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The mercury imaging X-ray spectrometer (MIXS) on BepiColombo

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1 **The Mercury Imaging X-ray Spectrometer (MIXS) on BepiColombo**

2

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47 **Abstract**

48 The Mercury Imaging X-ray Spectrometer (MIXS) on the BepiColombo Mercury
49 Planetary Orbiter (MPO), will measure fluorescent X-ray emission from the surface of
50 Mercury in the energy range 0.5 – 7.5 keV, which is induced by incident solar X-rays and
51 solar wind electrons and protons. These X-rays will reveal the elemental composition of
52 the surface of Mercury and aid the determination of the planet's evolution.

53

54 MIXS is a two component instrument. A collimated channel (MIXS-C) provides
55 measurements on scales of 70-270 km, sufficient to separate the major Mercurian
56 terrains. A second channel (MIXS-T) is the first imaging X-ray telescope for planetary
57 remote sensing and will make measurements on spatial scales of less than 10 km for
58 major elements during solar flares, sufficient to isolate surface landforms, such as craters
59 and their internal structures. The spatial resolution achieved by MIXS-T is made possible
60 by novel, low mass microchannel plate X-ray optics, in a Wolter type I optical geometry.

61

62 MIXS measurements of surface elemental composition will help determine rock types,
63 the evolution of the surface and ultimately a probable formation process for the planet. In
64 this paper we present MIXS and its predicted performance at Mercury as well as
65 discussing the role that MIXS measurements will play in answering the major questions
66 about Mercury.

67

68 **Keywords**

69 Mercury; BepiColombo; X-ray fluorescence; composition; instrumentation

70 **1 Introduction**

71 The innermost planet, Mercury represents an end member of the solar system in terms of
72 size, metal-to-silicate ratio and probably conditions of formation. Knowledge of
73 Mercury's history and formation is therefore essential to understand the formation and
74 evolution of the inner solar system as a whole. Mercury is also the least explored of all
75 the planets. Until recently, three brief flybys by Mariner 10 in 1974 and 1975 provided
76 the only detailed measurements of the planet. At the time of writing (January 2008) the
77 first data is being returned from NASA's MESSENGER mission to Mercury, which flew
78 by the planet on 14th January 2008. Following additional flybys in October 2008 and
79 September 2009, MESSENGER will ultimately go into orbit around Mercury in 2011.
80 These data, coupled with ground based measurements, have provided a picture of an
81 anomalously dense, airless and heavily cratered world which superficially resembles the
82 Moon. Mercury's very large core and an apparent paucity of iron at the surface
83 (estimated, on the basis of ground-based spectroscopy, at less than 3 wt % FeO) are only
84 two of the more striking differences between the two bodies (Strom and Sprague, 2003;
85 Solomon, 2003).

86

87 The major unanswered questions at Mercury may be divided into two categories

88

89 Primary questions:

90

- From what material did Mercury form, and how?

91

- How and when did Mercury become internally differentiated?

92 • Is there both primary and secondary crust on Mercury (as defined by Taylor,
93 1989)?

94 • Why does Mercury have a dipole magnetic field?

95

96 Secondary questions:

97 • What is the history of crustal evolution on Mercury?

98 • What is the crustal composition and how does it vary (i) across the surface, (ii)
99 with depth?

100 • How are the surface and exosphere related?

101 • How do the surface and magnetosphere interact?

102 • Does Mercury have a molten core?

103 • What are the deposits observed in craters near to the poles?

104

105 The Mercury Imaging X-ray Spectrometer (MIXS) on BepiColombo Mercury Planetary
106 Orbiter (MPO) will measure fluorescent X-rays from the surface of Mercury. Fluorescent
107 X-rays reveal the elemental composition of the surface to depths of a few micrometres for
108 low atomic number elements such as magnesium and for the L-shell emission lines of
109 heavier elements. For the harder, K-shell emission lines of heavier elements,
110 measurements of the fluorescent X-rays probes a deeper layer of the planetary surface (of
111 order tens of microns). Measurement of the composition of the regolith in this way is a
112 tool for determining the geological history and ultimately the formation mechanisms for
113 the planet. X-ray spectroscopy is complementary to measurements at optical and infrared
114 wavelengths which indicate chemical bonding and mineralogy, and to gamma ray and

115 neutron measurements which provide low spatial resolution measurements of certain
116 elements at depths of approximately 10 cm. In this paper we describe the production of
117 X-rays on Mercury's surface, the MIXS instrument and its capabilities and the expected
118 contribution that measurements by MIXS will make towards answering the major
119 questions about Mercury.

