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USE OF UNDULATORS FOR SPECTROSCOPY WITHOUT MONOCHROMATORS

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ABSTRACT

A new spectroscopic device consisting of a multiperiod undulator and an electron storage ring for X-ray and soft X-ray spectroscopy without monochromator is proposed. The properties of the new device are described and compared with the properties of undulators combined with conventional monochromators.

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I. INTRODUCTION

Synchrotron radiation (SR) of an electron storage ring is an extremely useful excitation source for spectroscopy in a wide spectral range extending from the visible to hard X-rays. In recent years, however, undulators and wigglers as excitation sources superior to ordinary SR get more and more important [1]. Whereas SR results from the centripetal acceleration of relativistic electrons in bending magnets of the storage ring, undulator and wiggler radiation (UR, WR) is emitted by relativistic electrons passing through a periodic multipole magnetic device with either a weak magnetic field (UR) or a strong magnetic field (WR). Such devices are inserted in straight sections between bending magnets of a storage ring. Their properties were reviewed recently by, e.g., Ternov et al. [2] and by Brown et al. [3].

An undulator emits a quasimonochromatic line (first harmonic of UR) the wavelength of which is a function of the electron energy, the magnetic field strength, and the geometry of the undulator. In the center of UR, the intensity of higher harmonics is neglegible compared with the intensity of the first harmonic ($k \lesssim 1$, k being defined below).

Up to now, experiments with UR are performed with fixed electron energy of the storage ring. The wavelength of the first harmonic then can be tuned by varying the strength of the magnetic field. In this case, a change of the wavelength is accompanied by a change in the spectral shape and of the intensity of the first harmonic.

In any case, using either SR or wiggler radiation for spectroscopy, an important part of the experimental set-up is a monochromator for spectral dispersion of the radiation. Especially in the soft X-ray region, the transmission of monochromators is low due to reflection losses and due to the aberrations of the reflection optics used ($T \approx 10^{-2}$). Moreover, the transmission strongly depends on the wavelength. On a long time scale, it is not stable due to radiation damage and contamination of the optical surfaces. Of special importance is the influence of optical elements on the polarization properties of the radiation. In many cases, the higher orders are a severe problem for spectroscopy with monochromators. Nevertheless, at present, monochromators are indispensable for spectroscopy with SR and WR. In the X-ray range (including soft X-rays), a spectral resolution $\Delta\lambda/\lambda \approx 10^{-3} \dots 10^{-4}$ is obtained.

The special properties of UR enable spectroscopic experiments without monochromators. This exciting aspect of UR is discussed in the present paper. A device consisting of an undulator and a storage ring for spectroscopy without monochromator is proposed.

II. PROPERTIES OF UNDULATOR RADIATION

The properties of UR were already calculated about 10 - 15 years ago [4-7]. The properties, which are important for the use of undulators, can be summarized as follows.

1. Intensity enhancement. In the first harmonic of UR, the intensity can be enhanced by about three orders of magnitude compared with SR at the same wavelength and bandwidth.

2. Small band width. In the first harmonic of UR, the bandwidth (fwhm) is given by

$$\frac{\Delta\lambda}{\lambda} \approx \frac{1}{N} \qquad (1)$$

N is the number of periods of the magnetic field of the undulator.

3. Strong collimation. The main part of the intensity of the first harmonic is emitted into a cone, the divergence of which is comparable with the (extremely small) vertical divergence of SR.

