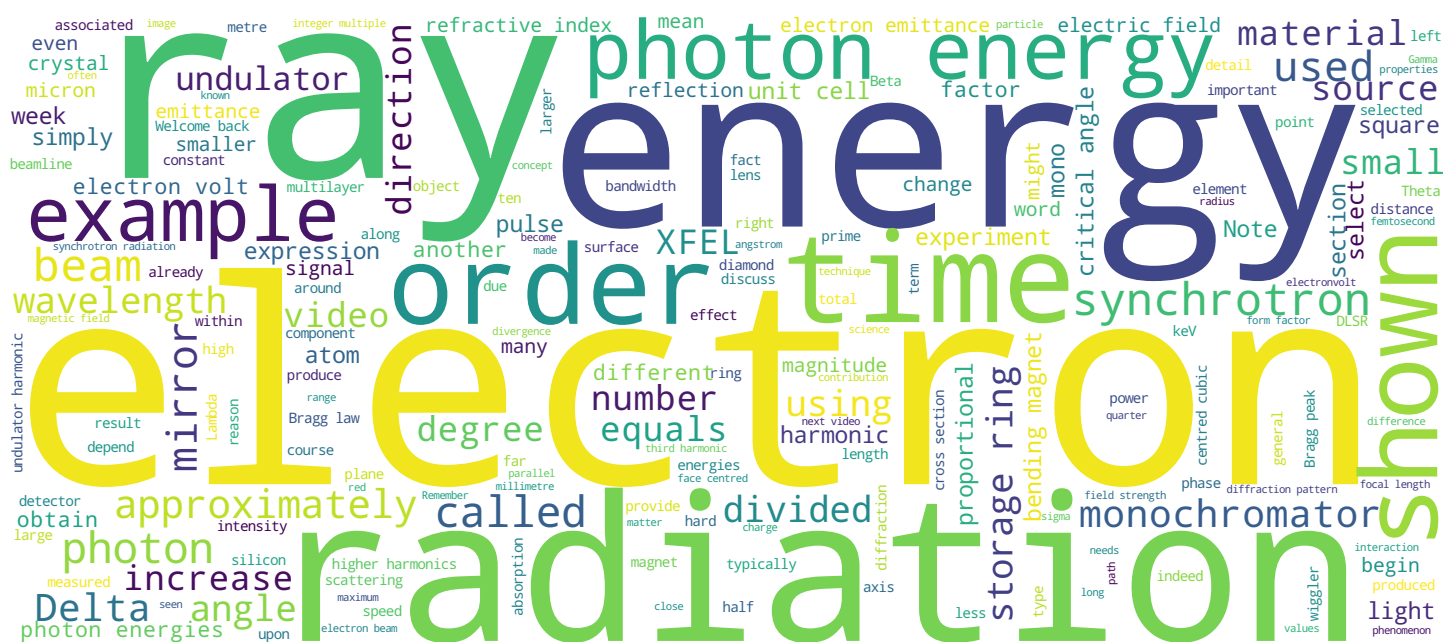


# Synchrotrons and x-ray free-electron lasers

## Techniques and applications

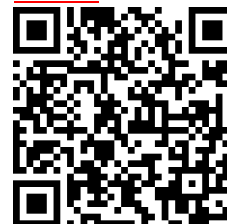
Prof. Philip Willmott



## Search MOOC



## Video



# Contents and objectives of this video



- Harmonic suppression
  - The problem
  - Suppression via reflection
  - Suppression via crystallography
  - Suppression via refraction
    - Multilayers
    - Prisms
    - Lenses

Welcome back to the final video this week. In this video, we will look at the problem of eliminating higher harmonics and the suppression of unwanted higher photon energies in general.