120 **2 X-ray remote sensing**

121 X-ray fluorescence has been used for remote sensing on Apollo 15 and 16 at the Moon
122 (Adler et al., 1973), on the Near Earth Asteroid Rendezvous (NEAR Shoemaker) mission
123 to asteroid 433 Eros (Trombka et al., 2000), on the Hayabusa mission to asteroid 25143
124 Itokawa (Okada et al., 2006) and on the SMART-1 mission to the Moon (Grande et al.,
125 2003). The Chandrayaan 1 and Kaguya (Selene) missions to the Moon also carry X-ray
126 spectrometers (Grande et al., 2008 and Shirai et al. 2008). The X-ray spectrometer on
127 MESSENGER (Leary et al., 2007) is derived from those on Apollo and NEAR
128 Shoemaker and uses collimated gas proportional counters as the detectors of X-rays
129 (Schlemm et al., 2007). The instruments on SMART-1 and Chandrayaan 1 were based on
130 silicon Swept Charge Device (SCD) detectors (Lowe et al., 2001), while those on
131 Hayabusa and Kaguya use silicon Charge Coupled Device (CCD) detectors. The
132 detectors on MESSENGER have an energy resolution of ~ 880 eV Full Width at Half
133 Maximum (FWHM) at 5.9 keV (Schlemm et al., 2007) and, as was the case for Apollo
134 before them, the separation of the K shell emission lines from Mg (1.25 keV), Al (1.49
135 keV) and Si (1.74 keV) is not possible. Instead, three separate detectors are employed
136 with thin Be windows, two of which bear an additional thin Mg or Al filter. The
137 differential X-ray attenuation of the three counters is then used to infer the relative

138 heights of the three peaks and produce elemental abundance ratios. The MESSENGER
139 X-ray spectrometer's field of view (FOV) is selected by a 12° collimator which, when
140 coupled with the highly elliptical orbit, results in a surface footprint of approximately
141 3000 km at apoherm (15193 km), and 40 km at periherm (200 km), the later resolution
142 being available for approximately 15 minutes in each 12 hour orbit. (Schlemm et al.,
143 2007).

144

145 MIXS differs radically from previous X-ray instruments for planetary remote sensing,
146 offering unprecedented spectral and spatial resolutions. MIXS has two complementary
147 instrument channels shown in Figure 1; MIXS-C (collimator) and MIXS-T (telescope).
148 MIXS-C has a 10.4° Field Of View (FOV), which defines its angular resolution, and is
149 optimised to provide the largest X-ray throughput at all energies and for all solar states.
150 The MIXS-C FOV results in a surface pixel size of 70 km at periherm (400 km orbital
151 altitude) and 270 km at apoherm (1500 km orbital altitude). MIXS-T is an imaging X-ray
152 telescope with a 1.1° FOV and has an angular resolution better than 9 arc minutes, which
153 may be used to full effect during solar flares when the incident (and thence the
154 fluorescent) X-ray flux is highest. MIXS-T's angular resolution is sufficient to provide a
155 spatial resolution better than 1 km at periherm and 4 km at apoherm. Together these two
156 channels ensure comprehensive measurements of the compositions of the major terrains
157 and, where solar conditions allow, the compositions of landform elements such as crater
158 peaks at spatial scales less than 10 km.

159 3 The relationship between Mercury's composition and its formation

160 Mercury has an extraordinarily large uncompressed density (5.3 g cm^{-3} compared with
161 4.0 g cm^{-3} for Earth), which is incompatible with models of formation by equilibrium
162 condensation (Cameron et al., 1988) and indicates that Mercury's metallic mass fraction
163 is at least twice that of the other terrestrial planets (Solomon, 2003). A large iron-rich
164 core is postulated, which occupies about 42% of the planet's volume and 75% of the
165 radius and there is evidence that it is at least partly molten (Margot et al., 2007).

166

167 Several models have been proposed to explain the relative sizes of Mercury's core and its
168 silicate fraction (mantle plus crust). These models fall into three basic categories:
169 selective accretion, post accretion vaporisation and massive impact.

170

171 In the first of these models, the oxidation gradient during solar nebula condensation,
172 aided by gravitational and drag forces, resulted in an enrichment of metallic iron
173 compared with other terrestrial planets (Weidenschilling, 1978). In the second, intense
174 solar radiation in the early Solar System led to the vaporisation and loss of silicates from
175 Mercury's exterior after the planet had formed (Cameron, 1985), or possibly from the
176 differentiated exteriors of planetary embryos before they collided to form Mercury. In the
177 latter model, a giant impact stripped Mercury of much of its rocky exterior (Benz et al.,
178 1988, 2007). A range of credible compositions for Mercury's mantle plus crust, which
179 result from the proposed models, is tabulated in Table 1.

