Soft x-ray spectroscopy beam line on the NSLS X1 undulator: Optical design and first performance tests

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(Presented on 18 July 1991)

The layout and first data on the performance of the soft x-ray undulator beam line on the x-ray ring at Brookhaven are described. The undulator (X1) has 35 periods of 8 cm, resulting in a tuning range for the fundamental of about 200–700 eV at the nominal ring energy of 2.5 GeV. The monochromator is based on the Dragon concept with spherical grating, movable exit slit but with water-cooled optical elements in order to deal with the maximum flux of ca. 400 W. This system represents one of the next generation of soft x-ray undulator beam lines which will figure prominently at new synchrotron radiation facilities such as ALS, ELETTRA and BESSY II. During the first performance tests absorption spectra of simple molecules at the C, N, and O K edges have been recorded with resolution and flux so far unattained in the soft x-ray region.

I. INTRODUCTION

The next generation of synchrotron radiation (SR) facilities serving the soft x-ray region will be characterized by electron beam energies in the range 1.5–2.0 GeV. Undulators installed on such storage rings will have fundamentals covering the spectral range 100–1000 eV, thus providing extremely bright sources of vacuum ultraviolet (VUV) and soft x-ray radiation for a variety of innovative experiments in microscopy, structural research, and spectroscopy. Since SR facilities in a similar energy range already exist (e.g., the Brookhaven x-ray ring or Photon Factory), attention has recently focused on the performance and application of undulators on these storage rings. At Brookhaven, for example, it has been shown that the X1 undulator[1] has a central intensity of more than 10^{15} photons s^{-1} 0.1% BW^{-1} $mrad^{-2}$ at $h\nu = 345$ eV, which is within a factor of 2 of the design value.[2] X1 is thus probably the world's brightest source of soft x radiation currently available. The microscopy beam line (X1A) on the undulator is already in use for scanning transmission x-ray microscopy, scanning photoemission microscopy, and Gabor holography.[2] Installation of the spectroscopy beamline (X1B) has just been completed and the first performance tests carried out. The monochromator, based on the Dragon concept[3,4] has a spherical grating and a moveable exit slit. The two focussing premirrors, the entrance slit, and the grating are cooled in order to cope with the maximum flux of ca. 400 W.[5] The beam line will be used for a variety of photoionization-based experiments in atomic and molecular physics as well as in surface and solid-state studies.

There is extensive interest in performing such experiments in the soft x-ray region since the K levels of C, N, O, and F as well as the L levels of the first row transition metals fall in the photon energy range 250–1000 eV. The development of suitable grazing-incidence grating monochromators with high spectral resolution for such studies has now become of paramount importance. Electron energy loss and photoabsorption experiments, for example, have shown that the natural linewidths of the K levels of C, N, and O in free molecules can be below 100 meV.[4,6,7] At such high resolution it becomes difficult to match the size and divergence of the source to the phase space acceptance of the monochromator, such that the flux decreases no more than linearly with the resolution. In the past, most of the experiments conducted on bending magnet monochromators in this energy range have suffered either from low instrumental resolution or from low spectral flux. Thus on both the Dragon monochromator on the UV ring at Brookhaven[4,6] and the SX-700 II monochromator at BESSY,[7] the intensity at the highest spectral resolution is probably not sufficient for performing photoelectron spectroscopy on free atoms and molecules. On the other hand, the high-energy toroidal grating monochromator (TGM)[8] at BESSY offers sufficient intensity for such gas-phase experiments but only at very poor resolution. It is clear that an undulator offers considerable advantages in this situation: First, the spectral flux from an undulator, integrated over the central cone, is typically a factor of 10 higher than the flux from 10 mrad of a bending magnet source. For practical reasons including size, quality, and cost of the optical elements, horizontal acceptance angles larger than 10 mrad are difficult to realize in this energy region. Second, the undulator source can be matched to the monochromator more efficiently because of the inherently higher spectral brilliance. It transpires that at the ultimate reso-