4. Tunability by varying the electron energy. The wavelength λ of the first harmonic can be tuned by varying the energy of the electrons (fixed magnetic field). This is seen from [8,9],

$$\lambda = \frac{\lambda_o}{2\gamma^2}\cdot(1+k^2)\cdot(1+\psi^2) \quad , \quad \lambda \simeq E^{-2} \qquad (2)$$

with

$$\gamma = \frac{E}{mc^2} \quad ; \quad k = H_o \cdot \lambda_o \frac{e}{2\sqrt{2}\pi mc^2} \qquad (3)$$

E: energy, m: rest mass, e: charge of the electrons, c: velocity of light, H_o: magnetic field (amplitude), λ_o: period of the magnetic field. The expression for k is valid only for sinusoidal magnetic fields

$H(x) = H_o \sin(\frac{2\pi}{\lambda_o}\cdot x)$. ψ in equ. (2) is the reduced angle of observation of UR, $\psi = \Theta/\varepsilon$. Θ is the angle between the direction of the radiation and the axis of the radiation cone; ε is given by

$$\varepsilon^2 = (1+k^2)\cdot\gamma^{-2} \qquad (4)$$

5. Constant spectral shape. For fixed H_o, the spectral shape of the first harmonic is independent of the energy of the electrons. Moreover, the number of photons in the maximum of the first harmonic of UR is independent of E for fixed H_o [9].

6. Tunability by varying the field strength. For fixed E, the wavelength of the first harmonic can be tuned by varying H_o. This can be seen from eqs. (2) and (3),
$$\lambda \propto (1+k^2)$$
In contrast to property 4, in this case the intensity and the spectral shape are changed [4-9].

7. High degree of polarization. In so-called "plane undulators", UR is completely linearly polarized, unlike SR with its elliptical polarization. In the "circular undulator", UR is circularly polarized [5].

8. Change of polarization. Any desired degree of polarization between 100 % linear and circular polarization can be obtained using, e.g., two identical plane undulators along the x-axis if the second one is rotated by some angle around the x-axis and if the distance between both undulators can be changed [10].

9. Variable spectral shape. The spectral shape of the first harmonic can be chosen arbitrarily (within certain limits) if an undulator with variable "periodicity" of the magnetic field is used [11,12].

10. UR is calculable. The theories are already well developed to calculate the spectral and angular distribution and the polarization properties [13].

Experimental investigations of UR were performed in various laboratories [2,3,14]. Presently existing UR sources do not make use of all the ten properties listed above. Mainly properties 1-3, 6 - and in a few cases -

7,10 are used. The properties 4,5,8,9 are nearly ignored up to now. Of central importance in view of this paper is property 4 which was successfully checked for the first time with an undulator inserted into an electron synchrotron [7,15,16] and more recently in an electron storage ring [3,14]. Only if we make use of property 4, all the other properties can be used at the same time.

III. UNDULATOR RADIATION AND SPECTROSCOPY WITHOUT MONOCHROMATOR (USR-SYSTEM)

Already in refs. 7,13,15,16 it was shown experimentally that in principle a system consisting of an undulator and an electron synchrotron can serve as a quasimonochromatic tunable light source. The special properties of the undulator render unnecessary a monochromator for tuning the wavelength making use of the change of the electron energy during the period of acceleration in the synchrotron.

In view of the fundamental advantages of a spectroscopic device consisting of an undulator + accelerator it is indispensable to discuss a system consisting of a multi-period undulator with a storage ring in which the energy of the electrons can be varied slowly (undulator + storage ring (USR-) system). There is no fundamental difficulty to design such a USR-system. Already in existing storage rings like PETRA, ramping of the electron energy over a factor of 3 is performed routinely with a feedback system.

For an operation of the USR-system, the following parameters are critical, namely the range of variation of the electron energy, the divergence of the electron beam in the undulator and the length of the straight sections of the storage ring. The energy range limits the tunability of the wavelength. The beam divergence leads to a wavelength spread of the first harmonic due to the $(1+\psi^2)$-term in equ. (2). This wavelength spread should be small compared with the bandwidth of the first harmonic given by equ. (1). The length of the straight section is an upper limit for the product $\lambda_o \cdot N$.

For two storage rings (E_o = 1 GeV and 6 GeV), beam optics have been already calculated, in which the spectral line width as determined by the beam divergence is equivalent to the line width due to a 100 period undulator. The length of the straight section is L = 4 m [17]. The new ESRF source under discussion contains even longer straight sections (L = 5 m) but a somewhat larger beam divergence [18]. In view of these machine studies,

the parameters given for two undulators for a 1 GeV and a 5 GeV ring (table 1) are realistic.