Notes

Summary



0m 04s

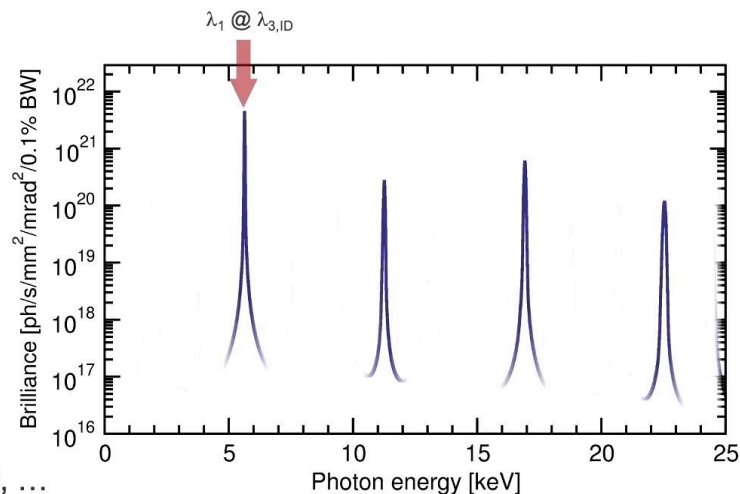
# Harmonic suppression

- The problem

- $m\lambda_m = \text{constant}$
- $\lambda_1, \lambda_1/2, \lambda_1/3, \dots$
- $\equiv h\nu, 2h\nu, 3h\nu, \dots$

- The goal

- Remove signal @  $\lambda_1/2, \lambda_1/3, \dots$



Let's begin by spelling out clearly what the problem is. Any monochromator that uses Bragg's law to select a given wavelength or photon energy will also select for integer multiples of that energy. This is simply because for a given instant angle  $\theta$  and lattice spacing  $d$ ,  $2d \sin \theta$  is a constant. Hence, both the wavelength  $\lambda_1$ , which is equal to this constant, and another wavelength  $\lambda_2$ , which is equal to  $\lambda_1$  divided by 2, will also satisfy the Bragg condition, as will indeed  $\lambda_3$ , which is equal to  $\lambda_1$  divided by 3, and so on, and so forth. The goal is to remove these harmonics with twice, three times, etc, etc, the energy of the so-called fundamental for  $m$  equals 1. This is a problem not only for broadband sources such as bending magnets and wigglers, but also for undulators, as they also produce harmonics evenly separated in energy from one another. If one tunes the monochromator to select the first harmonic of the undulator, all the higher undulator harmonics will also be selected if no other measures are taken to suppress them. Hopefully, obviously, however, if the mono is tuned to the third undulator harmonic, only that the sixth, the ninth, etc, will survive the monochromator selection.

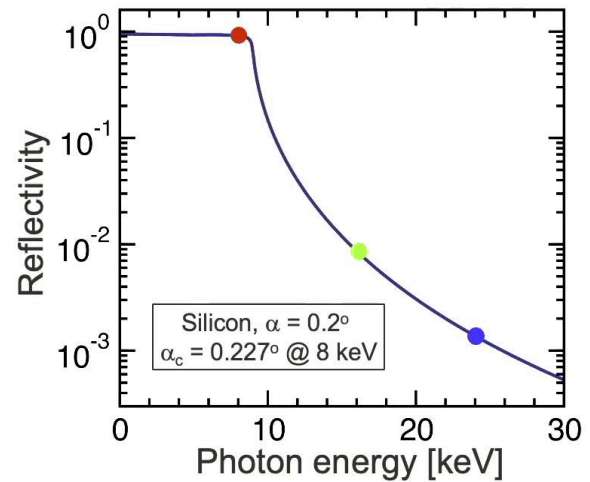
Notes

Summary



# Harmonic suppression via mirrors

- Set incident angle on mirror  
@ ca. 80%  $\alpha_c$  for desired energy  $h\nu$
- Reflectivity @  $2h\nu$  and above  $\ll 1$
- Use two mirrors – effect is squared!



So the mono itself can remove undulator harmonics, depending on which undulator harmonic is selected by the monochromator fundamental energy. The next common way of removing or significantly suppressing all harmonics higher than a selected energy is through reflection of an X-ray mirror. As we've already discussed earlier this week, the critical angle for total external reflection is inversely proportional to the photon energy. Hence, if one adjusts the instant angle of a polychromatic beam on a mirror so that it is marginally larger than the critical angle associated with a desired photon energy and the mirror material, higher photon energies will be suppressed. There are two distinct situations: one where the incident beam is truly polychromatic and broadband, such as radiation emerging from a bending magnets or a wiggler, or one where the energy is concentrated into narrow bands of energy either associated with an undulator source, in which case the total incident power is still high, measured in several hundreds of Watts, or after filtering by a monochromator. In the case of broadband bending magnets or wiggler radiation, all the raw undulator spectrum mirrors...

