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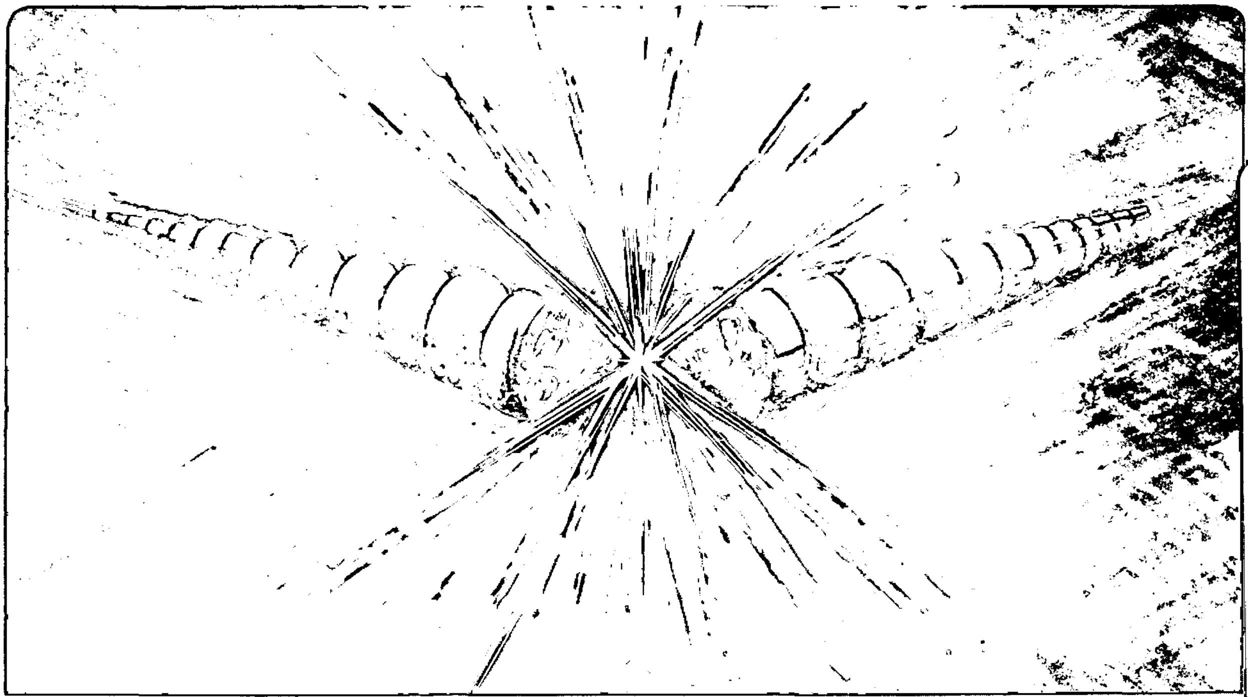

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The Advanced Light Source U8 Beam Line, 20 - 300 eV

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The U8 is a beam line under construction at the Advanced Light Source (ALS). The beam line will be described along with calculations of its performance and its current status. An 8 cm period undulator is followed by two spherical collecting mirrors, an entrance slit, spherical gratings having a 15° deviation angle, a moveable exit slit, and refocusing and branching mirrors. Internal water cooling is provided to the metal M1 and M2 mirrors as well as to the gratings. Calculations have been made of both the flux output and the resolution over its photon energy range of 20 - 300 eV. The design goal was to achieve high intensity, 10^{12} photons / sec, at a high resolving power of 10,000. The U8 Participating Research Team (PRT) is planning experiments involving the photoelectron spectroscopy of gaseous atoms and molecules, the spectroscopy of ions and actinide spectroscopy.

I. Introduction

The ALS U8 is an example of a Spherical Grating Monochromator (SGM).[1,2] Several limitations on monochromator resolution have been addressed by the SGM optical design. Errors in the fabrication of the gratings (and collecting mirrors) are minimized by using spherical surfaces. The contribution from fabrication tolerances is further reduced by having only one optic in between the entrance and exit slits. Aberrations are small compared with Toroidal Grating Monochromators (TGM), which have large astigmatic coma. Finally, slit width limits are diminished by increasing the radius of the grating, which is also equivalent to making the distances between the grating and the slits larger.