180 **4 Crust formation on Mercury and effects on surface elemental composition**

181 The measured abundance of elements on Mercury's surface cannot, however, be
182 representative of the bulk silicate fraction (mantle plus crust). The crust, whether
183 "primary" or "secondary" (Taylor, 1989) or both, must be chemically differentiated from
184 the mantle by processes dependent on its emplacement mechanisms. Space weathering
185 may further change the surface elemental abundances, so none of the models in Table 1 is
186 likely to correspond to the detected surface composition.

187

188 Primary crust is the oldest surviving crust, and would have derived from a magma ocean
189 (a highly-likely eventuality in any planetary growth scenario involving embryo-embryo
190 collision and/or a final 'giant impact'). Primary crust would be comprised of minerals
191 that grew by fractional crystallisation from a magma ocean melt of mantle (bulk silicate)
192 composition and floated to the surface. This crustal material would be analogous to, and
193 enriched in certain elements in ways comparable to, the anorthosites of the lunar
194 highlands which are enriched in Al and Ca relative to the mantle's bulk composition. Na
195 may be enriched to detectable concentrations in primary crust, although Na
196 concentrations are less than 1.5% in lunar anorthosites, and both Fe and Mg would be
197 depleted. The final crystallisation products of a magma ocean would be expected to have
198 enrichments in the incompatible elements such as K and the rare Earth elements,
199 analogous to the KREEP (Potassium, Rare Earth Elements and Phosphorus) component
200 identified on the Moon.

201

202 Secondary crust results from partial melting in the mantle and will have been emplaced
203 volcanically. Secondary crust will tend to be enriched in Fe (Robinson and Taylor, 2001)
204 but depleted in Mg relative to the bulk composition. Secondary crust will also have a
205 greater abundance of Al, Ca and Na than the mantle (but less than primary crust), and
206 will be richer in K, Ti and Cr than any other major silicate component of the planet.
207 Silicon abundance will probably be less in secondary crust than in primary crust, but the
208 fractional change in Si abundance between crustal types will be small compared to that
209 for other elements, depending on the extent of partial melting. Material erupted after
210 storage and differentiation in large-volume basaltic magma chambers will be lower in Fe
211 and Ti but richer in alkalis than in directly-erupted basalts (Jeanloz et al., 1995).

212
213 Extensive tracts of exposed primary crust on Mercury have yet to be identified. The
214 planet's surface may prove to be largely secondary crust, but it will be important to
215 identify and characterise any exposures of primary crust that have survived resurfacing
216 (or have been re-exposed through tectonism or impact cratering). With the understanding
217 that the Moon is not necessarily a close analogue for Mercury, we present data in Table 2
218 to indicate the sorts of variation in crustal composition at Mercury that an instrument
219 such as MIXS needs to be able to measure. The diagnostic significance of the elements
220 shown in Table 2 is discussed further in Section 5 of this paper.

221 Long-term exposure to meteorite impacts and energetic particles may further alter surface
222 elemental abundances, by processes often described as 'space weathering'. One
223 consequence of this may be the reduction of Fe bonded to oxygen within silicates to
224 metallic 'nanophase iron', alternatively known as submicroscopic metallic iron (SMFe)

225 particles (Blewett et al., 2002). Infrared – ultraviolet spectroscopy is not sensitive to
226 metallic Fe and so X-ray spectroscopy provides the only mechanism for detection of Fe
227 in SMFes. These provide a possible explanation for the apparent deficiency of Fe in
228 surface minerals. MIXS is therefore a crucial complement to the optical and infrared
229 spectrometers on BepiColombo (Simbio-Sys (this issue) and MERTIS (this issue)).

230

231 Determination of Mercury's bulk silicate composition on the basis of surface
232 measurements requires the identification and understanding of the history of crust
233 formation and of the subsequent surface processes. This requires a combination of
234 elemental analysis by X-ray, neutron and gamma ray spectroscopy, visual interpretation
235 of geological features on high-resolution optical images, and infrared – ultraviolet
236 spectroscopy to infer mineralogy.

237

238 **5 The importance of different elements at Mercury**

239 The following arguments describe the diagnostic significance of various elements whose
240 fluorescent X-ray emission is within the energy range detectable by MIXS.

241

242 **Si:** Expected in a narrow range, 19-25% (15–33% in some lunar specimens). Si as a
243 stand-alone element is unlikely to allow determination of mechanisms for Mercury's
244 formation or the evolution of the surface but is useful, not least as a reference to which
245 other elements may be compared.

