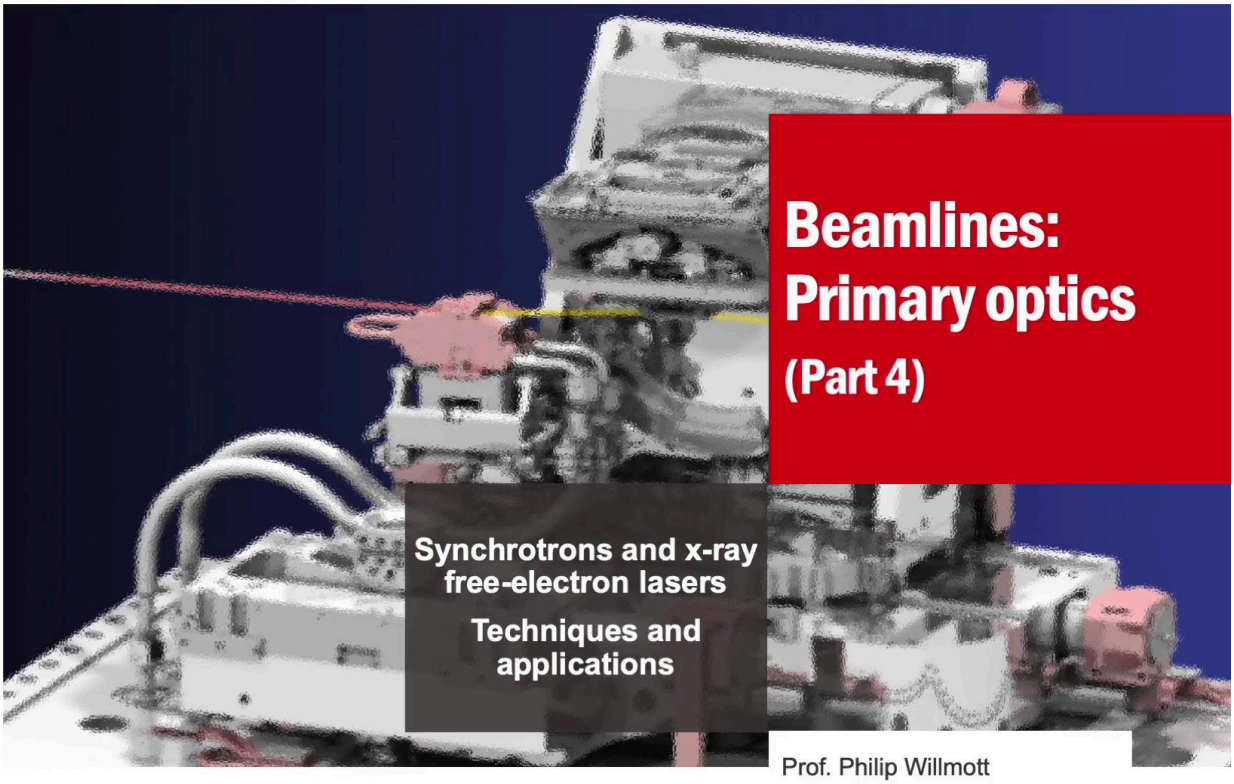

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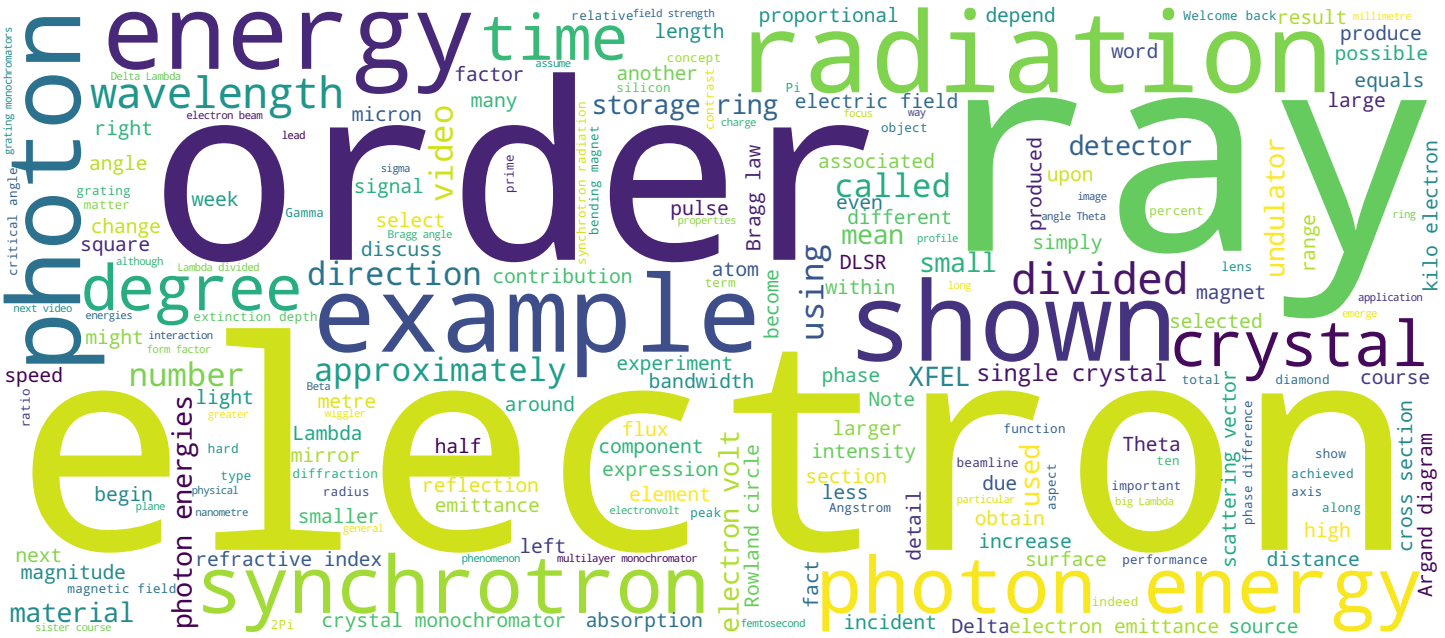
photon
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XFEL
single crystal
Bragg law
electron volt
Rowland circle
Argand diagram
cross section
scattering vector
refractive index
crystal monochromator
absorption
electron emittance source
Delta
incident
surface
performance
distance
increase
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Note
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Bragg angle
Gamma
lead
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grating monochromators
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Bragg angle
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Argand diagram
cross section
scattering vector
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Welcome back
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properties

Contents and objectives of this video

- Monochromators
  - Grating monochromators
  - Crystal monochromators
  - Multilayer monochromators

Welcome back to the fourth of five videos in this section on primary optics. In this video, we will look in more detail at aspects of Grating, Crystal, and Multilayer monochromators.