Let the undulators be of the weak field type, k = 0.35, and the first harmonic may be observed in the center of the radiation cone. Note, that the undulators are of the weak field type throughout the whole range of tunability of the wavelength in contrast to those undulators in which the magnetic field gap is changed.

Concerning the tunability of the electron energy, the most pessimistic estimate is that the possibility for ramping a beam cannot be improved in the future. Nevertheless, the values of the wavelength of the first harmonic for different electron energies given in table 1 show that both the X-ray and the soft X-ray range can be covered by USR-systems. The tunability range of λ of each of the undulators roughly corresponds to the wavelength range covered by monochromators.

For a storage ring especially designed for a USR-system, one should try to increase the range of energy ramping from E_{max}/E_{min} = 3 at least to 5. With a value of about 10, a unique wavelength range by far superior to the scanning range of monochromators would be achieved. A large value of E_{max}/E_{min} has also the advantage that longer wavelengths can be produced with short period undulators leading to a moderate length of the straight sections even for high resolution (large N) devices.

IV. SOME PROPERTIES OF THE USR-SYSTEM FOR SPECTROSCOPY WITHOUT MONOCHROMATOR

IV.1 Spectral resolution

The undulators proposed in table 1 have a spectral resolution $\Delta\lambda/\lambda \approx 10^{-2}$. At first glance this seems to be not attractive compared with $\Delta\lambda/\lambda \lesssim 10^{-3}$ of crystal monochromators [19] or grazing incidence Rowland mountings [20]. We would like to point out, however, that the spectral resolution of the various non-Rowland mountings presently used in the soft X-ray range (toroidal grazing incidence monochromators [20], the FLIPPER-type monochromators [21]) is between 10^{-2} and 10^{-3}. The spectral resolution of the USR-system is not far from the resolution of such systems.

The parameters given in table 1 are based on a design of storage rings not optimized for a USR system. The emittance of a storage ring can be made even smaller than proposed in [17,18] if, e.g., the size of the storage ring is increased. Note, that the emittance scales as $E^2 \cdot \Phi^3$, where Φ is the bending angle between quadrupoles [17]. A reduction of the beam divergence by a factor of 2 which is entirely reasonable, leads to an improved $\Delta\lambda/\lambda \approx 2.5 \times 10^{-3}$ (provided the straight section is long enough for 400 periods).

Besides the beam divergence [22], the practical value of the period of the magnetic field, λ_o , is a limiting factor for the spectral resolution of the USR-system. The smallest values of λ_o are achieved with permanent magnets consisting of $SmCo_5$ alloys [23]. There is no reason to say that the present minimum for λ_o also holds for the future. Recently the use of antiferromagnetic materials was proposed to improve the properties of an undulator [24]. With such devices, in principle, 10^4 or more periods could be used. If the beam divergence of the electrons could be reduced considerably, a really exciting new era of X-ray and soft X-ray spectroscopy would start.

It must be admitted, however, that the ultimate resolution of a USR-system is also determined by additional spectral broadening of the first harmonic by various effects like, e.g., the finite beam size, the stability of the beam during ramping, the energy spread of the electron beam, the accuracy of the periodicity, and the homogeneity of the magnetic field. Various broadening effects have been discussed in the literature [22,25].

IV.2 Intensity, higher order- and stray light-rejection

Concerning the number of photons per resolution interval and per second at the sample, the USR-system has to be compared with a system consisting of an undulator and a monochromator. The USR-system avoids the transmission losses of the monochromator. In the soft X-ray range this means a gain in intensity by up to two orders of magnitude.