246

247 **Ti:** Between 1% and 8% in lunar and terrestrial basalts. Abundances greater than 3% on
248 Mercury would indicate sufficient oxygen fugacity to form Ti-oxides (as opposed to Ti
249 merely substituting for other cations within silicates). A Ti abundance of approximately
250 0.1% or less in lavas would support an enstatite chondrite model for Mercury's
251 composition (Taylor and Scott, 2004).

252

253 **Al:** By analogy with the Moon, expected to be abundant in primary crust (~18%), but
254 between 4% and 10% in basalts. Distinguishing between, for example, 18% and 10% Al
255 content would allow the separation of primary and secondary crust.

256

257 **Fe:** The confirmation or otherwise of a low Fe abundance in Mercury's crust is of key
258 importance. Fe abundance is expected to be less than 2% in primary crust, but could be at
259 least 4% in secondary crust. Fe concentration of less than 0.3% would support an
260 enstatite chondrite origin for Mercury's composition (Taylor and Scott, 2004).

261

262 **Mg:** Should be rare in primary crust (less than 2%), but abundant (4-12%) in secondary
263 crust unless the outer part of Mercury has been stripped to reveal inner mantle Mg-rich
264 cumulate. A Magnesium concentration less than 7% would support a refractory-volatile
265 mixture model of Mercury, whereas more than 10% in lavas would support other models
266 (Taylor & Scott, 2004).

267

268 **Na:** Possibly as much as 1% in primary crust and expected to be less abundant in most
269 basalts, although some terrestrial basalts contain more than 1% Na. Detection of Na

270 would place constraints on the volatile budget within Mercury. The liberation of Na into
271 the exosphere from surface material may occur through interplanetary dust impacts, large
272 impacts and the subsequent exposure of fresh regolith, thermal desorption and
273 evaporation, recycling processes from cold craters and ion sputtering.

274

275 **Ca:** By analogy with the Moon, Ca should be abundant in primary crust (18-20%) but
276 rarer in secondary crust (8-14%). A Ca concentration of less than 9% in units recognised
277 as lava would support an enstatite chondrite model of Mercury's composition (Taylor and
278 Scott, 2004). Like Na, Ca is also a constituent of Mercury's exosphere.

279

280 **P:** Reaches concentrations of about 0.1% in lunar mare basalts and double that in the
281 petrologically significant KREEP basalts of the lunar highlands. P and Ti have similar
282 partitioning behaviour during partial melting, and the Ti/P ratio in chondrites is about 1.
283 Thus, a Ti/P of order 10 in volcanic terrains on Mercury would indicate previous
284 scavenging of P into the core and thus provide compelling confirmation of Mercury core
285 formation prior to volcanism.

286

287 **Mn:** Reaches about 0.3% in lunar mare basalts but is much less abundant in primary
288 crust. If detectable on Mercury, it would be expected in secondary crust only.

289

290 **K:** Effectively absent in lunar primary crust, but up to as much as 1% in some kinds of
291 lunar secondary crust and higher in some impact melts. If detected on Mercury,

292 potassium may be used in conjunction with other elements to constrain basalt

293 petrogenesis. K is also a major component of the exosphere.

294

295 **S:** Fe sulphides could provide the sulphur observed in the exosphere and inferred from
296 radar backscatter from Mercury's poles (Sprague et al., 1995, 1996). S concentration is
297 probably much less than 1% except possibly in areas of high-radar reflectivity in polar
298 craters, where sulphur is an alternative candidate to water ice for the material making up
299 the reflective layer. X-ray emission from S inside polar craters would have to be induced
300 by incident electrons (and/or protons) in the absence of direct illumination by the Sun.

301

302 **Cr:** Averages 500 – 600 ppm in the lunar crust. Cr of order 1% in rocks identified as lava
303 would support a refractory-volatile mixture model of Mercury, whereas 0.1% would
304 support other models (Taylor and Scott, 2004).

305

306 **Ni:** Present in abundances less than 400 ppm in the lunar crust, and potentially diagnostic
307 in conjunction with Cr. On the Moon the Cr:Ni abundance ratio has been used to
308 constrain formation models (Taylor, 1975).

309

310 **O:** It is conventionally assumed that in silicate rocks cations (all elements in Table 2 apart
311 from S) are oxidised. O is therefore likely to be about 44-46% in surface materials. A
312 significant departure from this abundance would call into question the whole mineralogy
313 of Mercury's crust.

314

315 In addition, the acquisition of volatile elements will indicate whether Mercury conforms
316 to the approximate trend of increasing depletion with decreasing heliocentric distance,
317 defined by C-type asteroids in the outer belt, to S-type, to E-type in the inner belt, to
318 Mars, to Earth (Bland and Benedix, 2006). Determining volatile abundances will also
319 allow constraints to be placed on volatile depletion during a putative giant impact.