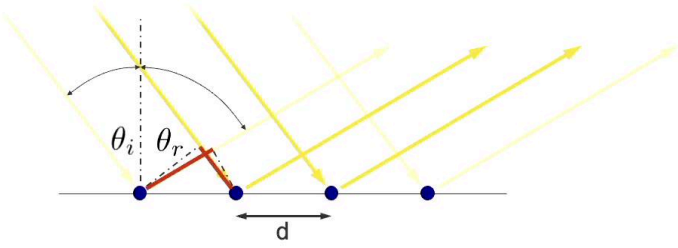
Notes

Summary

0m 05s

Grating monochromators

- N_f = # illuminated facets ~ 10^4
- Resolving power: $\frac{\lambda}{\Delta\lambda} = mN_f$



$$m\lambda = d(\sin\theta_i - \sin\theta_r)$$

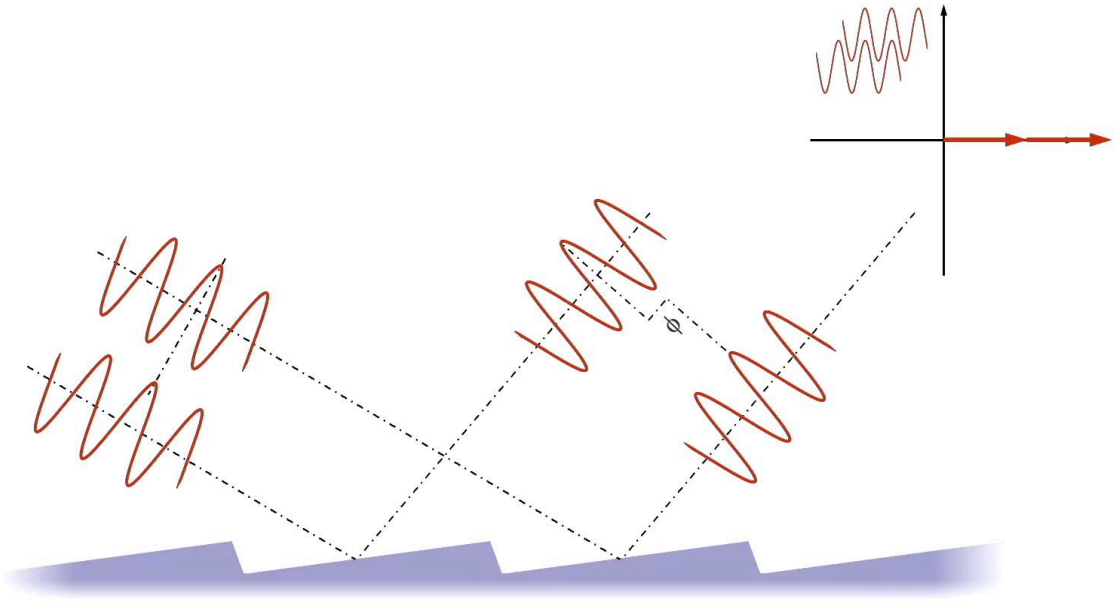
We begin with Grating monochromators. The profile of the grating grooves can vary. Blaze profiles are the most common, which display a saw-tooth-like profile. They work most efficiently when the incident and reflective beams reflect specularly of the blaze surface. For a grating evenly illuminated across N_f facets, which can be of the order of around 10,000, the resolving power of the Nth harmonic is Lambda divided by Delta Lambda is equal to mN_f.

Notes

Summary

0m 19s

Grating monochromators



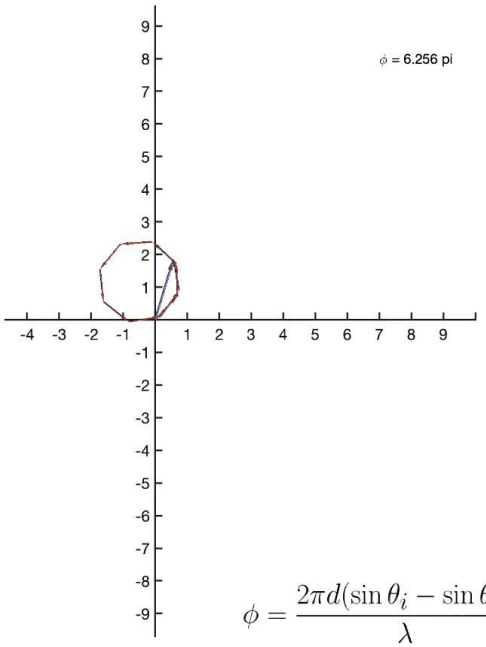
Let's look at this aspect more closely. How is the performance of grating monochromators affected by the number of illuminated facets N_f. To understand this better, we again resort to the use of Argand diagrams and the contribution to the interference signal from each facet. Note, by the way, that the exact same argument and mathematical approach can be used to describe diffraction from single crystals. For example, in crystal monochromators, whereby instead of considering scattering from individual facets, we substitute this with scattering of individual scattering planes. So we assume that illumination of each facet is the same, and that therefore, this scattering amplitude is also the same. How these scattered wavelets add up depends on their relative phase. In other words, how they interfere with each other. If we just consider the contribution from two adjacent facets as shown here, we see that although the incident radiation is in phase, the two scattered waves are out of phase by an amount Phi which can be between 0 and 2Pi, as we see here in this small Argand diagram.