The resolving power of SGMs has already been a proven success.[2,3] Monochromator resolutions have been demonstrated smaller than the natural linewidths for core-hole excited molecules.[4] At smaller excitation energies valence hole states may have considerably longer lifetimes and correspondingly smaller linewidths. A number of experiments have not been possible at the highest resolution, such as angle resolved photoemission of gases or coincidence experiments. The U8 beam line will achieve high flux because of two reasons. The source is a 4.5 m long undulator. Secondly, the small dimensions of the electron beam passing through the undulator are further demagnified in order to maximize the transmission through a 10 μm entrance slit.

The energy range of the beam line extends from 20 - 300 eV. At the low photon energy limit, 21.2 eV will be accessible, where many He I photoelectron spectra are available for comparison. At high energies the monochromator will reach the K ionization edge of C, important for the spectroscopy of organic molecules.

Figure 1 displays the layout of the U8 beam line. Not shown are the 8 cm period undulator source or the front end. The first optical element, the M1 spherical mirror focuses the beam horizontally at the sample chamber. A second spherical mirror, M2 provides the vertical focus at the fixed entrance slit with a demagnification of 15 to 1. The grating chamber houses three spherical gratings, which have a deviation angle of 15°. The M1 and M2 mirrors and the gratings are made of Glidcop^{TM} with internal water cooling channels to reduce the thermal distortion. The exit slit is moveable to satisfy the grating focus condition. Finally, the M3 bendable mirror will refocus the beam vertically and plane mirrors may deflect the beam horizontally to provide a focus in different experimental chambers.

This report presents calculations of the resolution and flux of the ALS U8 beam line.

II. Monochromator Resolution

The resolution goal of our monochromator design is a resolving power of 10,000. The results of analytical calculations are shown in figure 2. This calculation considers different terms in the optical path function expansion according to the method of Hogrefe et al.[1] The full width at half maximum (FWHM) of a particular aberration is computed. In Fig. 2 the dashed curve for each grating represents the most important aberration of SGMs, coma. Except at the Rowland circle energy (where coma vanishes), both spherical aberration and line curvature are about an order of magnitude smaller than coma. The contribution of 10 μm slit openings are shown by the solid curves in Fig. 2. The effect of the entrance slit or of the exit slit is shown, whichever is greater. At low energies for each grating, the exit slit contribution is larger.

Including aberrations and slit width limits, a resolving power of 10,000 can be obtained except for the small photon energy range below 25 eV. Depending on the energy, either the contribution from the slit widths or the coma aberration is more important. In addition, figure errors from the grating fabrication are also critical. Our specification for the tolerance of the slope error is 0.5 μrad rms. Similar resolution values have already been achieved by different SGM monochromators.[2,3] For example, at the LBL SGM at the Stanford synchrotron, we have determined the resolution from fitting the vibrational peaks of the nitrogen 1s - π^* resonance. A resolving power of 6600 was achieved with 5 μm slit openings.

III. Photon Flux

The beam line flux is constructed from the undulator output together with the separate efficiencies of all the elements of the U8 beam line: M1 and M2 mirrors, the entrance slit, the diffration grating and the exit slit. The curves for the undulator output are derived from formulae of Kwang-Je Kim.[5] The 10^{15} photons / sec. are delivered in a 0.1 % bandwidth, which represents an integration over the central cone with the undulator gap chosen to position the maximum of the appropriate harmonic at the given photon energy. Gratings 1 and 2 are matched with the fundamental and grating 3 with the third harmonic. The undulator gap must be varied so that the appropriate harmonic contains photons of the correct wavelength on axis, in the central cone.

The reflectivity of the collecting mirrors is calculated from a routine based on the method of Henke.[6] Fresnel's equations are used together with tabulated values of the f1 and f2 optical constants. The U8 M1 mirror will have two coatings, carbon for 20 - 260 eV and nickel for 80 - 300 eV. To switch between coatings will require a vertical translation of the M1 mirror chamber. The U8 M2 mirror with its nickel coating will give an 18 % dip at 68 eV because of the Ni 3p edge.