320 **6 Solar X-ray induced fluorescence from Mercury's surface**

321 The primary mechanism for producing X-ray fluorescence from airless planetary bodies
322 in the inner solar system, within approximately 3 AU of the Sun (Adler and Trombka,
323 1970; Adler et al., 1972), is excitation by solar coronal X-rays, although fluorescence can
324 also be induced through bombardment by charged particles. Solar X-ray induced X-ray
325 fluorescence spectroscopy as an observational technique is therefore limited to the Moon,
326 Mercury, asteroids and comets in the inner solar system.

327
328 The intensity of X-ray fluorescence from the various elements on a planet's surface
329 depends on the energy and intensity of incident solar X-rays, but solar X-ray intensity can
330 vary by several orders of magnitude and can be highly variable on time scales of minutes.
331 It is therefore essential that measurements of planetary fluorescent X-ray emission are
332 accompanied by simultaneous measurements of the solar X-ray spectrum. On
333 BepiColombo, solar X-rays will be measured by the Solar Intensity X-ray and Particle
334 Spectrometer, SIXS (Huovelin et al., this volume), which also characterises the particle
335 environment local to the spacecraft. These measurements by SIXS allow normalisation of
336 fluorescence measurements from different orbits allowing the correction of data in order
337 to give a self-consistent picture of the surface.

338

339 Figure 2 shows the solar X-ray flux as a function of energy for various solar flare states
340 measured at 1 AU by the X-ray Solar Monitor (XSM) on SMART 1 (Huovelin et al.,
341 2002). Solar flare states are defined according to the total energy output of the sun
342 measured in the wavelength range 1-8 Å, as measured by the NOAA's GOES spacecraft,
343 in orbit around the Earth. Flare states are designated as : solar quiet (A1 flare), B, C, M
344 or X on a scale where an X1 flare is 10 times an M1 flare is 10 times a C1 flare etc. The
345 largest solar flare to date, in November 2003, is believed to have peaked at around X40
346 (Brodrick et al., 2005). Also shown in Figure 2 are polynomial approximations to solar
347 spectra taken from Truscott et al. (2000). The polynomial approximation to the solar quiet
348 spectrum below 4 keV is smoothed and extrapolated from the 0.3-2.7 keV spectrum
349 reported by Fichtel and Trombka (1997) who in turn used earlier (semi-empirical) work
350 by Tucker and Koren (1971) based on observations from Apollo 15. Above 4 keV, data
351 from Clark et al. (1997) are added. Line emissions were not included in these spectra
352 because the hotter the solar coronal plasma (i.e. the more active the Sun), the more the
353 total continuum emission will dominate. Nevertheless, Tucker and Koren (1971) include
354 more than 450 lines in their solar coronal model; these lines will be included in future
355 MIXS calculations. The detection of lines in the measured solar spectra of Figure 2 is
356 limited by the spectral resolution of the XSM detector. The Fe-K α line is resolved in the
357 M-flare XSM data at 6.6 keV, shifted from 6.4 keV for cold iron because of the increased
358 ionization state for Fe in the solar corona.

359 The solar spectrum will be scattered from the planetary surface as well as initiating
360 fluorescence. However, the energy resolution of the MIXS instrument will allow it to

361 detect the shift in energy between elastically and inelastically scattered X-ray line
 362 emission. The XSM “C1 flare” data shown in Figure 2 was recorded during a C2 flare
 363 event and reduced by a factor of 2. The divergence of the XSM solar quiet data from its
 364 representative polynomial, above 4 keV, is probably due to the inclusion of the diffuse X-
 365 ray background (DXB) and galactic X-ray background within the 52° XSM field view.
 366 The predicted contribution to the measured flux due to the DXB (whose intensity is given
 367 by Zombeck, 2007) is also shown in Figure 2.

368

369 BepiColombo will arrive at Mercury shortly after solar minimum in August 2019, with a
 370 nominal mission duration of 1 year, extensible to 2 years. Representing the years of
 371 operation at Mercury with the corresponding years, two solar cycles earlier, around solar
 372 minimum in 1997, we can estimate the fractions of a year for which the Sun is expected
 373 in various flare states in 2019 and 2020 (Huovelin et al. (this volume)).

374

375 If E is the X-ray energy and the incident intensity of parallel solar X-rays on Mercury’s
 376 surface is $I_0(E)$ (photons $\text{cm}^{-2} \text{s}^{-1}$) then the intensity of fluorescence from a given X-ray
 377 line (photons $\text{cm}^{-2} \text{s}^{-1} \text{steradian}^{-1}$) can be determined in terms of fundamental physical
 378 parameters by the relationship shown in Equation 1, adapted from Clark and Trombka
 379 (1997).