Notes

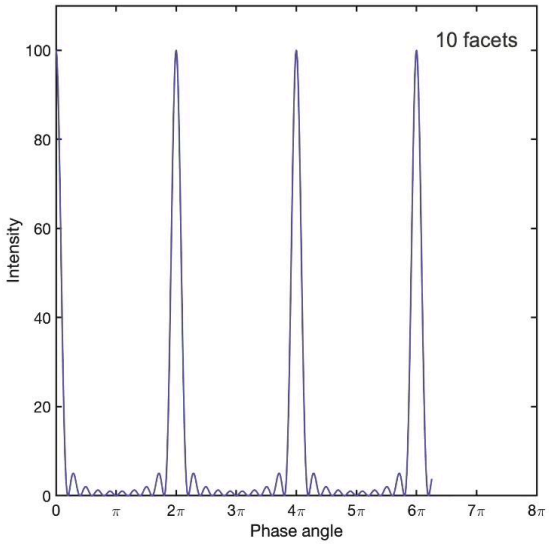
Summary

0m 59s

Grating monochromators



$$\phi = \frac{2\pi d(\sin\theta_i - \sin\theta_r)}{\lambda}$$



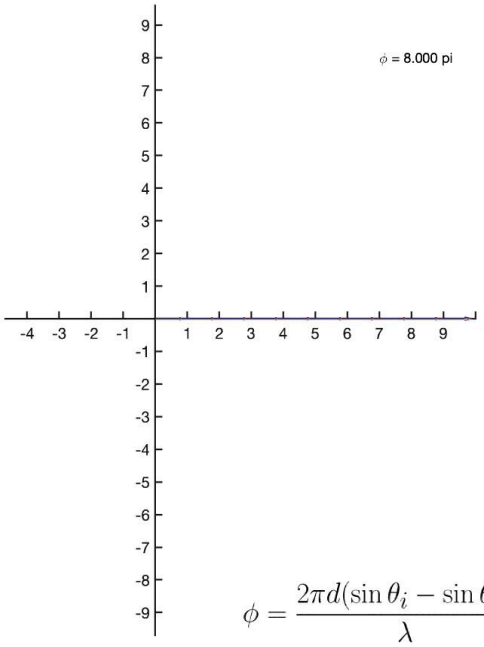
Let's now consider the case of illumination of 10 facets. If the optical path difference between scattering of adjacent facets is an inter-multiple of wavelengths, the phase difference Phi will be an integer multiple of 2Pi, and the sketching amplitudes will all add up in one direction to produce a total amplitude ten times the length of the individual scattering amplitude from one facet, as can be seen here. Now, let's gradually change the incident and/or exit angle so that the phase difference Phi increases from the starting value of 0. On the left is the Argand diagram in which you will clearly see how the ten individual contributions begin to curl around, and the total amplitude will decrease. On the right, the intensity of the radiation is plotted as a function of Phi. This is simply the square of the amplitude, which is, itself, the vector sum of the individual contributions. In other words, the blue arrow in the Argand diagram movie, which I will begin now. The first minimum occurs when the individual vectors form a closed polygon with N_f sides, whereby N_f is equal to 10 in this example. And hence, the phase difference between the scattered radiation of neighbouring facets is 2Pi divided by 10, which is 36 degrees.

Notes

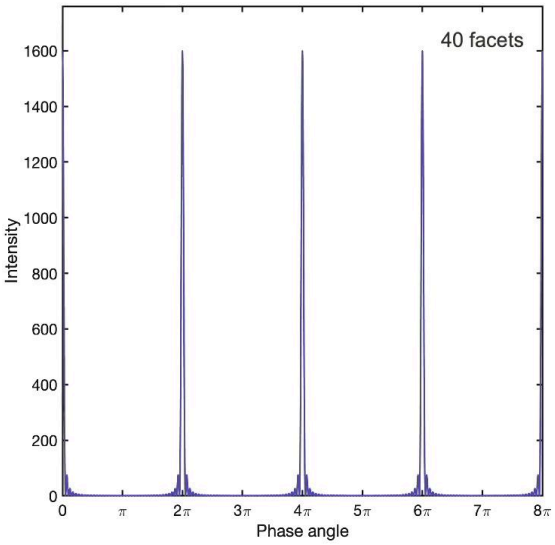
Summary

2m 19s

Grating monochromators



$$\phi = \frac{2\pi d(\sin\theta_i - \sin\theta_r)}{\lambda}$$



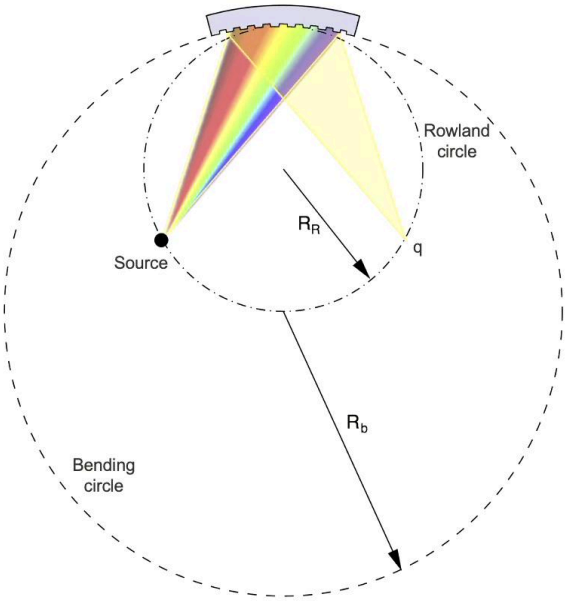
The vectors continue to curl up on themselves, with minimal occurring for each advance of 36 degrees until we reach a value for Phi of Pi or 180 degrees, where the vectors alternate between being positive and negative along the real axis and cancel one another out. Thereafter, the vectors begin to uncurl again until a maximum is reached at Phi is equal to 2Pi. The width of the peaks is 2Pi divided by N_f, and hence, the relative bandwidth is 1 divided by mN_f or the inverse of the resolving power. An increase in the number of facets, therefore, improves the resolution proportionally. See, for example, the intensity distribution for a grating containing 40 facets. Indeed, modern soft X-ray monochromators N_f can easily be several thousand and bandwidths comparable and often superior to those demonstrated by crystals such as silicon can be achieved.

Notes

Summary

3m 53s

Spherical grating monochromators



- Grating
  - Spherical concave surface, radius R_b
  - Lines ⊥ to Rowland circle, radius $R_R = R_b/2$
- Divergent source
  - Sits on Rowland circle
  - Grating refocuses selected wavelength to q
- Energy selection
  - Rotate and slide the SGM or source around Rowland circle to access different photon energies

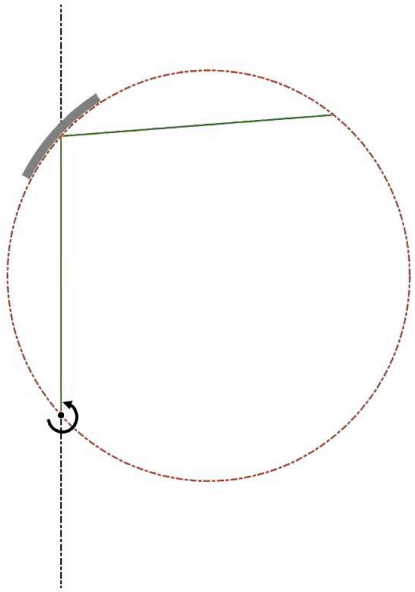
Now, it's possible to bend dispersive elements such as crystals or gratings in order to simultaneously disperse the radiation, in other words, to monochromatise, and to focus it. In spherical grating monochromators or SGMs, the grating surface has a concave, spherical form with a radius R_b. The grating grooves or lines are perpendicular to the so-called Rowland circle, which lies tangential to the centre of the grating and has a radius that are half that of the spherical grating. Any source lying somewhere on the Rowland circle will select a certain wavelength and refocus it at another position on the same Rowland circle.