To evaluate the transmission through the entrance slit, the effects of the demagnified source and of the spherical aberration of the condensing mirror are combined. The spherical aberration is the dominant aberration for spherical mirrors with large demagnifications. For both effects intensity distributions are calculated vertically across the entrance slit. In the case of spherical aberration, the distribution of rays on the condensing mirror is first considered. Then, this distribution is projected onto the slit resulting in a function that is infinite at zero with a tail at positive heights above the slit center. The 15 times demagnified source corresponds to the perfect image of the gaussian electron beam. The extended nature of the undulator source is included through using the diffraction limited source size. Finally, the spherical aberration distribution and the demagnified source distribution are convoluted together and then integrated over the entrance slit opening. The entrance slit width is varied in order to fix the slit-limited resolving power at

10,000. The slit width varies from 11 to 66 μm for this resolving power with the grating aberrations are not included. The transmission through the entrance slit is roughly 70 %.

The efficiency of the gratings includes three factors: the collection, the diffraction efficiency and the reflectivity. The grating collects most of the incident beam on its optical surface. The collected fraction is derived from the beam divergence, which in turn depends both on the geometric divergence of the undulator central cone, increased by the mirror demagnification and on the diffraction from the entrance slit. The contribution from diffraction is approximated by a gaussian, whose standard deviation is given by $\sigma = \lambda / 2d$, where λ is wavelength of the radiation and d is the slit opening. In general, the grating acceptance is unity and then decreases as the horizon energy is approached.

The calculation of the first order diffraction efficiency is based on the thesis of Bennett.[7] This scalar theory for laminar gratings includes the interference between the top and bottom of the grooves and the masking of the bottom by the top of the grooves. The groove depths are chosen to place the diffraction efficiency maximum in the center of the energy range over which the gratings have high resolving power. Laminar gratings are preferable because of the relatively wide energy range with good efficiency. The limited scanning range of each grating (E to 3E) is an unavoidable consequence of the SGM having a fixed deviation angle.

The reflectivity of the gratings is computed from the optical constants in the same way as the reflectivity of the mirrors. However, the appropriate angle to use with gratings, i.e. which combination of α or β, is not obvious. The grating reciprocity theorem states that the efficiency for the grating to diffract the beam from the entrance slit in first order onto the exit slit must be the same as the efficiency for the grating to diffract a hypothetical beam from the exit slit in negative first order onto the entrance slit. Following experimental work of Werner Jark[8] and Howard Padmore,[9] the deviation angle has been used here in the calculation of the grating reflectivity. The reflectivity is high for the two lower energy gratings, but worse for the high energy grating. This variation results from the critical angle becoming more grazing at higher energies.

The exit slit opening is varied to always have a slit-width limited resolving power of 10,000. Because the initial undulator flux is calculated for a fixed bandwidth, this choice of varying the exit slit width results in a constant transmission. The resolution is irrelevant for the exit slit efficiency because a broadened image results in equal amounts of the correct wavelength hitting the slit and of the wrong wavelength passing through the slit.

The final, resolved flux after the exit slits is shown in figure 3. (The refocussing optics is not included). An overlap is provided from one grating to the next of 20 eV. An intensity in the range of 10^{12} - 10^{13} photons / sec. is obtained at a resolving power of 10,000 (neglecting grating aberrations and figure errors).

IV. Summary

Analytical calculations have been described, which predict the resolution and flux from the ALS U8 beam line. The coma aberration and slit widths give the largest contributions to the monochromator resolution. Nevertheless, except for a small energy range, 10,000 resolving power should be achieved. The U8 beam line design attempts to preserve the high brightness of its undulator. After losses on the optical elements and at the slits, the U8 beam line still has a flux of 10^{12} - 10^{13} photons / sec. at high resolution.

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Figure Captions

Figure 1: The layout of the beam line: the horizontal (M1) and vertical (M2) focussing mirrors, the entrance slit, the three spherical gratings having a 15° deflection angle, the moveable exit slit and the M3 refocusing mirror. Not shown are the 8 cm period undulator and the front end.