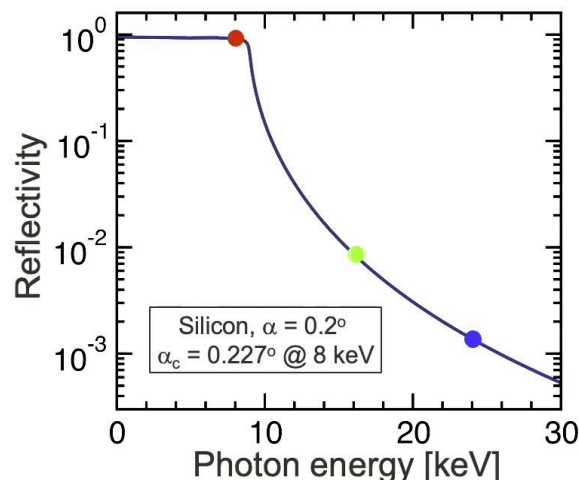
Notes

Summary



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any mirror placed in the path of the beam will absorb a significant fraction of the radiation and very often, therefore, needs to be cooled. Radiation that is emerged from the synchrotron source and bounced off a mirror before being monochromatised is referred to as pink beam radiation. This is because the reflection properties of the mirror will select for the radiation that has its critical angle higher than the mirror tilt angle. The higher energy radiation for which the critical angle is below the mirror tilt angle will be poorly reflected. The power of the radiation after monochromatisation is measured in a few milliwatts to a few tens of milliwatts. Hence, any mirror after a monochromator does not need to be cooled. Consider, for example, the fundamental radiation selected by a mono at 8 keV. Depending on the mono type, it is most likely that the higher harmonics at 16, 24, 32 keV, etc, will also be selected by the mono as a consequence of Bragg's law. However, if a mirror is used to bounce its radiation after the mono and the angle is judiciously set, the higher harmonics will all be suppressed, and only the 8 kilo keV will be efficiently reflected. If two mirrors are used, this effect is squared.

Notes

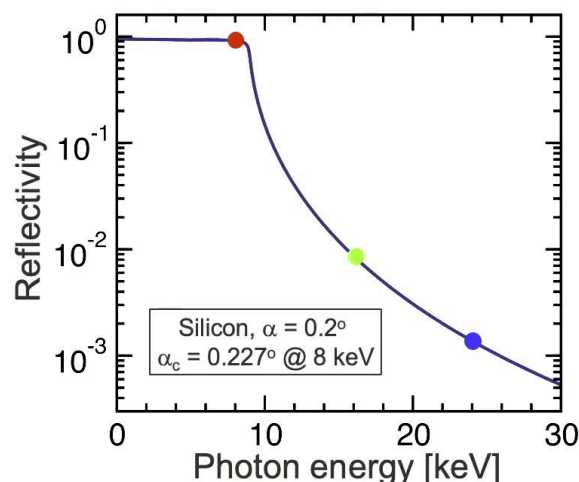
Summary



3m 22s

# Harmonic suppression via mirrors

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@ ca. 80%  $\alpha_c$  for desired energy  $h\nu$
- Reflectivity @  $2h\nu$  and above  $\ll 1$
- Use two mirrors – effect is squared!



So in the example shown on the right for a reflection of 8 keV radiation and its harmonics, a silicon mirror at an angle of 0.2 degrees will 100 percent reflect the 8 keV fundamental, but attenuate the 16 keV radiation more than 100 fold and the 24 keV nearly 1,000 fold. A second mirror at the same relative angle would increase the attenuation of the second and third harmonics by over 10,000 and nearly 1 million, respectively.

