation travelling from a medium with a smaller real part of the refractive index to one with a larger NR.

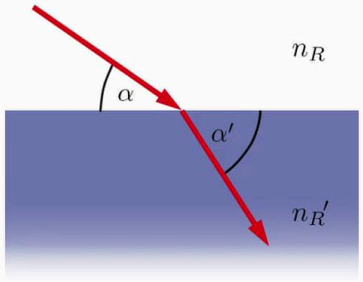
Notes

Summary

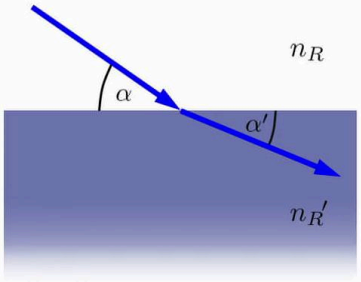
4m 46s

Refractive index in visible v x-rays

- Visible
  - $n_R > 1.0$
  - Light bent to steeper angles when entering denser medium
  - Most (normally all) electrons have binding energies > hν



- X-rays
  - $n_R = 1 - \delta < 1.0$
  - Light bent to *shallower* angles when entering denser medium
  - Most (often all) electrons have binding energies < hν



BUT: $v_p = c/n_R > c$… Really?? Yes!!

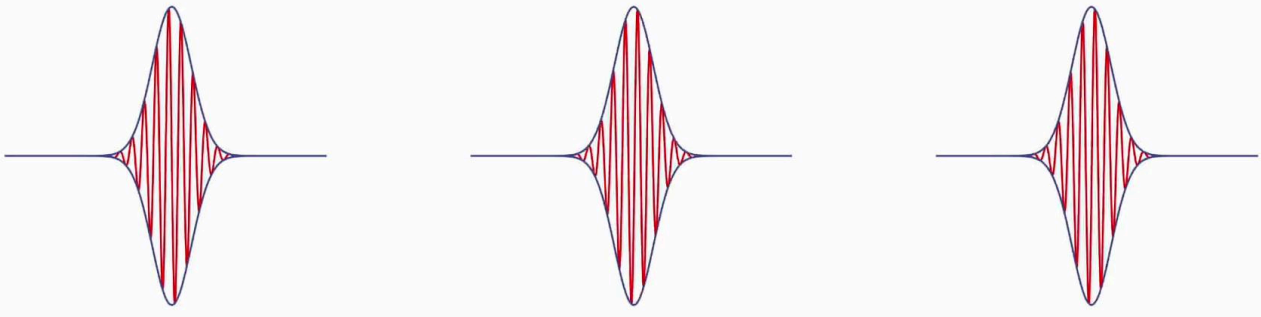
Because matter has refractive indices that are greater than one in the visible and less than one in the X-ray regime, we can expect different refraction effects. In the visible, light is bent to steeper angles when passing from a lighter to a denser medium. For X-rays, the opposite is true, as a refractive index of matter is less than unity. This might start alarm bells ringing, as it seems to imply that the velocity of X-rays in the medium equal to C divided by NR is greater than C the speed of light. Well, this is actually true. But it's the phase velocity VP, which it exceeds C. Before we continue with our discussion of the refractive index for X-rays, we briefly address the difference between phase velocities and group velocities.

Notes

Summary

5m 04s

Phase and group velocities



X-rays in matter: $v_p = c/n_R > c$; $v_g = n_R c < c$

Shown here are three light pulses propagating to the right. In vacuum, the crests and troughs of the electromagnetic wave travel at the same speed as the envelope Gaussian pulse. In a medium though, the crests and troughs can move faster than the envelope, as shown in the middle. The speed of the crests and troughs is the phase velocity, while that of the Gaussian envelope is the group velocity. For X-rays, it is the group velocity that carries the energy, and this is equal to NR times C, which is smaller than the speed of light. For completeness, I also show the case in which the phase velocity is slower than the group velocity, in which case the former slipped backwards relative to the latter. We will not need to concern ourselves with such a situation in this course, however.