Figure 2: The calculated resolution, where the solid lines show the slit width limit (10 μm) and the dashed lines show the worst aberration coma.

Figure 3: The calculated photon flux for 10,000 resolving power (slit width limit) and 400 mA. Three gratings span the energy range 20 - 300 eV.

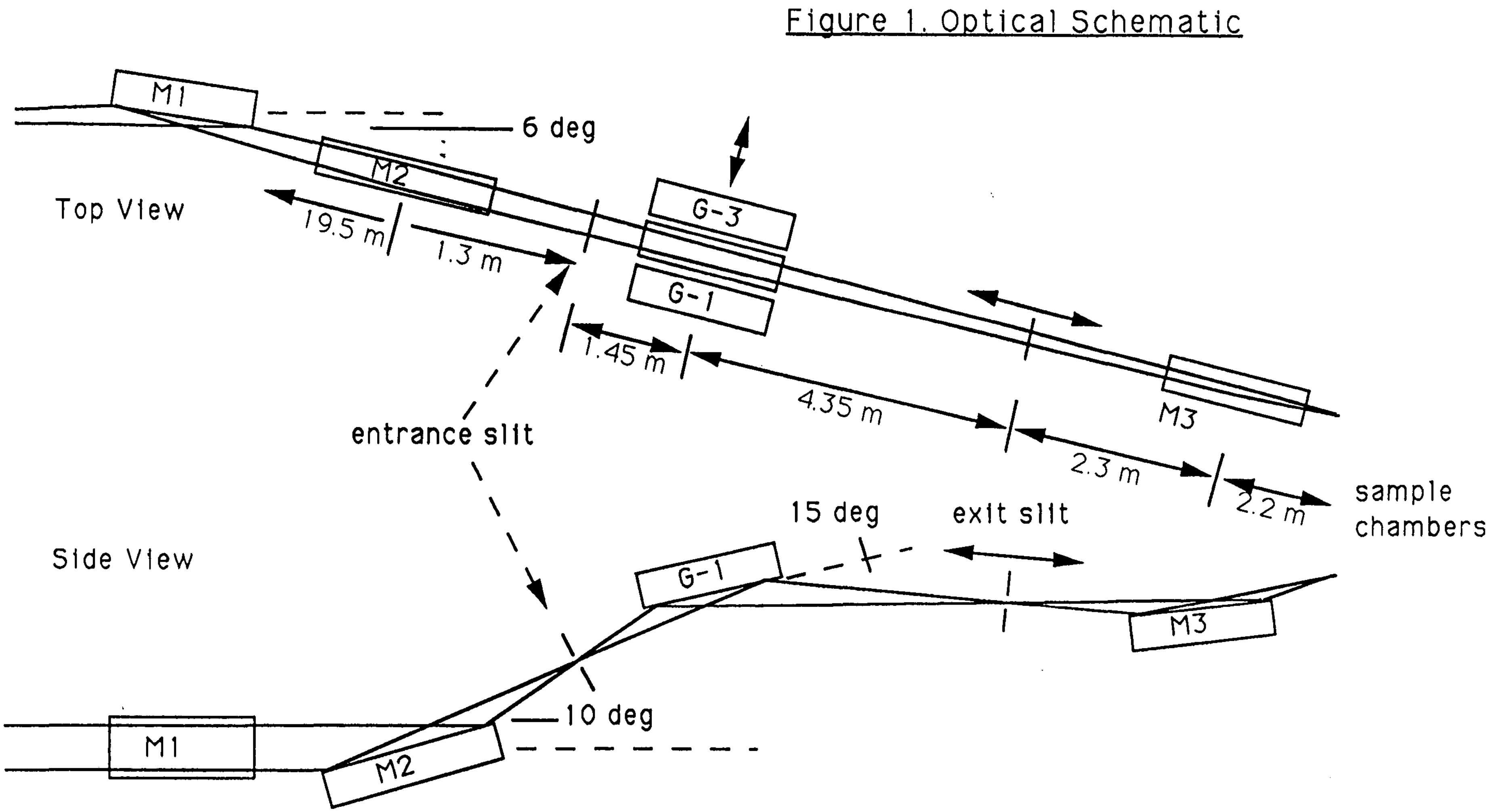
Figure 1. Optical Schematic
M1
6 deg
M2
Top View
19.5 m
1.3 m
G-3
G-1
1.45 m
4.35 m
M3
entrance slit
2.3 m
2.2 m
sample chambers
15 deg
exit slit
Side View
G-1
M3
M1
10 deg
M2