Notes

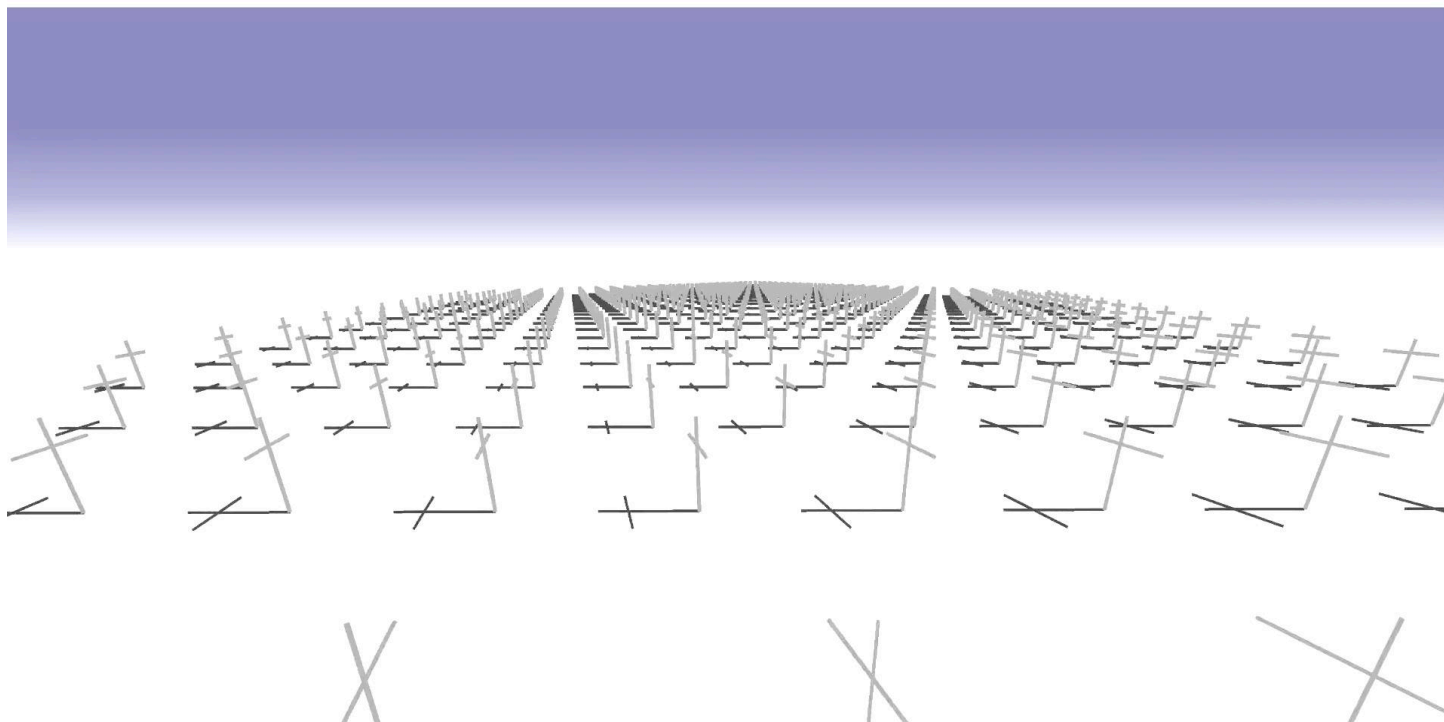
Summary



4m 58s



# Harmonic suppression via choice of mono crystal



The next method to suppress harmonics is a little difficult to appreciate without some background in crystallography, though I will try my best to provide a heuristic explanation, even if the details may remain somewhat opaque for some of you. There are different crystal planes in a crystal, just as there are different apparent straight lines of crosses through a military cemetery. Each aisle between the lines of crosses or planes of atoms in 3D crystals has a different width, which, in the terms of the Bragg law can be equated to  $D$  and a different orientation related to  $\Theta$ .

Notes

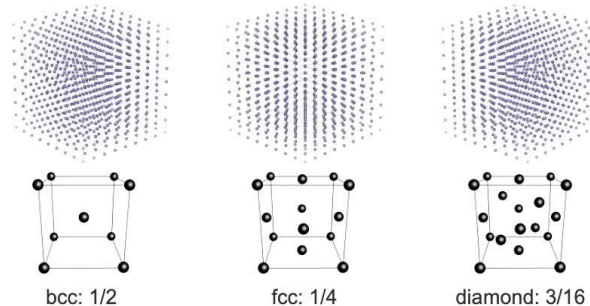
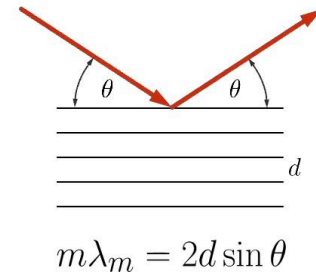
Summary