Notes

Summary

6m 04s

Refractive index in the x-ray regime

$$n = 1 - \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_i(0)$$

$f = f_1 + if_2$ Complex quantity

atoms/unit volume

$$n = 1 - \delta + i\beta$$

$Z_i + f_i'$

$$\delta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{1,i}(0) \qquad \beta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{2,i}$$

$$\delta \propto (h\nu)^{-2}$$

See also derivation of the equations for n_R and n_I in the supplementary text "The complex refractive index"

It turns out that the refractive index is given by this expression, Fi(0) is the complex atomic form factor for Q equals zero. In other words, in the forward sketching direction, while Ni is the number density of atom type I. Again, take a closer look at the supplementary text, The Complex Refractive Index. Now we've just stated that N is equal to one minus delta plus I beta. Hence by separating the real and imaginary parts of both of these expressions, we obtain this expression for delta, whereby we only consider the real part of the atomic form factor, Zi plus F1i(0). The sum of Nif1i(0) is simply the electron density as seen by the X-rays. Remember from the last section of this week that this is not necessarily the same as the physical electron density due to possible destructive interference between the incident and scattered radiation. Here is the expression for beta, which only includes the magnitude of the imaginary components of the atomic form factor, F2i. It's noted that assuming that we are far from an absorption edge and the summation in our expression for delta, is indeed equal to the physical electron density, then the only variable is lambda. Which implies that delta is inversely proportional to the square of the photon energy. This is an important relationship to remember for later in this course.

Notes

Summary

7m 01s

How big are δ and β?

- Why do we need to know these?
  - Reflectivity properties
  - Absorption properties
  - Transmission properties
- Make simple assumptions
  - $h\nu \gg E_B$
  - Ignore absorption edges
  - Use elements as examples
    - Compound materials act similarly
  - Values correct to factor 2 - 3

So let's try to calculate the magnitudes of delta and beta as these will provide information about the reflectivity, absorption and transmission properties of X-rays in matter. We make the assumption that the photon energies are significantly larger at any electron binding energy in the material and can thus ignore absorption edges. We will use elements as examples, but extension to compound materials is trivial, and the values are anyway accurate to within a factor of two or three.

Notes

Summary

8m 41s

How big is δ?

$$\delta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{1,i}(0)$$

Z_i ≃ ρ

$4.49 \times 10^{-6}\ (\lambda\ [\text{Å}])^2$

Let's begin with the refractive index decrement delta. The factor shown in red is equal to 4.49 times 10 to the minus six, times the wavelength expressed in angstroms squared. F1i(0) is equal to Z minus any dumping term F prime. But we agreed we would assume that the photon energy was far from an absorption edge. So we can set F prime to zero. The summation is therefore simply equal to the electron density of the material. This holds true for elements or compounds for which I is greater than one. Can we generate a rule of thumb for the electron density rho?

Notes

Summary

9m 13s

How big is δ?

$$\delta = \frac{r_0}{2\pi}\lambda^2 \underbrace{\sum_i N_i f_{1,i}(0)}_{\simeq \rho}$$

Z_i

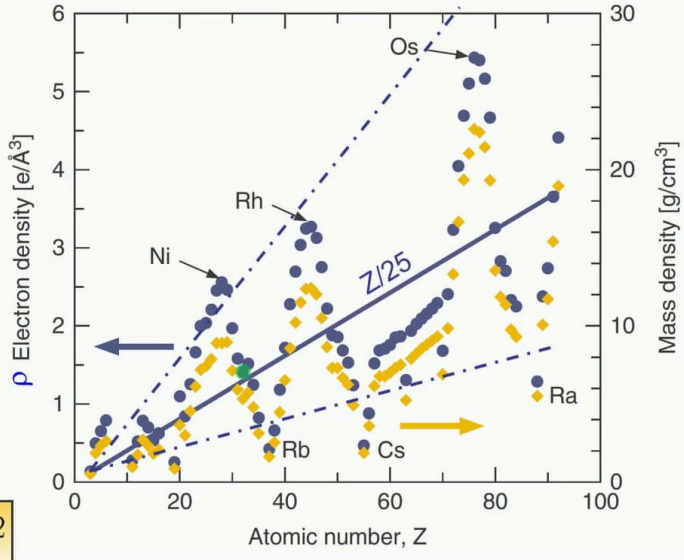
$4.49 \times 10^{-6}\ (\lambda\ [\text{Å}])^2$