Notes

Summary

4m 59s

Spherical grating monochromators



- Grating
  - Spherical concave surface, radius R_b
  - Lines ⊥ to Rowland circle, radius $R_R = R_b/2$
- Divergent source
  - Sits on Rowland circle
  - Grating refocuses selected wavelength to q
- Energy selection
  - Rotate and slide the SGM or source around Rowland circle to access different photon energies

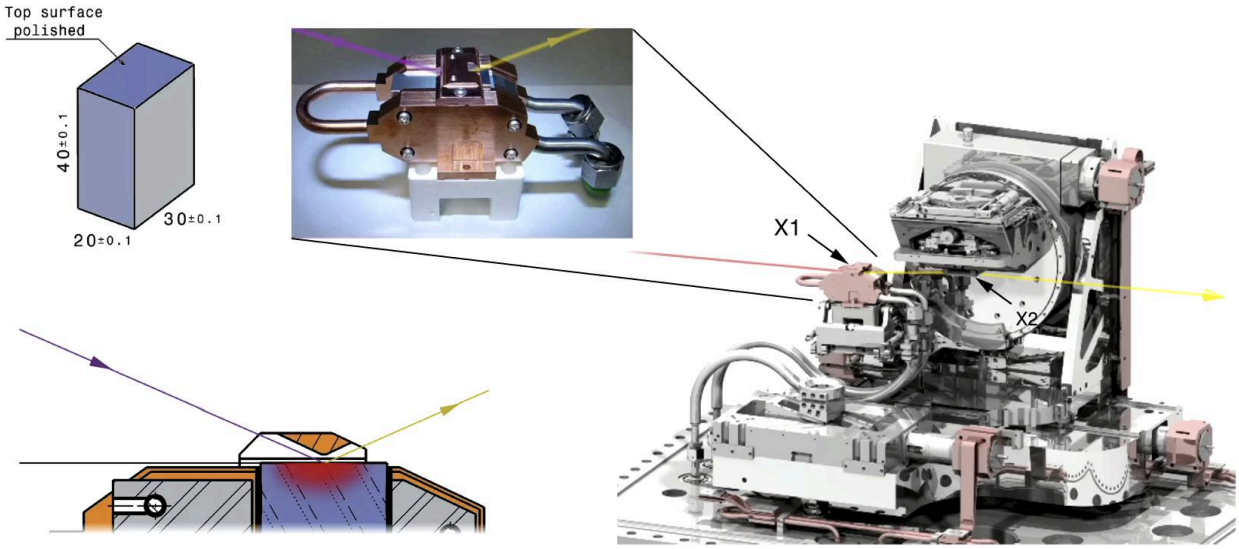
Different energies can be selected by moving the Rowland circle around at axis parallel to the grooves and sliding the grating around the Rowland circle as shown here. The detector also moves around the Rowland circle at twice the rate as that of the grating.

Notes

Summary

5m 52s

Crystal monochromators



Adapted from: Willmott *et al.*, J. Synchrotron Rad. **20** 667-682 (2013)

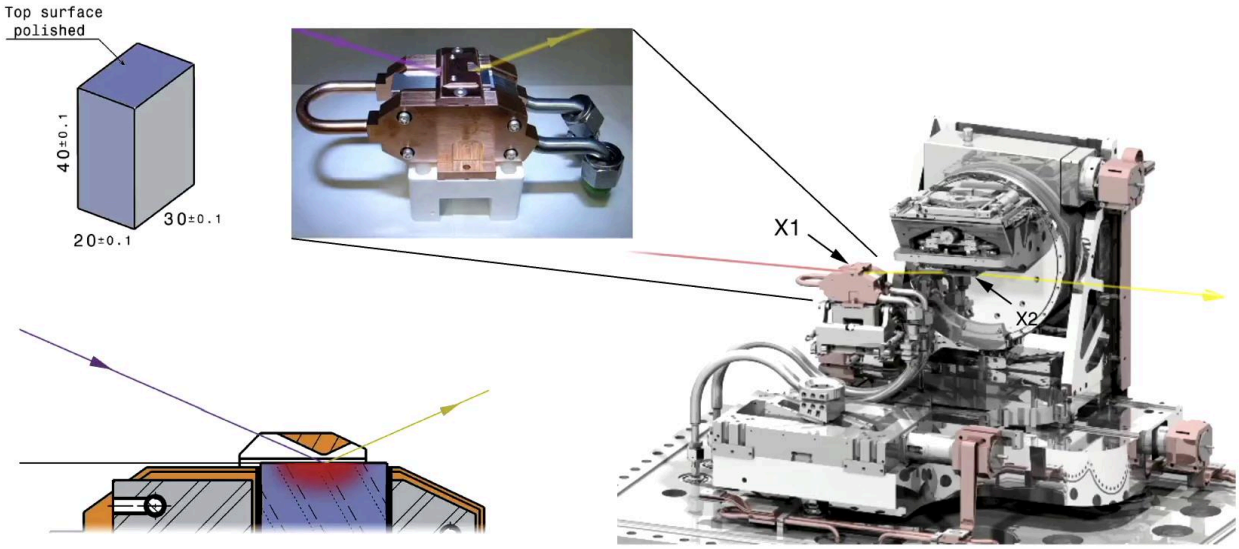
We now move on to Crystal monochromators. Crystal monochromators use perfect bulk-sized crystals, commonly called single crystals, to select a given energy using brag diffraction. The most commonly used crystal material is cilicon. Silicon has a reasonable thermal conductivity and can be efficiently cooled by water or, more commonly, liquid nitrogen in order to minimise the mechanical strain induced by a local thermal bump where the incoming polychromatic beam impinges on the crystal surface. Remember, even in the case of undulator radiation, less than a percent of the incident power will be transmitted and the remainder absorbed in the small volume defined by the footprint of the radiation on the surface and the absorption depth of the crystal material. Importantly, silicon can be produced as a near perfect single crystal with linear dimensions up to tens of centimetres thanks to its ubiquitous use in the semiconductor industry, where large and exceedingly perfect wafers are produced on mass. The most common crystallographic orientation is the (111) orientation.

Notes

Summary

6m 09s

Crystal monochromators



Courtesy Cinel SrL, Padova, Italy

Adapted from: Willmott *et al.*, J. Synchrotron Rad. **20** 667-682 (2013)

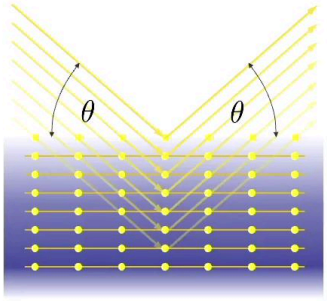
The crystal is typically mounted on a rotation stage or so-called goniometer head as part of the monochromator in order for it to be oriented at such an angle to select a certain photon energy as shown here in this technical rendition of the double-crystal monochromator developed for the Material Science Beamline at the Swiss Light Source.