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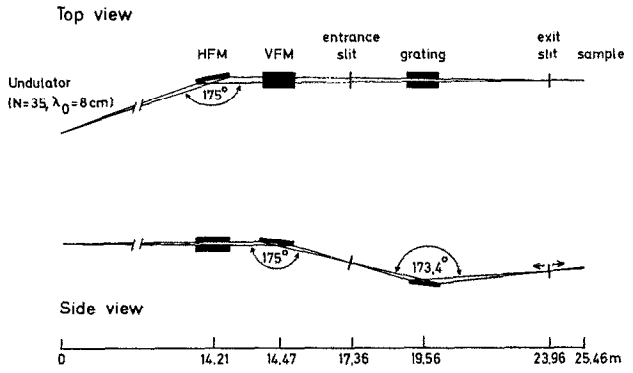

FIG. 1. The layout of the X1B monochromator.

lution at least another order of magnitude in flux may therefore be available for the experiment concerned.

In the present paper we describe the layout of the new X1B spectroscopy beam line at Brookhaven and, in order to obtain some indication of the resolution, show core-level photoabsorption data taken for the molecules CO, N_2, and O_2.

II. DESIGN CONSIDERATIONS AND LAYOUT OF X1B

The two most important requirements for a soft x-ray monochromator on a spectroscopy beam line are high intensity and high resolution. For X1 we have chosen a version of Chen's cylindrical element monochromator (CEM), similar to the Dragon on the Brookhaven UV ring. The CEM combines high resolution with high transmission, since only three reflecting elements are required and the resolution is determined largely by the slope error of the cylindrical or, in this case, spherical grating. The latter is located between the entrance slit and a moveable exit slit, thus giving rise to a layout similar to the TGM. However, the CEM is capable of higher resolution than the TGM because of the movable exit slit which fulfills the focusing condition and because of the rectangular beam cross section. Similarly, the CEM design has certain advantages over the BESSY/Zeiss SX-700 monochromator, which has no entrance slit. The ultimate resolution of the latter instrument is determined by the vertical source size and the slope error of the aspherical focusing mirror. We note that a resolution comparable to that of the Dragon is only obtained with the SX-700 by stopping down the optics and working in second order.[7]

For more details of the undulator and of the X1 beam line up to the main mirror box, where the two branch lines separate, the reader is referred to Ref. 2. For the microscopy and imaging experiments[2] a water-cooled plane metal mirror intercepts the beam at a grazing angle of 40 mrad, deflecting it into the X1A beam line. When this mirror is withdrawn the undulator radiation falls upon the horizontally focusing cylindrical mirror (HFM) of X1B. The layout of the monochromator is shown in Fig. 1; the detailed design parameters are given in Ref. 5. The HFM focuses the source onto the sample in the experimental chamber, reducing it in size by a factor of 0.8, which, ignoring aberrations, gives an image of approximately 300 μm wide (σ). This mirror absorbs most of the power radiated by the undulator, thus protecting the more critical optical elements. In addition, it fulfills the requirement that X1A and X1B are separated horizontally. The second cylindrical mirror (VFM) focuses the undulator radiation vertically onto the water-cooled entrance slit. With a 5:1 demagnification the image size at the slit is approximately 5–10 μm(σ) in height, thus still giving maximum transmission efficiency even at the smallest slit settings required for the ultimate resolution. Demagnifying the image also has the concomitant effect of increasing the vertical divergence by a factor of 5 to 300 μrad (σ). A vertical divergence of less than 100 μrad would mean that the grating would be under-illuminated to such an extent that the resolution would be diffraction limited. On the other hand, with a vertical divergence greater than 500 μrad the grating would be over-illuminated and hence the resolution aberration limited. This is a particular problem at near-to-grazing angles of incidence, corresponding to the photon energy range 180–300 eV.

Both mirrors have been manufactured in aluminium by Zeiss (Oberkochen, Germany) and coated with Kanigen and gold; each is water cooled and mounted with five independent degrees of freedom on bellows for *in situ* adjustment (two linear motions, pitch, roll, and yaw).