Experiments with a conventional system consisting of a SR- or WR-source and a monochromator often suffer from higher orders and from stray light. A USR-system with a weak field undulator and an observation angle $\psi = 0$ is free of higher orders in the whole spectral range. A combination of a USR-system and an additional monochromator which is synchronized to the

USR-system, acts as a double monochromator concerning stray light rejection. Especially in the soft X-ray range this would be a substantial improvement compared with the presently existing systems.

IV.3 Polarization

The unique polarization properties of UR were already summarized in section 2 [13,26,27]. They hold independent of whether an additional monochromator is used or not. However, each additional optical element between the radiation source and the sample can change the polarization properties. From experience it is known that an exact control of these changes is extremely difficult in the short wavelength range.

The USR-system is the only quasimonochromatic, tunable radiation source in the X-ray and soft X-ray range, the polarization properties of which can be chosen arbitrarily.

IV.4 Variation and measurement of the wavelength

It is expected that the ramping of the electron energy will be performed computer controlled. Then various kinds of operation are possible from a stepwise to a continuous scanning mode.

Though it is no central point in this paper, we would like to propose the following law for the time dependence of the electron energy E,

$$E = E_{max} \cdot e^{-\alpha t} \qquad (5)$$

(α: rate of decrease of the electron energy). This law has an interesting consequence. Given a fixed time interval, Δt , of registration of a point of the spectrum, the relative change in electron energy, $\Delta E/E$, during Δt, is constant, independent from E itself. From equ. (2) it is seen that the relative change of the wavelength of the first harmonic, $\Delta\lambda/\lambda$ = constant, too. This is quite different from conventional monochromators in which the wavelength is changed by steps of fixed $\Delta\lambda$, independent of the respective wavelength.

The actual wavelength of the light emitted by the USR-system can be calculated from the actual energy of the electrons (equ. (2)). This requires an accurate measurement of E with $\Delta E/E \approx 10^{-4} \ldots 10^{-5}$ depending on the spectral resolution of the USR-system.

If, however, users of a USR-system would like to have at their disposal an independent calibration system for the actual wavelength of the first harmonic of the undulator (period $\lambda_{o,1}$) this can easily be done by comparison with a second undulator (period $\lambda_{o,2}$) equipped with a conventional monochromator because from equ. (1) we see

$$\frac{\lambda_1}{\lambda_2} = \frac{\lambda_{o,1}}{\lambda_{o,2}} \qquad (6)$$

This holds for the same E and the same k. We point out this special possibility because the calibration of the actual wavelength can be done routinely in a different wavelength range in which the experimental requirements may be much more simple. Such a combination of two undulators could be regarded as a "wavelength transformer".

V. CORRECTION OF THE ELECTRON TRAJECTORY IN UNDULATORS

A USR-system requires a change of electron energy in a wide range, combined with a fixed magnetic field. This leads to a great importance in designing the correction sections at both ends of the undulator. For a USR-system, it is indispensable that the axis of the trajectory of the electrons remains fixed for different electron energies, because a fixed radiation cone is required.

Presently, in general, only one correction section is used at each end of the undulator (with $1/2\ H_o$). This is shown schematically in fig. 1a. In this case, the axis of the electron trajectory does not coincide with the axis of the undulator [28]. We have to distinguish two possibilities depending on the number of magnetic sections, N' (one magnetic section is half of the period of the magnetic field of the undulator).

(i) With an even number of sections, $N' = 2k$, $(k = 1,2,3 \ldots)$ the axis of the trajectory is tilted by an angle φ inside the undulator (fig. 1b).

(ii) With on odd number of sections, $N' = 2k-1$ $(k = 1,2, \ldots)$ the axis of the trajectory is displaced parallel to the axis of the undulator by an amount of a (fig. 1c).

The values of a and of φ depend on the strength of the magnetic field and on the energy of the electrons.