$\delta = 1.8 \times 10^{-7}\ (\lambda\ [\text{Å}])^2\ Z$

$\delta = 2.77 \times 10^{-5}\ Z/(E\ [\text{keV}])^2$

e.g. Ge, Z = 32, 2 Å:
RoT: $\delta = 2.3 \times 10^{-5}$
CXRO: $\delta = 2.42 \times 10^{-5}$

$$\delta \propto Z/(h\nu)^2$$



Here is a plot for rho, for all the condensed matter elements at room temperature and pressure up to uranium. The electron density is given in blue, and the mass density also given in gold. Both show very similar dependencies with respect to Z. The oscillations reflecting the periodic qualities of the elements in the periodic table. The best linear fit to rho, is rho equals Z upon 25. Although this is only very approximate, it's good to a factor of two or three. The dash lines for rho equals Z upon 50 and rho equals Z upon twelve and a half encapsulate over 80 percent of the elements. We can therefore combine our expression for the factor in red with our approximation of rho equals Z upon 25 to obtain a rule of thumb, delta equals 1.8 times 10 to the minus seven times lambda in angstrom squared times Z. Or expressed instead as a function of the photon energy, delta equals 2.77 times 10 to the minus five times Z divided by E expressed in kilo electron volts squared. Using this rule of thumb, we obtain, for example, for Germanium and an X-ray wavelength of two angstroms, a value for delta of 2.3 times 10 to the minus five. The precise number which can be calculated or simply found at the CXRO website is 2.42 times 10 to the minus five.

Notes

Summary

10m 03s

How big is δ?

$$\delta = \frac{r_0}{2\pi}\lambda^2 \underbrace{\sum_i N_i f_{1,i}(0)}_{\simeq \rho}$$

Z_i

$4.49 \times 10^{-6}\ (\lambda\ [\text{Å}])^2$

$\delta = 1.8 \times 10^{-7}\ (\lambda\ [\text{Å}])^2\ Z$

$\delta = 2.77 \times 10^{-5}\ Z/(E\ [\text{keV}])^2$

e.g. Ge, Z = 32, 2 Å:
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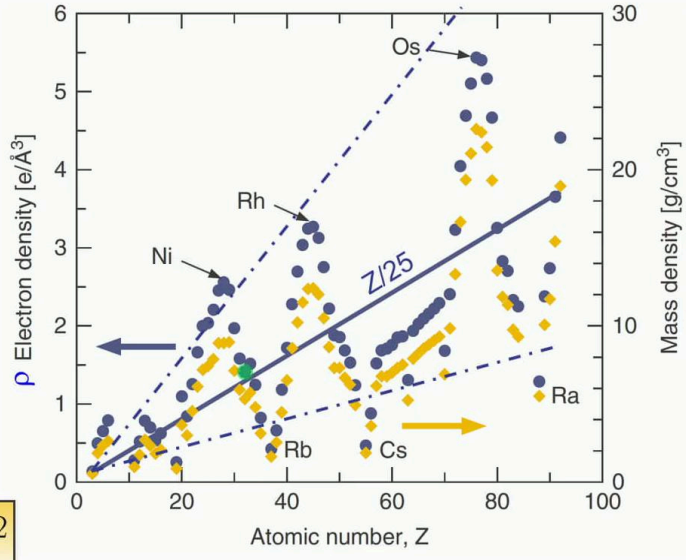
$$\delta \propto Z/(h\nu)^2$$



Take-home message: even for high Z and low photon energies, $\delta \ll 1$

Only about 5 percent different. Note that the rule of thumb is proportional to Z and inversely proportional to the square of the photon energy. Lastly, from the numbers obtained it should be clear that delta is much smaller than unity, even for high Z and low photon energies. For example, the effective index decrement of tungsten, which has an atomic number of 74, is at one-kilo electron volt, still only two times 10 to the minus three.

Notes

Summary

11m 37s

How big is β?

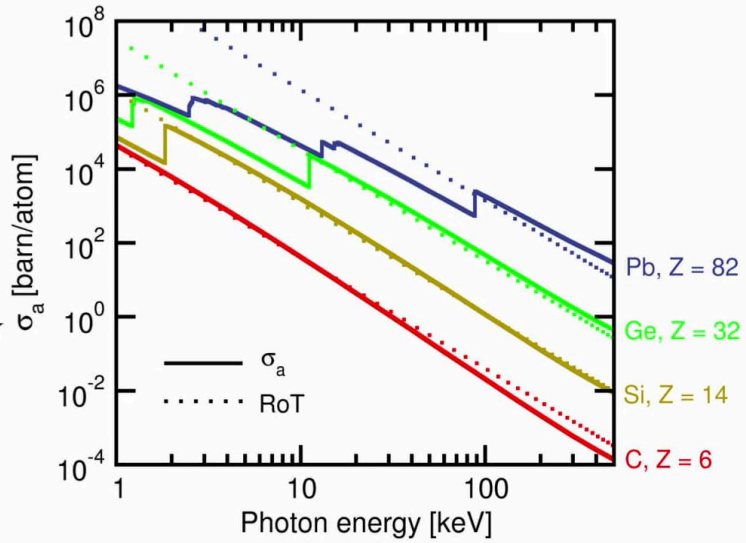
$$\delta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{1,i}(0)$$