The entrance slit is also water cooled for better stability. The monochromator will eventually have a grating exchange mechanism, which will allow three gratings to be installed. At present, the single 800 l/mm grating is mounted in a holder which is water cooled along the sides to minimize distortion. It was mechanically ruled by Hyperfine Inc. (Boulder, Colorado, USA) into Au on a spherical fused silica blank. The exit slit moves in order to fulfill the focusing condition and to maintain the best resolution during a wavelength scan. At present, this slit is not water cooled, because the power load is much less than at the entrance slit. After the exit slit the beam diverges vertically resulting in a spot in the sample chamber less than a square millimeter in size.

The calculated spectral resolution for the X1B monochromator is shown in Fig. 2 as a function of photon energy for an 800-l/mm grating, 5-μm entrance and exit slits and a 0.5-arc sec slope error. The calculation has been performed using Eqs. (1)–(5) in Chen's paper.[3] At the same time, the individual contributions of the coma, the entrance and exit slits and the slope error are indicated. Not shown is the contribution due to the diffraction limit which has been included in the "total" curve assuming a vertical divergence of 300 μrad (σ). If the nominal slope error of 0.5 arc sec of the spherical grating is achieved in practice, a resolution $E/\Delta E$ of $\sim 8 \times 10^3$ at the N K edge and $> 1 \times 10^4$ at the C K edge would appear possible. As will be shown below, there is a strong possibility that this calculated resolution will actually be reached. We also note from these model calculations depicted in Fig. 2 that for 5-μm slits the slope error effectively determines the resolution. For 10-μm slits (not shown) the contribution of

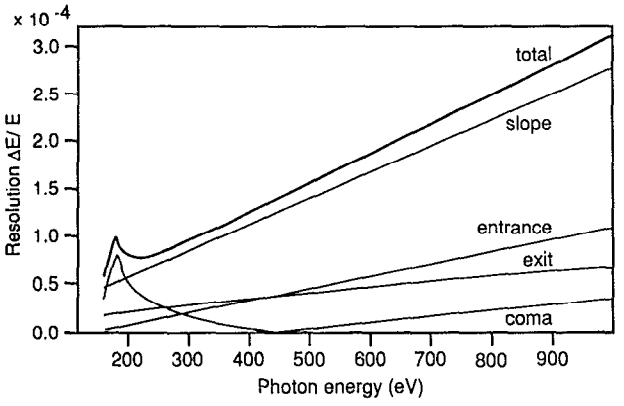

FIG. 2. The calculated resolution of the X1B monochromator as a function of photon energy for exit and entrance slits of width 5 μm, 0.5 arc sec slope error on the 800 l/mm spherical grating and a vertical divergence of 300 μrad (σ). Also shown are the contributions to the total resolution from coma, slit width, and the slope error.

each of the other parameters is of the same order of magnitude as that of the slits.

III. PHOTOABSORPTION DATA FOR CO, N_2, AND O_2

The C1$s\rightarrow\pi^*$ transition in the core-level photoabsorption spectrum of CO is shown in Fig. 3. The spectrum was measured directly in absorption using a GaAsP diode as detector. The gas cell was 25 cm long and filled to a pressure of $\sim$10 mTorr. Both entrance and exit slits were set for maximum resolution at 5 μm; the total measuring time was 5 min. The photon energy scale was calibrated by reference to the electron-energy-loss spectroscopy (EELS) data of Tronc *et al.*[9] The vibrational structure in the spectrum of Fig. 3 is clearly resolved; the separation between the $v'=0$ and $v'=1$ lines is ca. 250 meV, in agreement with the analysis of Domke *et al.*,[7] who give a value of 256$\pm$2 meV. The instrumental resolution is undoubtedly

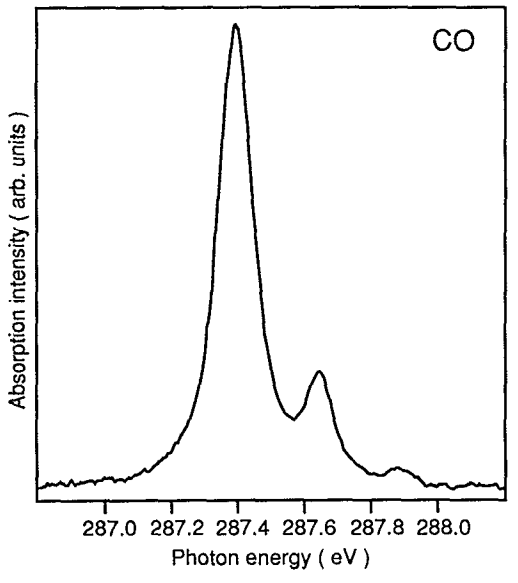

FIG. 3. The C1$s\rightarrow\pi^*$ transition in the core-level photoabsorption spectrum of CO.