For USR-systems, it is preferable to use two correction sections at each end of the undulator (fig. 2a). The length of the correction section should be the same as the length of the main section in order to maintain the spectral shape of the first harmonic. The x-variation of the magnetic field should be the same in all sections (e.g., sinusoidal). In the first and in the last section, the amplitude of the magnetic field should be $1/4\ H_o$, in the adjacent sections $3/4\ H_o$, and in all other sections H_o [12,28,29]. It was shown that in this case the radiation cone and the axis of the undulator coincide, independent of H_o, N', and the electron energy [29] (fig. 2b).

VI. CONCLUDING REMARKS

In this paper we discussed the potential properties of a new source of quasimonochromatic, tunable, highly collimated X-ray and soft X-ray radiation consisting of an electron storage ring and an undulator with a high number of periods and with a fixed magnetic field. Tunability of the wavelength is achieved by ramping the electron energy.

The various aspects of such a system lead to the following parameters for the storage ring.

(i) $E_{max}/E_{min} = 5 \ldots 10$. With $E_{max} \approx 5$ GeV, the X-ray and the soft X-ray range could be covered. $E_{max} \approx 1$ GeV would even make accessible the VUV spectral range.

(ii) For a spectral resolution of $\Delta\lambda/\lambda \lesssim 2.5 \times 10^{-3}$, the beam divergence of the storage rings proposed in ref. 17 have to be reduced to ~ 50 %.

(iii) The length of the straight section must be ~ 6 m, provided $E_{max}/E_{min} \approx 10$. Otherwise, either the spectral range must be restricted, or L should be longer.

Detailed machine studies are required now to check whether such systems are feasible.

USR-systems could bring about considerable progress in various fields of spectroscopy. The increase of excitation intensity by up to two orders of magnitude may perhaps lead to a breakthrough for the investigation of secondary effects like X-ray fluorescence under primary state selective excitation.

The most exciting aspect of the USR-system is the fact that it is the only radiation source in the X-ray range known so far, which allows for a free choice of polarization from the linear via any degree of elliptic to the right or left hand circular type. Various types of experiments in atomic, molecular, and solid state spectroscopy could benefit from this property.

Finally, we want to point out, that the USR-system could also be used as a quasimonochromatic, tunable radiation standard for, e.g., calibration of radiation sources, of photon detectors, determination of the transmission function of monochromators, and optical elements. This highly interesting aspect, however, was not discussed in detail because it is beyond the scope of this paper.

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TABLE 1

Parameters of two undulators (k = 0.35; λ_o = 1.5 cm and 4 cm) inserted into storage rings with E_o = 5 GeV (case 1) and 1 GeV (case 2). An energy ramping by a factor of 3 is assumed. The wavelength of the first harmonic given as a function of the electron energy holds for ψ = 0. For the numbers in brackets see text.

Number of periods, N		100	(400)
Band width, $\Delta\lambda/\lambda$ = 1/N		10^{-2}	(2.5×10^{-3})
	e^--energy range	wavelength (λ_o=1.5 cm)	- scanning range (λ_o=4 cm)
case 1	5 to 1.67 GeV	0.879 to 7.88 Å	2.93 to 26.3 Å
case 2	1 to 0.33 GeV	22 to 202 Å	73.3 to 673 Å

FIGURE CAPTIONS

Fig. 1 Schematic concept of an undulator with one correction section (1/2 H_o) at each side (a) and an electron trajectory for an even (b) and an odd (c) number of sections.

Fig. 2 Schematic concept of an undulator with two correction sections (1/4 H_o, 3/4 H_o) at each side (a) and the corresponding electron trajectory (b).