Notes

Summary

7m 33s

Crystal monochromators



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

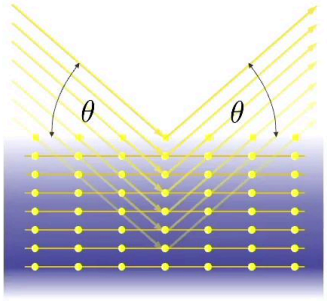
Bragg's law predicts that if one were to have a perfect, non-absorbing and very weakly scattering crystal of infinite depth and a perfectly-collimated incoming polychromatic beam, the bandwidth of the selected radiation would be infinitely narrow. However, reality fall short of this ideal.

Notes

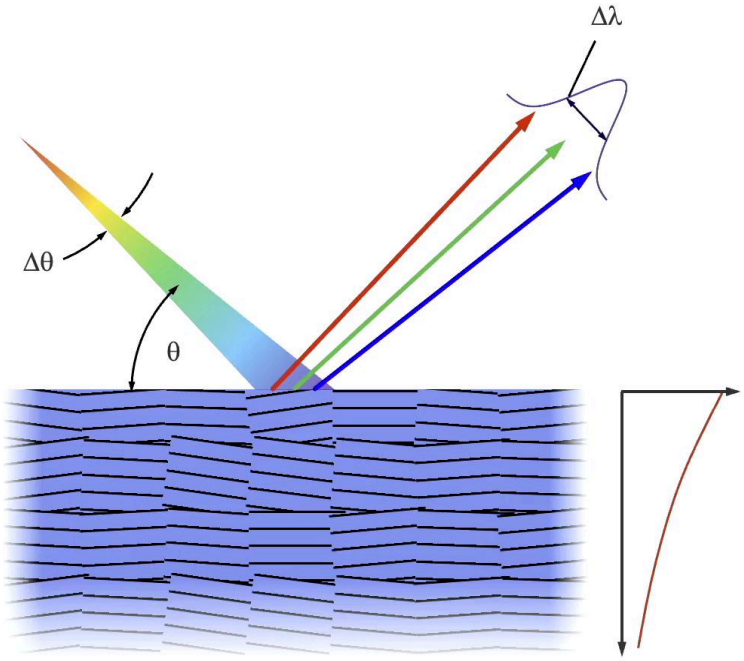
Summary

7m 58s

Crystal monochromators



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



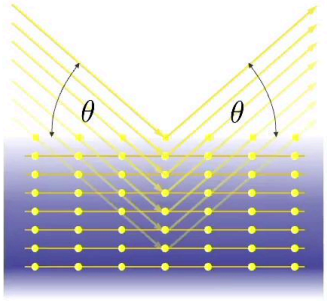
First, there is always some residual beam divergence, which means a band of photon energies is selected slightly lower energy photons from the steeper impinging part of the beam, higher energies towards the shallower end according to Bragg's law. Secondly, crystallographic defects such as edge and screw dislocations result in slightly misaligned crystallites that make up the imperfect single crystal. This phenomenon is referred to as mosaicity. Lastly, finite absorption and extinction depths mean that the radiation does not penetrate infinitely deep into the bulk, which, in itself, all other imperfections excluded will set a lower limit to the bandwidth. Note that this finite penetration of the incident B is essentially the same, at least qualitatively as the finite number of grating lines that can be illuminated in a grating dispersive element, also limiting the bandwidth there as we covered in the first off of this video. In the case of silicon crystals, the contribution that normally dominates is indeed due to the finite extinction depth, resulting in a so-called Darwin width of the Bragg reflection, which results in a relative spectral bandwidth a little larger than 10 to the minus 4.

Notes

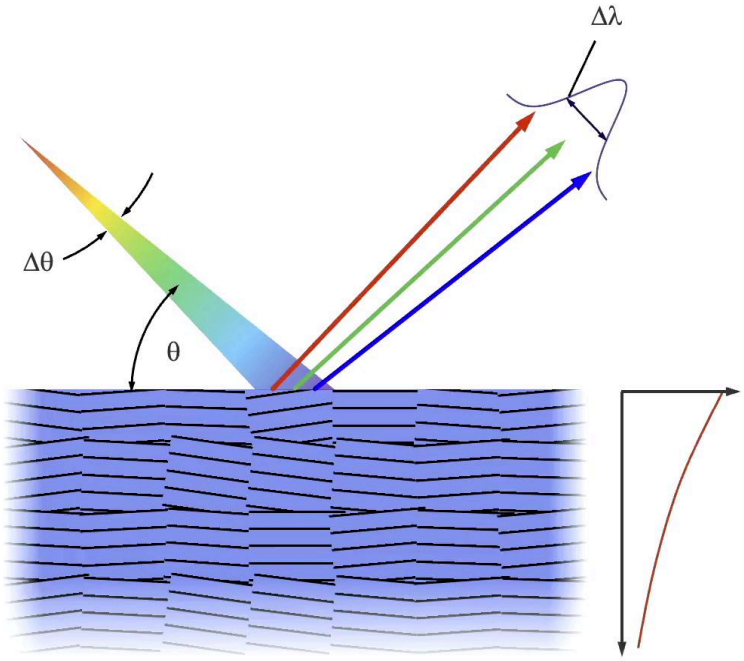
Summary

8m 21s

Crystal monochromators



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



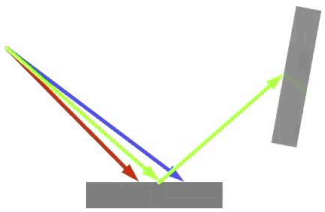
Hence, it emerges that one Angstrom radiation with an energy of 12.398 kilo electron-volts has a minimum bandwidth of approximately 1.7 electron-volts. Note that the corresponding width in Theta, the Bragg angle, is Delta Lambda divided by Lambda times tan Theta, and thus, the crystal also accepts a fine angular range of the order of a thousandth of a degree. In summary, all these factors contribute to a given crystal, always selecting a bandwidth Delta Lambda, which is greater than zero.