5m 35s

# Harmonic suppression via choice of mono crystal

- “Systematic absences”
  - Symmetry of atoms in crystal  $\Rightarrow$  some diffraction peaks have zero intensity due to destructive interference among scattered waves from individual atoms
- e.g. Si(111) reflection allowed but (222) forbidden
  - For same incident angle  $\theta$ 
    - $\lambda_{(111)} = 2d_{(111)} \sin \theta$   
observed Bragg peak
    - $\lambda_{(222)} = \lambda_{(111)}/2$
    - $d_{(222)} = d_{(111)}/2$
    - $\Rightarrow \lambda_{(222)} = 2d_{(222)} \sin \theta$   
missing Bragg peak



The Bragg law predicts that each of these high symmetry avenues will produce a Bragg peak in the diffraction pattern. However, in a 3D crystal, each repeat element or so-called unit cell will contain a set of atoms numbering from one up to many thousands, in the case of a protein crystal. This is known as the basis. For example, three types of cubic unit cell are shown here. The body-centred cubic containing two atoms or identical configurations of atoms per unit cell, the face-centred cubic containing four identical sub-units, and the diamond cell, which is actually a face-centred structure whereby each sub-unit contains atoms at its origin and at a quarter, a quarter, a quarter relative to the unit cell size. This might seem complicated, but the important take-home message here is that elastically-scattered components of the incident X-rays from the atoms within the unit cell will interfere. And for certain orientations, certain crystal planes, this can result in perfect destructive interference between them, and the Bragg peak will have zero intensity. This is called a systematic absence. Examples of this are that in BCC structures which are...

Notes

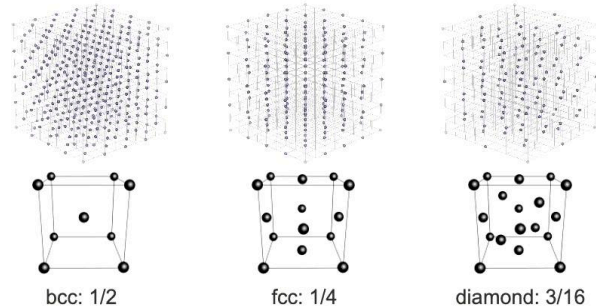
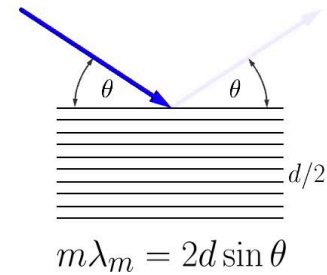
Summary





# Harmonic suppression via choice of mono crystal

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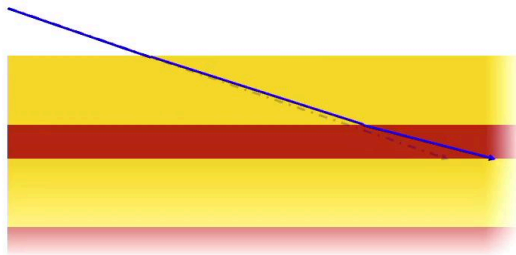
in which half of the Bragg peaks are missing, FCC, for which three quarters are missing, and the diamond structure for which only three sixteenths are allowed. Look carefully at the three-dimensional diffraction patterns above each structure. We begin by ignoring interference between scattered radiation from individual atoms within the unit cell, for which we would, thus, obtain non-zero intensity Bragg peaks for each location in reciprocal space. But if we do take the atomic structure into account, we see how the diffraction patterns, that is, the regularly spaced array of Bragg peaks, becomes much sparser for body-centred cubic, face-centred cubic, and diamond that among would obtain for a simple cubic structure. For example, for reasons of symmetry, the (111) reflection of silicon is allowed, or as the (222) is nominally forbidden. I say, nominally, as it complete suppression assumes that the electron cloud surrounding the silicon atoms have perfectly spherical symmetry, which we know not to be 100 percent valid. Four of the 14 electrons in silicon are associated with  $sp_3$  covalent bonding, which is far from spherically distributed. Hence, these reflections tend to be very weak but not entirely absent.