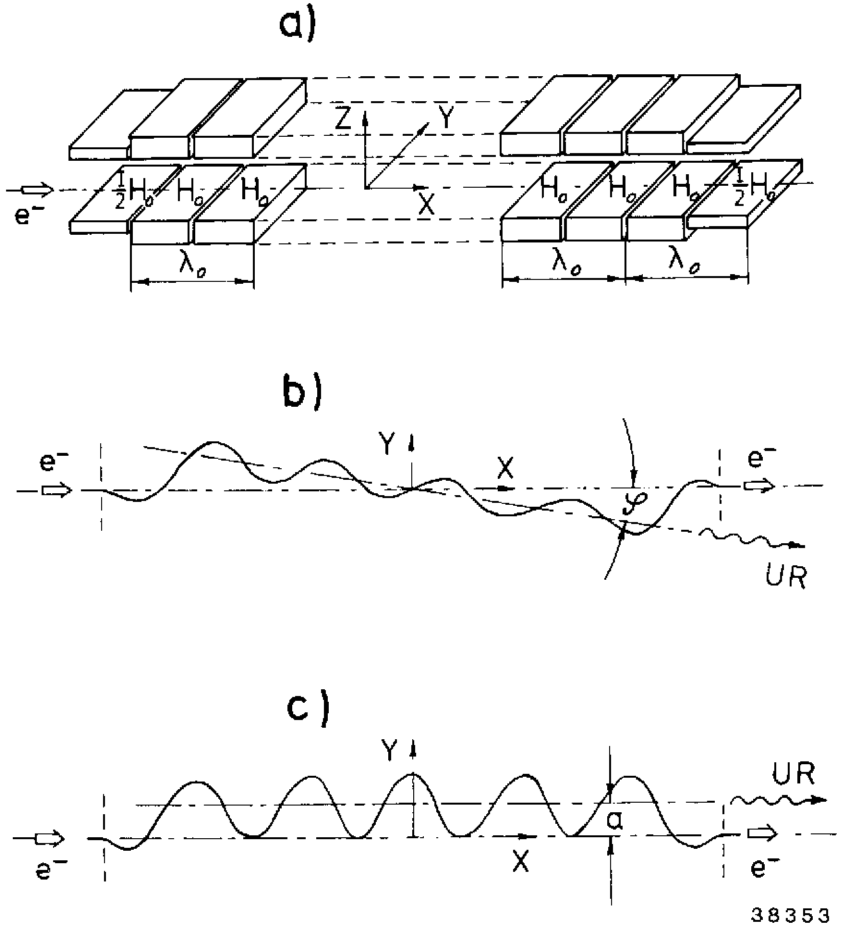

Fig. 1

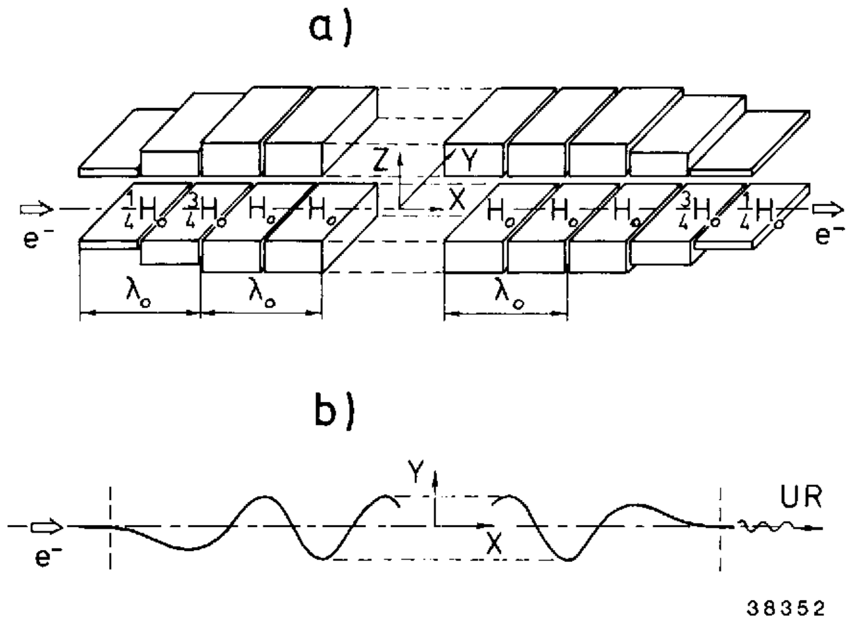

Fig. 2