Notes

Summary

9m 53s

Crystal monochromators



J. W. M. DuMond, Phys. Rev. **52** 872 (1937)

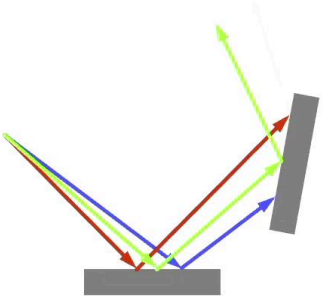
This leads us to the concept of dispersive or nondispersive configurations in monochromators. We've already argued that the incoming radiation is polychromatic and divergent to a certain degree, and that the crystal, thus, selects a band of wavelengths from this incoming beam. We were, therefore, expect a range of photon energies to be reflected off the crystal, the lower energy photons being selected at slightly steeper angles and those with the high energies at shallow angles according to Bragg's law. These will be reflected specularly with respect to the diffracting planes. Now, if we place an identical crystal in the path of the reflected rays, we can adjust its orientation so that all of those wavelengths selected by the first crystal are preserved after reflection of the second crystal as their respective impinging angles remain unchanged relative to the crystals diffracting planes. This is a non-dispersive configuration. Now, let's consider an alternative set up. We concentrate, to begin with, on the central energy shown here in green. In the previous slide, this was intercepted by the second crystal and reflected back parallel to its initial direction, but we could also reflect the beam in the opposite sense shown here.

Notes

Summary

10m 33s

Crystal monochromators



J. W. M. DuMond, Phys. Rev. **52** 872 (1937)

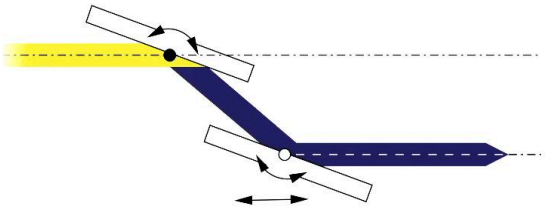
Now, what about the other energies? In this new setup, these no longer impinge on the surface of the second crystal at the same angle as they do on the first crystal. And as a result, they will be lost or strongly attenuated. This is a dispersive set up, as a narrower range of wavelengths is selected by the second crystal done by the first. This configuration is, therefore, more monochromatic, but at the expense of flux. A similar effect can be achieved by using a different crystal type or crystal orientation for the second element. This is succinctly explained using so-called Du Mond diagrams for which I direct you to the reference given here.

Notes

Summary

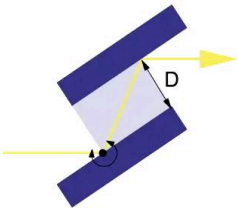
12m 13s

Crystal monochromators

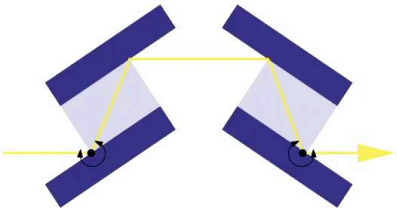


Double-crystal monochromator (DCM)

Channel-cut monochromator (CCM)



$\Delta y = 2D\cos\theta$



Four-bounce monochromator (4BM)

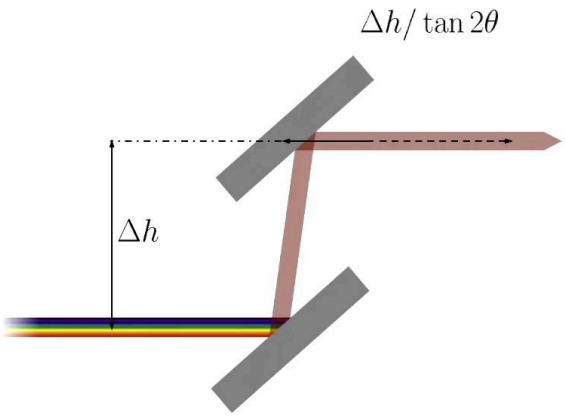
There are different types of crystal monochromators. A common configuration is the double-crystal monochromator using two identical crystals in the non-dispersive mode. This not only provides maximum flux but also allows the beam to emerge from the monochromator parallel to the incident beam. Channel-cut monos are fabricated using just one single crystal, which has had a central channel milled out of it. This adds simplicity and speed to changing the photon energy, requiring a single rotation stage, a definite advantage when performing rapid energy scans in certain types of spectroscopic experiments where physical and/or chemical changes are to be followed rapidly with as many as 40 energy scans per second in modern beamlines. The disadvantage is that the exit beams height will change as the channel-cut monochromator or CCM is rotated, though this can be made to be minimal by making the channel width D to be as small as possible and scanning over a not too large range of photon energies, which in turn determines the angular range of Theta. Lastly, the problem of this varying exit beam height of a CCM can be overcome by using a four-bounce configuration shown here on the right. Here, the disadvantage is that this is a dispersive set up associated with a certain loss of flux.

Notes

Summary

13m 05s

Fixed-exit DCM



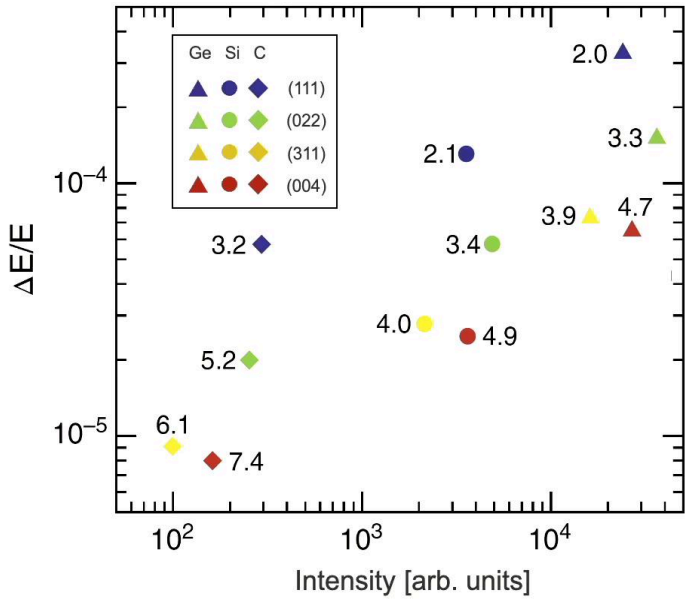
If the height offset Delta h in the monochromatised beam emerging from a double-crystal monochromator is to remain constant for all photon energies, not only do both crystals have to rotate to the Bragg angle, but also one of them, in this animation, the second upper crystal, must be translated along the beam axis. It is a simple trigonometric exercise to show that the relative horizontal position of the two crystal phase centres for a given instant angle Theta is given by Delta h divided by tan 2Theta.