380

$$381 \quad I_{line} = \frac{1}{4\pi} w_i g C_i \left(\frac{r-1}{r} \right) \int_{E_{abs}}^{\infty} I_0(E) \rho \cos \theta \frac{\left(\frac{\mu(E)_i}{\rho_i} \right)}{\mu(E) + \mu(E_{line}) \frac{\cos \theta}{\cos \phi}} dE \quad (1)$$

382 where w_i is the fluorescence yield of a given emission series (K,L etc.), g is the weight
383 fraction of a given line within a series (α, β etc.), C_i is the mass fraction of a given
384 element, r is the jump ratio at the absorption edge of interest, ρ is the bulk density of the
385 surface material, ρ_i is the partial density of the element of interest, θ is the angle of
386 incidence of the incident solar X-rays, measured from the surface normal and ϕ is the
387 viewing angle measured from the surface normal. $\mu(E)$ is the mass absorption coefficient
388 of the bulk material and $\mu(E)_i$ is the linear absorption coefficient for the element of
389 interest. E_{line} is the energy of the elemental emission line of interest.

390

391 Equation 1 assumes a perfectly smooth and homogeneous planar surface; no allowance is
392 made for effects due to the real properties of the planetary regolith, including surface
393 roughness and packing density. Also unaccounted for in Equation 1 are shadowing effects
394 due to large scale topography. Energy independent effects of the regolith and topography
395 (e.g. shadowing) may be removed by the use of elemental abundance ratios (e.g. Mg:Si,
396 Al:Si) instead of absolute abundances, however the use of ratios cannot remove any
397 effects for which there is an energy dependency, and it has been shown in preliminary
398 measurements that for large values of θ and ϕ the measured ratios of elemental line
399 intensities varies as a function of surface roughness by 10% - 20% (Näränen et al.,
400 2007, Okada et.al, 2004). Work is continuing at the University of Leicester, the
401 University of Helsinki and Birkbeck College to quantify the effects of regolith properties
402 on line intensities, in order to provide a more complete interpretation of X-ray
403 fluorescence data from planetary surfaces.

404

405 To indicate the fluorescence emission spectrum expected from Mercury's surface, line
406 emissions calculated from Equation 1 are shown in Figure 3. Solar input spectra for the
407 simulation are the polynomials shown in Figure 2, scaled to an average Mercury-Sun
408 separation of 0.39 AU. Also shown in Figure 3 is the scattered X-ray continuum,
409 calculated using Equations 2 – 9 of Clark and Trombka (1997). The surface is simulated
410 as a smooth high-K lunar basalt with a composition given by Taylor (1975) (Table 2). A
411 lunar basalt composition may not be a close analogue for much of Mercury's surface, but
412 basalt contains a rich mix of elements and is used here to give an indication of the
413 fluorescence intensities that might be expected from the various elemental lines of
414 interest. The lines shown are for solar quiet, B1, C1, and M1 flare states. The ability of
415 MIXS to resolve individual lines is discussed in Section 10.

416 **7 Magnetospheric Phenomena and X-ray emission**

417 X-ray emission may also result directly from magnetospheric phenomena (for reviews of
418 Mercury's magnetosphere see Ness, 1979; Russell et al., 1988; Slavin, 2004; Milillo et
419 al., 2005). Mariner 10 showed that Mercury has a largely dipolar magnetic field tilted
420 only slightly to the planetary spin axis. Interaction of this magnetic field with the solar
421 wind creates a miniature magnetosphere, capable of standing off the solar wind to a
422 distance of $\sim 1.5 R_M$ (where $1 R_M$ is 2439 km). However, the nature of the internal
423 dynamo is yet to be fully understood. Nevertheless, Mariner 10 observations left the
424 impression that Mercury's magnetosphere is potentially one of the most dynamic in the
425 solar system, showing evidence of familiar terrestrial magnetospheric processes. These
426 include dayside magnetic reconnection phenomena (or Flux Transfer Events - FTEs)
427 similar to those seen at the Earth, ULF wave activity (indicative of closed field lines), and

428 extremely rapid substorm activity on time-scales of a few tens of seconds. It is possible
429 that these processes will produce X-rays at the surface of the planet (or even in the
430 exosphere) due to precipitation and/or acceleration of electrons and/or ions in large scale
431 current systems associated with solar wind-magnetosphere-exosphere-surface coupling
432 (for example, see Grande, 1997; Burbine et al., 2005). Burbine et al. (2005) have
433 suggested that electron-induced X-ray emission from Mg, Al and Si should be detectable
434 by the MESSENGER X-ray Spectrometer (XRS) on the dark side of Mercury.