$$\beta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{2,i}$$

$$\frac{\delta}{\beta} = \frac{Z}{f_2}$$

$$f_2 = f'' = \frac{\sigma_a}{2\lambda r_0}$$

$$\beta = \frac{f_2\delta}{Z} = \frac{\sigma_a\delta}{2r_0 Z\lambda}$$



$$\sigma_a[\text{barn/atom}] = 30\frac{Z^4}{(h\nu[\text{keV}])^3}$$

So now let's proceed to the absorption index beta. First, from our two expressions for beta and delta, we obtain a ratio for them equal to Z divided by F2, the magnitude of the imaginary component of the atomic form factor. So now let's look at F2 to see if we can make some generalizations here as well. I have already stated that F2 is equal to sigma A divided by two lambda R(0). So let's look again at the photo absorbing cross-section sigma A. In the first video of this week, we saw that Z drops off as the third inverse power of the photon energy and increases as Z to the fourth. Above the highest energy absorption edge, the so-called K edge, the best fit is sigma A upon A in barns per atom is equal to 30 times Z to the four divided by H mew in kilo electron volts cubed. From our ratio of delta and beta, we therefore obtain beta equals F2 delta upon Z or sigma A delta divided by two R not Z lambda.

Notes

Summary

12m 12s

How big is β?

$$\beta = \frac{f_2\delta}{Z} = \frac{\sigma_a\delta}{2r_0 Z\lambda}$$

2.82×10^{-5} Å

$$\sigma_a[\text{barn/atom}] = 30\frac{Z^4}{(h\nu[\text{keV}])^3}$$

$$\sigma_a[\text{Å}^2/\text{atom}] = 30 \times 10^{-8}\frac{Z^4}{(h\nu[\text{keV}])^3}$$

$$\delta = 1.8 \times 10^{-7}(\lambda[\text{Å}])^2 Z$$

$$\lambda[\text{Å}] = \frac{12.3984}{h\nu[\text{keV}]}$$

$$\beta = 1.19 \times 10^{-8}\frac{Z^4}{(h\nu[\text{keV}])^4}$$

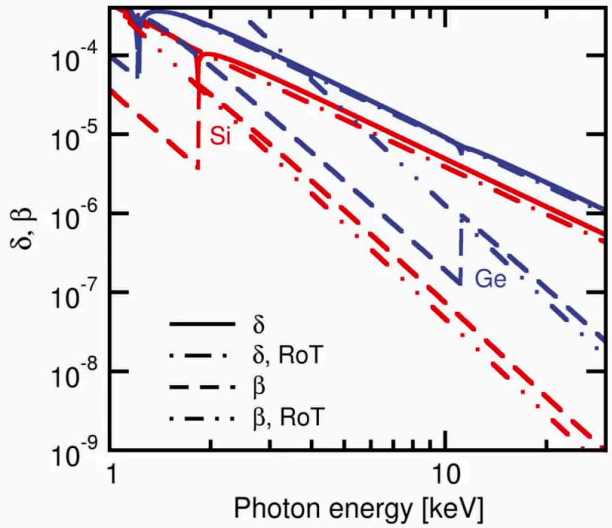
So we can now combine our rule of thumb for sigma A, remembering to convert to square angstroms from barns and our rule of thumb for delta and our numerical expression for the photon wavelength and the known value for the Thomson scattering length to obtain a rule of thumb for beta, which is equal to 1.19 times 10 to the minus eight times Z to the power of four divided by the photon energy in KV to the fourth power.

Notes

Summary

13m 29s

Summary of magnitudes for δ and β



$$\delta \propto Z/(h\nu)^2$$

$$\beta \propto Z^4/(h\nu)^4$$

n = 1 – very little + i(almost nothing)

Summarising these back of the envelope estimates for the magnitudes of delta and beta, we see for the examples of Silicon and Germanium that both terms are very small and that beta drops off more sharply with photon energy than does delta, owing to its stronger inverse proportionality to H mew. We encapsulate the contents of this video by making the perhaps only semi-serious statement that N is equal to one minus very little plus I times almost nothing. In the next video, we will take this nonetheless, very important, very little and almost nothing to describe total external reflection of X-rays and their associated penetration depth beneath the surface.

Notes

Summary

14m 02s