Notes

Summary

14m 45s

Bandwidths of crystal monochromators



- Most common Si(111)
- Numbers: max Q-value in Å^{-1} assuming θ = 70°
- Ge only used at high energies due to absorption edge @ 11.1 keV
- Very narrow ΔE/E for diamond makes it interesting for seeding of SASE FELs

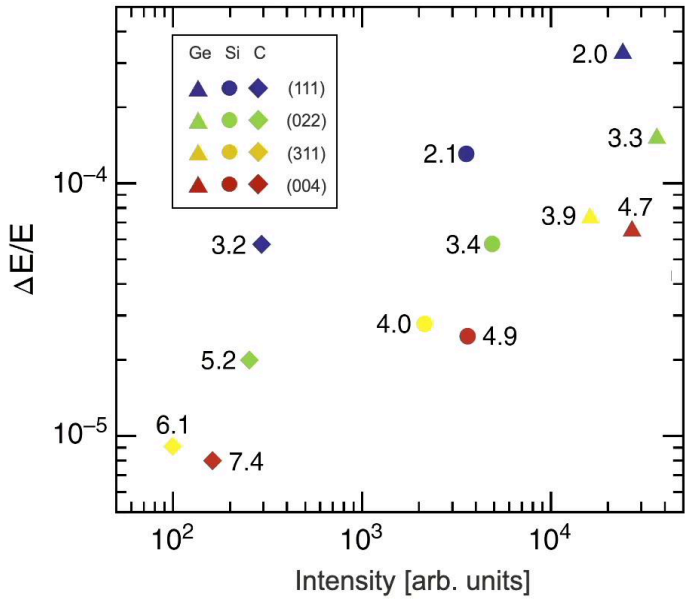
Now, as we have just mentioned, even a perfect single crystal will not select an infinitely narrow band of radiation from a perfectly parallel incident mono-poly chromatic beam due to the extinction depth of that crystal. The extinction depth reflects the fact that each atomic plane of the crystal elastically scatters the instant radiation even if only weekly, meaning that the instant beam will become weaker as it penetrates further and further into the material. They should not be confused with the absorption depth of the material, which is some are obviously associated with photo absorption and not elastic scattering. In the plot shown here, the relationships are highlighted between crystal material and it's a top atoms intrinsic elastic scattering cross sections, the crystal orientation and the bandwidth of the diffracted beam. We know that the Thomson scattering cross section increases with the square of the atomic number Si. It is also larger for smaller scattering vectors. Hence, one can expect that the (111) reflections with their large interplanes spacing and small Q will scatter more strongly than the (004) reflections.

Notes

Summary

15m 21s

Bandwidths of crystal monochromators



- Most common Si(111)
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- Ge only used at high energies due to absorption edge @ 11.1 keV
- Very narrow ΔE/E for diamond makes it interesting for seeding of SASE FELs

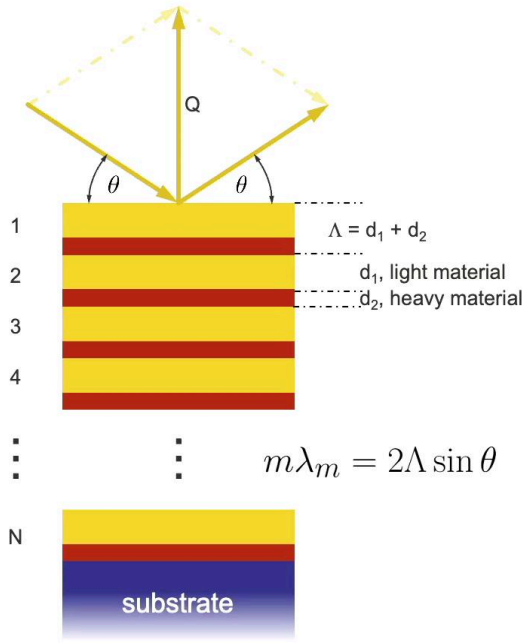
One might, therefore, predict that the strongest reflection is, thus, for Germanium (111), the blue triangle. However, the so-called structure factor determined by the details of the relative positions of the atoms within the crystal actually means that the (022) reflection is marginally stronger than the (111). We will look at this more closely when discussing diffraction theory in the sister course. The relative bandwidth Delta E divided by E of the monochromatised radiation is proportional to the structure factor, hence, goes down with decreasing set and increasing scattering vector Q. Diamond, therefore, has the narrowest bandwidth, making it interesting for monochromators use to XFELs, in particular, for seeding. The numbers adjacent to each data point represent the minimum accessible photon energy in kilo electron-volts that can be accessed assuming a practical maximum instant Bragg angle of 70 degrees, for which two Thetas, therefore, 140 degrees.