435
436 If this is the case, MIXS would sample the surface/exosphere effects of this dynamic
437 coupling, which *in situ* plasma and field measurements alone will not be able to establish.
438 Candidate processes which may produce surface X-ray emission are: cusp dynamics or
439 FTEs, substorms/Pi2 pulsations (irregular and damped ultralow frequency range magnetic
440 pulsations which occur in connection with magnetospheric substorms), and the effects of
441 active solar wind conditions (i.e. Solar Energetic Proton events (SEPs) and Coronal Mass
442 Ejections (CMEs)). To fully understand the magnetospheric phenomena, of which X-ray
443 emission is one manifestation, it will be important to coordinate measurements by MIXS
444 with *in situ* field and plasma measurements taken with instruments on both the MMO and
445 MPO spacecraft.

446 **8 The Mercury Imaging X-ray Spectrometer (MIXS)**

447 The optical elements for both instrument channels, shown schematically in Figure 1,
448 consist of microchannel plate (MCP) X-ray optics operating in two different modes and
449 manufactured by Photonis SAS (Brive, France). MIXS-T has radially packed, square-
450 pore MCPs in a Wolter Type I optical geometry (Willingale et al., 1998). MIXS-C has

451 square packed, square-pore MCP optics in a “slumped collimator” optical geometry.
 452 Figure 4 shows a scanning electron microscope image of an MCP coated with a thin layer
 453 of Ir to optimise its X-ray reflectivity (Jefimovs et al., 2007). The MCPs for both
 454 telescope and collimator have a high reflectivity 60 nm thick Al film over their front
 455 faces, to reduce thermal load. Microchannels are arranged in square multifibres, which
 456 are then stacked in the appropriate geometry.

457

458 **8.1 The MIXS focal plane assembly**

459 Both MIXS-T and MIXS-C have identical focal plane assemblies, based on monolithic
 460 19.2 mm × 19.2 mm Active Pixel Sensors (APS). The sensor features Macropixels
 461 (Zhang et al., 2006), which combine the benefits of DEPFET (DEpleted P-channel Field
 462 Effect Transistor) structure (Treis et al., 2006) (i.e. low power consumption, fast readout,
 463 excellent energy resolution at low noise, intrinsic radiation hardness and arbitrary access
 464 to pixels) with those of a Silicon Drift Detector (SDD) (arbitrary scalable pixel sizes and
 465 an entrance window with low X-ray attenuation).

466

467 The FWHM energy resolution (ΔE) of the Gaussian detector response is given by

$$468 \quad \Delta E = 2.36w \left(\frac{FE}{w} + R^2 + A^2 \right)^{\frac{1}{2}}, \quad (2)$$

469 where w is the energy required to create an electron hole pair (3.62 eV in Si), F is the
 470 Fano factor (a factor describing the non-Poissonian variance in the number of electrons
 471 generated in a detector by an incident X-ray photon, ~ 0.1 in Si) (Fraser, 1989), E is X-
 472 ray energy and R and A are the noise contributions from the readout electronics and

473 amplification (Fraser, 1989). Measurements of X-ray spectra obtained by DEPFET
474 detectors by Zhang et al. (2006) have shown that energy resolutions approaching the
475 theoretical Fano limits (~ 60 eV at 1 keV, 130 eV at 6 keV) are feasible with these
476 devices.

477

478 The MIXS detectors will measure X-rays in the energy range 0.5 – 7.5 keV, with a
479 spectral resolution of 100 eV at 1 keV at the start of operations, following the 6 year
480 cruise to Mercury. The resolution will degrade over the mission lifetime due to radiation
481 damage but should still be less than 200 eV after one year at Mercury (Treis et al., 2008)..
482 This resolution allows the separation of X-ray line emission from elements of interest
483 while the predicted sub-keV quantum efficiency permits the detection of lines not
484 accessible to previous instruments - including the Fe-L emission line at 0.7 keV. This
485 measurement is vital in elucidating the apparent low iron abundance indicated by
486 ground-based visible and infrared spectroscopy (which is sensitive to Fe-O bonds rather
487 than to Fe itself). Fe-L is of particular importance because the higher energy Fe-K lines
488 (6.40 keV and 7.06 keV) are practically visible only during high solar states.

489

490 The MIXS focal plane assembly (FPA) consists of a 64×64 array of $300 \mu\text{m}$
491 macropixels, each with a triple drift ring structure. Whereas in a charge coupled device
492 (CCD), charge is transferred across the whole device for readout by a single preamplifier,
493 in the macropixel array every pixel has its own readout FET (Field Effect Transistor).