Figure 1

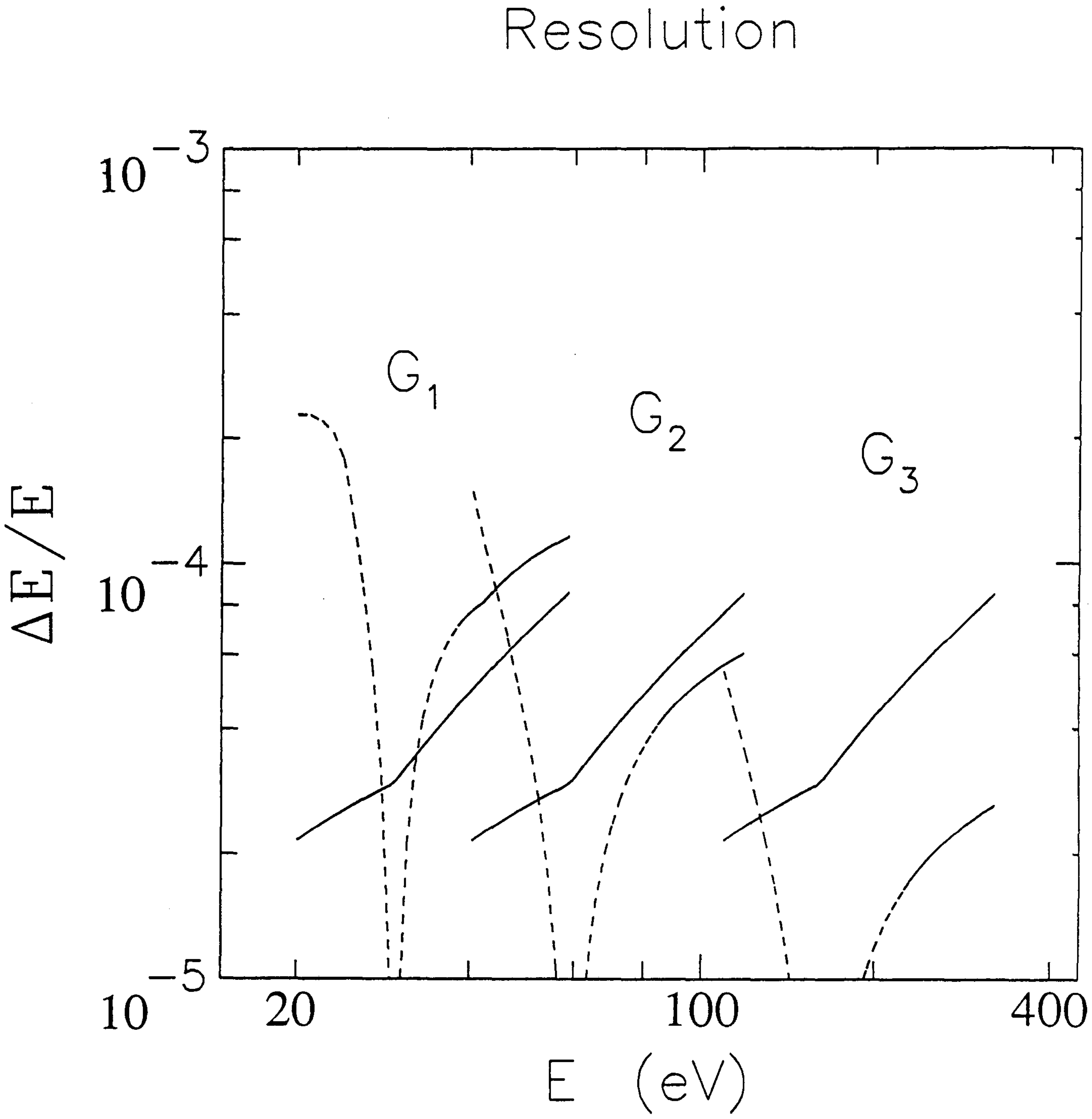

Figure 2

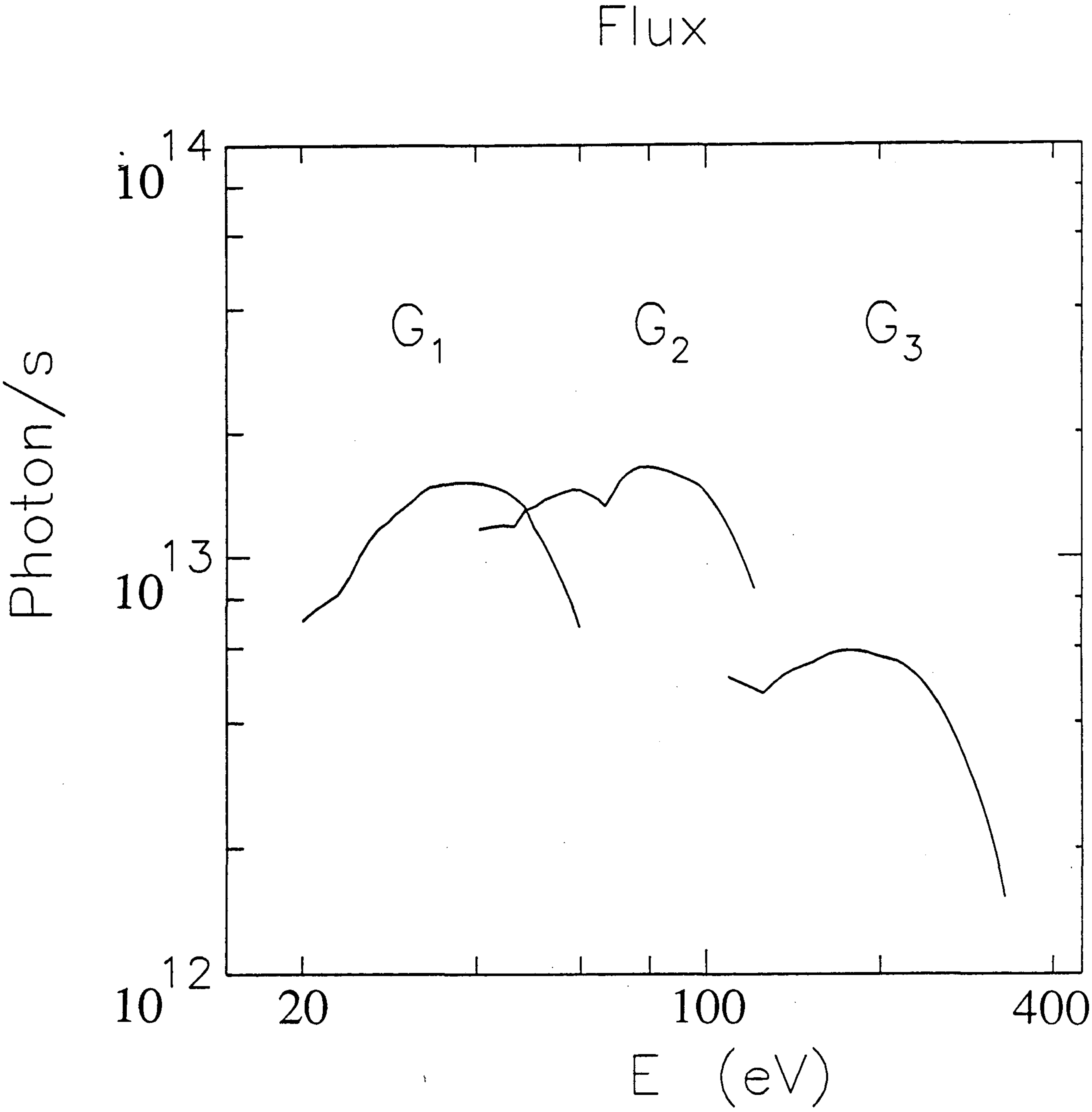

Figure 3

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