Notes

Summary



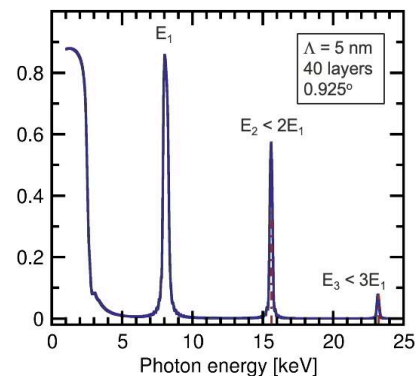
# Harmonic suppression via refraction in multilayers



$$m\lambda_m = 2\Lambda \sin \theta (1 - \kappa\Lambda^2/m^2)$$

$$\kappa \sim 2 \times 10^{-3} \text{ nm}^{-2}$$

- $\kappa$  material dependent
- $\kappa\Lambda^2/m^2$  biggest for  $m = 1 \sim 0.05$ 
  - Deviation of  $\lambda_1$  from “simple” Bragg law biggest
  - $E_m$  ( $m > 1$ )  $\neq mE_1$  [or  $\lambda_m$  ( $m > 1$ )  $\neq \lambda_1/m$ ]
  - Helps only for undulator radiation!!



Refraction plays a crucial role in harmonic suppression when using multilayer monochromators. Consider the example shown here. The first harmonic selected by the multilayer is shown to be at 8.00 keV. The second and third harmonics, however, are not at two and three times this value, respectively, as we might have expected from our simple Bragg-like equation shown here on the left, but instead are at 15.592 and 23.177 keV. The reason for this is that the equation is actually an approximation. The exact equation is shown here where the second correction term in the brackets, Kappa Lambda squared divided by m squared, accounts for refraction effects. The X-rays are bent to shallower angles, and this effect is most noticeable for the shallowest angles for the fundamental with m equals 1. Inserting typical values into this expression, we find that Kappa Lambda squared divided by m squared is of the order of 5 percent compared to the uncorrected expression. It is already four times weaker than this for the second harmonic and nine times weaker for the third harmonic. One might ask why this correction is not also employed for the normal Bragg equation for crystals.

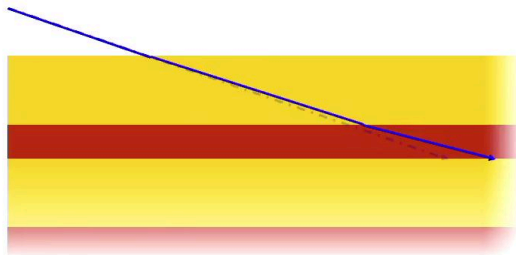
Notes

Summary



9m 16s

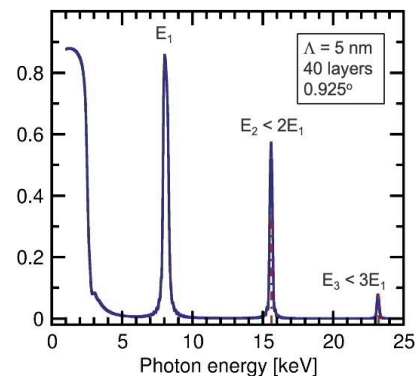
# Harmonic suppression via refraction in multilayers



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  - Helps only for undulator radiation!!



Well, first, in some cases requiring the highest accuracy, it actually is. However, the deviations are much smaller due to the fact that the wavelengths being selected in multilayers are very much smaller than the periodicity, resulting in shallow Bragg angles and a larger relative refractive effect. In other words, a larger relative change in angle of the X-rays as they cross the interface between spacer and reflecting layer. This phenomenon means that multilayers can be used to suppress higher harmonics, at least for undulator radiation for which the bandwidths are typically much narrower than the shift in the Bragg energy away from simple integer multiples of the first harmonic. For broadband radiation, this phenomenon will not help however.

Notes

Summary



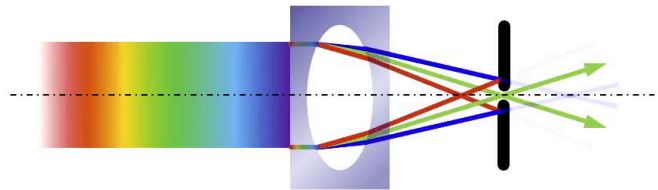
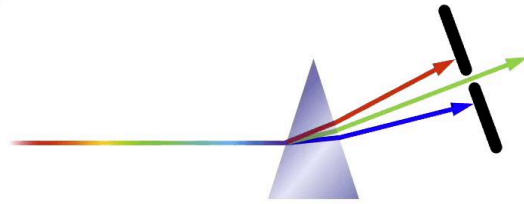
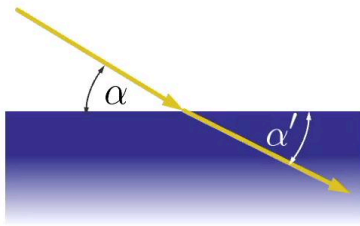
# Harmonic suppression via refraction by prism or lens