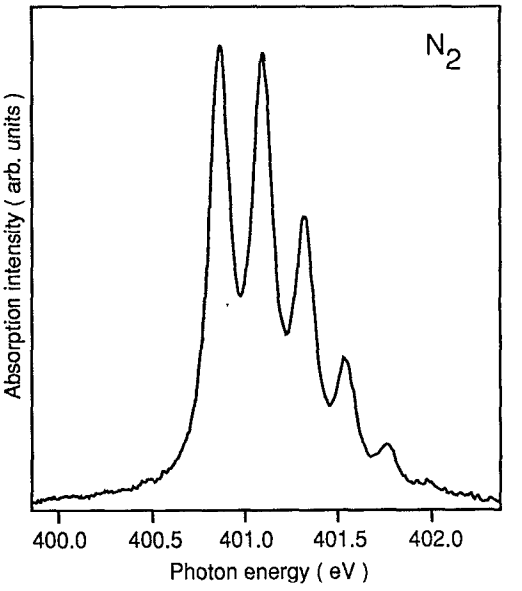

FIG. 4. The N1$s\rightarrow\pi^*$ transition in the core-level photoabsorption spectrum of N_2.

better (higher peak-to-valley ratio) than in the latter paper where a value of 80 meV is given. The as-measured linewidth of the $v'=0$ peak is 130 meV, compared to the natural linewidth of 100 meV quoted by Tronc *et al.*[9] Assuming addition in quadrature, this would indicate an instrumental resolution of 83 meV, which seems somewhat high compared to the 80-meV value quoted by Domke *et al.*[7] This short discussion highlights the problems associated with the quantitative determination of resolution in this spectral region. Deconvolution routines to separate out pure Gaussian and Lorentzian components also lead to misleading results in the C1s spectrum of CO.[10]

The corresponding N1$s\rightarrow\pi_g^*$ absorption spectrum for N_2 taken under the same conditions is shown in Fig. 4. The energy scale was calibrated via the $v'=1$ line in the EELS spectrum of Tronc *et al.*[11] Because of the pronounced vibrational fine structure, it is not possible to give a value here for the as-measured linewidth without deconvolution. Chen and Sette[4] find that such a deconvolution can be performed entirely with Lorentzians, a fact which they interpret as being due to a very small contribution from instrumental (Gaussian) broadening. The resolution of the Dragon monochromator at this photon energy is estimated to be lower than 40 meV based on a comparison with EELS data. Whereas this cannot necessarily be accepted as a definitive value, Chen and Sette do propose useful criteria for determining the comparative resolution of soft x-ray monochromators. They take the first valley to third peak ratio in the N1$s\rightarrow\pi_g^*$ absorption spectrum for N_2 (at 400.95 and 401.31 eV, respectively) which is about unity in the EELS data for 70-meV instrumental resolution.[12] Approximately the same value is obtained on the SX-700 II in first order but improves to $\sim$0.85 in second order.[13] The resolution of this monochromator in second order is thought to be $\sim$74 meV at 400 eV.[13] Chen and Sette[4,6] also obtain $\sim$0.85 compared to the value of 0.73 obtained on