Notes

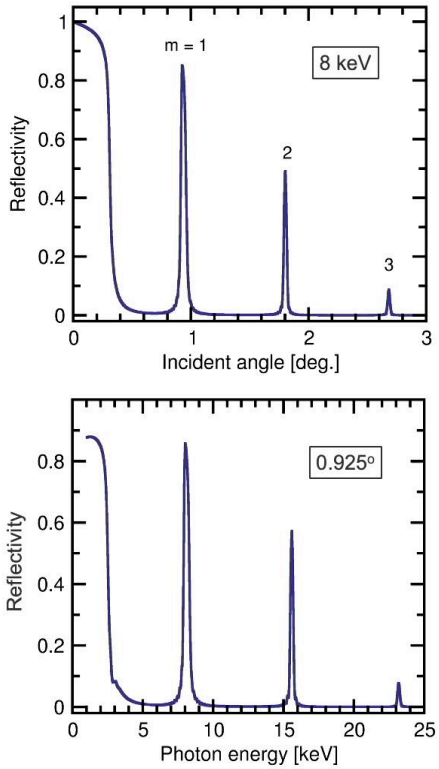
Summary

16m 48s

Multilayer monochromators



B_4C/Rh
Λ = 5 nm
d_1/d_2 = 1/3
40 layers



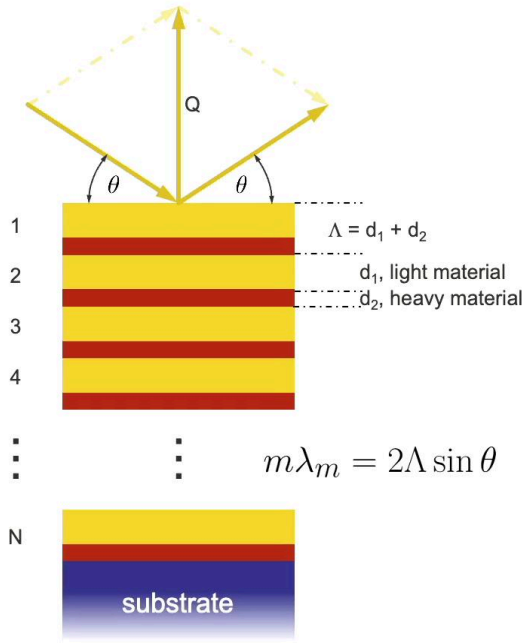
Finally, we discuss multilayer monochromators. Crystals diffract X=rays through scattering of plane of atoms. It is a three-dimensional system exploiting the periodicity in the direction parallel to the scattering vector. In the case of multilayers, scattering is produced by a contrast in the electron density at the interface between heavy reflection layers and lighter space of layers. The only required periodicity is in one direction: the direction of the scattering vector Q. Indeed, in many instances, on an atomic level, the materials which make up the reflection and space of layers can be amorphous with no periodicity at this spatial scale of Angstroms. So what motivates a beamline scientist to use a multilayer monochromator. First, the reflectivity can be very high. This, coupled with a bandwidth which, maybe typically, 100 times larger than that provided by single crystals, means that the flux output from multilayer monos can be very intense. Techniques such as X-Ray Computed Tomography profit from this as only seldomly, does a narrow bandwidth bring advantages, while rapid data acquisition can access structural and morphological changes on the sub-second or even the sub-millisecond time scale.

Notes

Summary

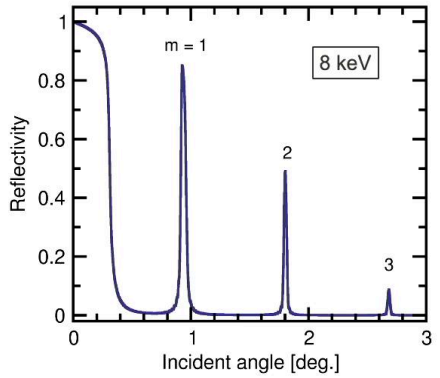
18m 02s

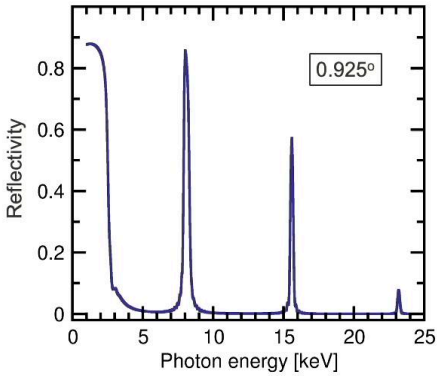
Multilayer monochromators



$$m\lambda_m = 2\Lambda \sin\theta$$

B_4C/Rh
Λ = 5 nm
d_1/d_2 = 1/3
40 layers





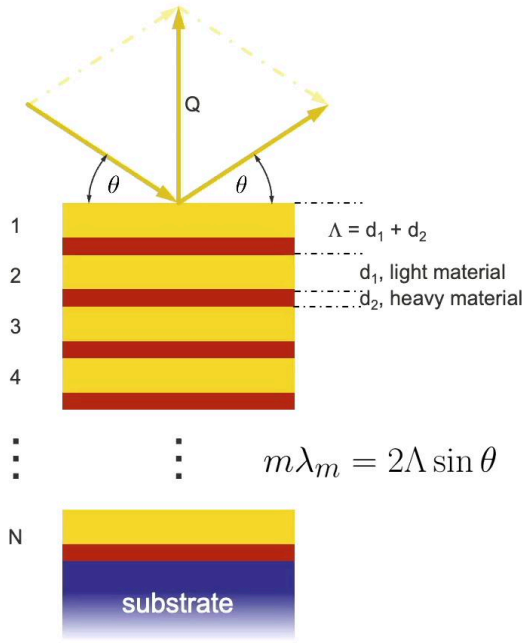
Lastly, as we will discuss in the following video, the larger periodicity of multilayers compared to crystals by an order of magnitude can lead to refraction effects that can be exploited in suppressing harmonic contamination. There are several designed parameters which determine the performance of a multilayer mono. We've already mentioned that one requires reflecting layers made of heavy metals, such as ruthenium or tungsten, separated by [inaudible 00:20:08] of space of layers made of boron, carbon, or a combination of these. The strength of the reflection is determined partly by the ratio of the thicknesses of the thick layer to the thin layer. Two thick layers means that the X-rays cannot penetrate deep enough into the multilayer, while two thin layers reduces the reflected intensity. A common ratio of thicknesses is 0.4 to 0.6, heavy to light, though this can vary depending on the applications. The total periodicity big Lambda is typically measured in a few nanometres, while the number of layers is commonly of the order of 100. The total thickness of the multilayer structure is equal to m big Lambda. So in the example here, this equates to 200 nm.

Notes

Summary

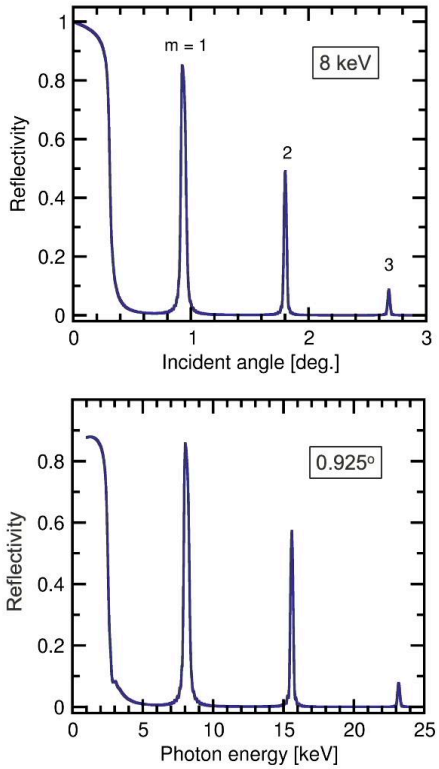
19m 33s

Multilayer monochromators



$$m\lambda_m = 2\Lambda \sin\theta$$

B4C/Rh
Λ = 5 nm
d1/d2 = 1/3
40 layers



Making this too large means that the X-rays cannot penetrate to the bottom of the structure obviating any advantages. Lastly, the layers should have atomically smooth interfaces in order to perform properly. The wavelengths that are selected are approximately given by the modified Bragg equation shown here. That is m Lambda_m, the photon wavelength, is equal to 2 times big Lambda, the multilayer periodicity, times sine Theta. For one Angstrom radiation, the example shown here results in an incident angle Theta of 0.573 degrees. Hence, the length of the multilayer surface must be big enough to accommodate the incident beam footprint and might need to be in excess of 5-10 centimetres.

Notes

Summary

21m 04s

In the next video…

In the next and last video of this week, we look at different strategies to remove unwanted higher harmonics emerging from monochromators. These include effects produced by reflection, refraction, and diffraction.

Notes

Summary

21m 58s