- Exploit inverse-square-dependence of  $\delta$  on  $(h\nu)$

$$\delta = \frac{\rho r_0}{2\pi} \lambda^2$$

- Refraction

$$\frac{\cos \alpha}{\cos \alpha'} = 1 - \delta$$



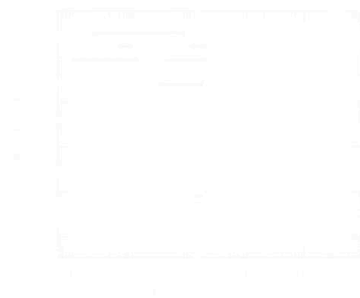
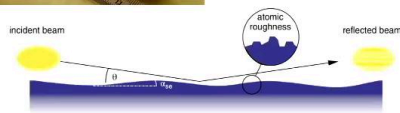
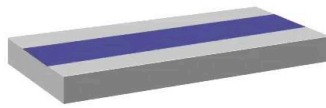
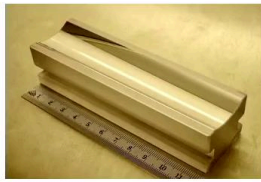
Finally, refraction can be used to spatially filter a band of radiation. Remember, the real part of the refractive index for X-rays is 1 minus Delta. And Delta itself depends on the square of the photon energy. So a simple prism placed in the path of the polychromatic beam, in conjunction with a narrow slit, will select a fraction of the beam. The prism needs to refract strongly enough, depending both on its shape and the material from which it is made. This leaves only very few materials that are mechanically and thermally robust enough and not absorb too strongly the X-rays. The most obvious candidate is diamond. The slit should be placed as far as possible downstream of the prism in order that the radiation fan becomes sufficiently large compared to the beamwidth. Vertical refraction is therefore preferred as the beam is narrower in this plane. Similarly, one can use compound refractive lenses. The focal length of a CRL is proportional to the inverse of Delta and is therefore, proportional to the square of the photon energy. A slit is positioned at the point where the desired photon energy is focused.

Notes

Summary



# Summary of this section



To summarise this section, we have looked in detail at variants of the two primary optical elements of X-ray mirrors and monochromators.

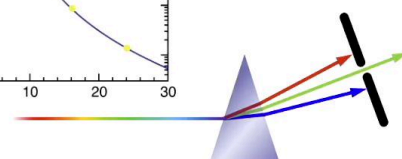
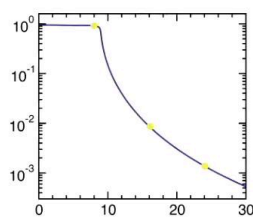
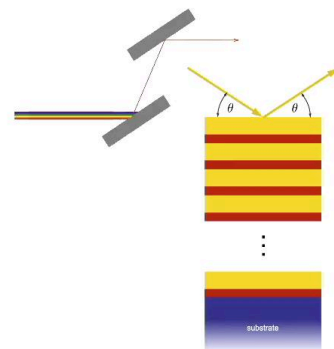
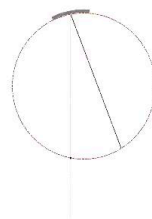
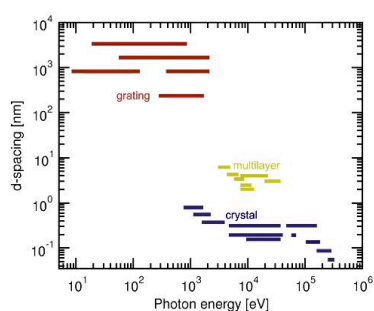
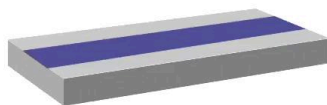
Notes

Summary



13m 17s

# Summary of this section



We have seen that monochromators, in general, filter for integer multiples of a fundamental photon energy, and that suppression of the higher harmonics can be achieved through a variety of approaches based on reflection, refraction, and diffraction.

Notes

Summary



13m 27s



## Next week...



Next week, we will take a closer look at secondary optics elements, in particular, micro-focusing elements such as capillary lenses, compound refractive lenses, and Fresnel zone plates. Moving on, we will also look at both photon and electron detectors, beginning with a summary of the handling of noise.

Notes

Summary



13m 44s