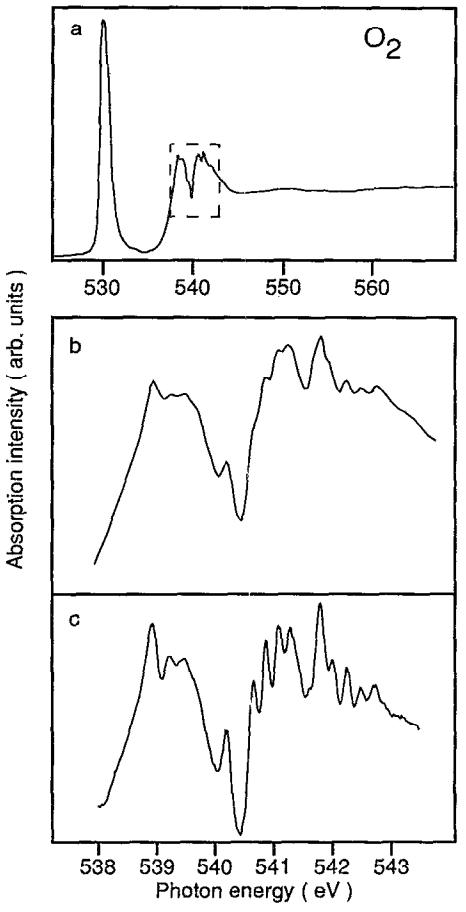

FIG. 5. The core-level absorption spectrum of O_2. (a) Overview spectrum from Ma *et al.*[14] (b) The expanded Rydberg region also from Ref. 14. (c) Same region as (b) taken on the X1B monochromator.

X1B and shown in Fig. 4. This is a clear indication of a significant increase in spectral resolution compared to the two bending magnet monochromators. A conservative estimate at this stage would therefore place the absolute value of the spectral resolution on X1B significantly below 70 meV at 400 eV.

A similar improvement in resolution compared to previous results is seen in the O1$s\rightarrow$Rydberg region of the photoabsorption spectrum of the oxygen molecule. The individual transitions have recently been assigned by Ma *et al.*,[14] whose spectra are shown in Fig. 5(a) and 5(b). Spectrum (b) is a magnified view of the Rydberg region enclosed by a dashed line in spectrum (a). The higher resolution in spectrum (c) taken on X1B is immediately apparent. The photon energy scale has been calibrated by reference to the EELS data of Hitchcock and Brion[15] ($4p\pi_u/3p\sigma_u$ line[14] at 541.8 eV). Note that there are two Rydberg series in the spectrum converging to the $^4\Pi$ and $^2\Pi$ ionization thresholds at 543.1 and 544.2 eV, respectively.

The first flux measurements at the exit slit of the X1B monochromator at 400 eV have given values of $\sim 1 \times 10^{11}$ photons s^{-1} using a Hamamatsu GaAsP diode as well as $\sim 4 \times 10^{11}$ photons s^{-1} using a calibrated (oxidized) aluminium photodiode of the sort previously used at Brookhaven.[16] For these measurements the monochromator was operated with 20-μm entrance and exit slits which then gives a spectral resolution similar to that measured on the Dragon under optimal conditions (N_2 adsorption spectrum, $v/p \sim 0.85$). In order to relate these figures to monochromators on bending magnets, we note that 1×10^{11} is a typical value measured with the same GaAsP diode at the exit slit of the HE-TGM 1 at BESSY where the resolution is only about 1 eV at 400 eV photon energy.

IV. CONCLUSIONS

The very first data from the X1B beam line, taken just a few weeks prior to this meeting indicate that there is a good chance that the design performance of the monochromator will be met in practice. Because natural linewidths are not known for the core-level absorption spectra of C, N, and O in small molecules, quantitative information on resolution cannot be given. It is, however, already clear that the resolution at 400 eV lies well below 70 meV, thus approaching the design value given by $E/\Delta E = 8 \times 10^3$ for this energy. Moreover, a comparison with the corresponding spectra from the Dragon (Brookhaven UV ring) and the SX-700 II (BESSY) suggests that the resolution on X1B is significantly higher. As expected, the flux is at least a factor of 10 higher than for similar monochromators installed on bending magnets and operating at comparable resolution. With cautious optimism we expect further improvements as commissioning proceeds.

ACKNOWLEDGMENTS

This project has been financed in part by the German Federal Ministry of Research and Technology under Contract 05 490 FXB/TP1. The work at Brookhaven is supported by the US Department of Energy under Contract DE-AC02-76CH000016.

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