494 The predicted quantum efficiency (QE) of the MIXS detector is shown as a function of

495 energy in Figure 5. The window is 30nm polyimide plus 50nm Al, with negligible X-ray
496 attenuation above 0.5 keV.

497 **8.2 MIXS-C optics**

498 An X-ray collimator is conventionally an array of parallel channels whose aspect ratio
499 (the ratio of channel length L and width d) alone defines the field of view (FOV). The
500 collimator is positioned directly above an underlying detector and the two have identical
501 areas. Such a geometry means that the effective area of a planar collimator falls off
502 linearly with off-axis angle; the angular response is triangular in form (Fraser 1989). In
503 contrast, MIXS-C uses a slumped or radial collimator geometry, shown schematically in
504 Figure 6. This geometry allows (a) the reduction of the required detector size for a given
505 collimator aperture and (b) the physical separation of the collimator and detector planes,
506 with consequent advantages in terms of cost, radiation shielding mass, cooling power and
507 sensitivity.

508
509 The MIXS-C collimator is an array of four slumped 40×40 mm square pack - square
510 pore glass MCPs with $20\mu\text{m}$ wide channels. The MCPs are spherically slumped to a
511 common radius of 550 mm and have a channel aspect ratio of 55:1. The open area
512 fraction of the MCPs is 0.6, comparable with that of a standard mechanical collimator.
513 The side length D of the square collimator is 80 mm and the detector is square, with a
514 side length of 19.2mm, identical to the MIXS-T detector. The detector is placed 550 mm
515 from the collimator along the optical axis, at the collimator's centre of curvature. In this
516 geometry, the FOV for collimated X-rays is determined by the sum of the angle
517 subtended by the slumped collimator and the acceptance angle of the channels, and is

518 equal to 10.4° . The design ensures that all X-rays transmitted through the collimator are
519 ultimately incident on the detector.

520

521 In addition to the collimated flux, X-rays can be reflected from the Ir-coated internal
522 faces of the microchannels. Figure 7 shows the effective areas (transmitted, transmitted
523 plus reflected rays) as a function of angle for MIXS-C at 1 keV, calculated using the
524 Monte-Carlo raytracing model of Price et al. (2002). Unlike a conventional collimated
525 instrument, MIXS-C's effective area is constant across most of its FOV. The FOV can be
526 described by two components (i) a core FOV defining the central "flat top" angular
527 response (6.5°) and (ii) the total FOV incorporating the fall-off in effective area to zero
528 (10.4°).

529 **8.3 MIXS-T optics**

530 MIXS-T uses radially-packed, $20\ \mu\text{m}$ square-pore MCP optics, in a conical
531 approximation to the Wolter type I focussing geometry, typically used in X-ray
532 astronomy (Ashenbach, 1985). The MCP embodiment of the Wolter optic geometry is
533 discussed in detail by Willingale et al. (1998); the path of an X-ray through an MCP
534 Wolter pair is illustrated in Figure 8. The focal length of MIXS-T is 1 m, determined by
535 the 4 m and 1.33 m slump radii of the front and rear MCP plates (Willingale et al. 1998).
536 X-rays entering a microchannel in the first plate are reflected at grazing incidence from
537 an internal channel wall, upon exiting the front MCP, the X-ray then enters a
538 microchannel in the rear MCP where a second reflection takes place. After two
539 reflections, the beam converges in the focal plane. Deviations from the optimal path of
540 an X-ray may occur due to multiple reflections within microchannels, misalignments

541 between microchannels and groups of microchannels (multifibres) or because of
542 scattering due to small deviations from a perfectly smooth Ir-coated reflective channel
543 walls. The achievable quality of the focus is ultimately limited by the practical
544 approximation to the radial packing geometry and by the conical approximation to the
545 true Wolter I geometry.

546

547 The 210 mm diameter MIXS-T optic, shown in Figure 1 and schematically in Figure 9, is
548 assembled from a mosaic of MCPs, each of which is a sector of a circle, slumped to the
549 figure of the surface of a sphere. Front and rear “sectors” together form “tandems” which
550 are arranged in three rings with different thicknesses (2.2 mm inner, 1.3 mm middle, and
551 0.9 mm outer) to approximate the ideal $1/r$ thickness profile which maximises the
552 throughput of the telescope by maximising the probability of a single reflection in each
553 MCP.

554

555 The on-axis effective area of the MIXS-T optics has been calculated using a Monte Carlo
556 ray-tracing model incorporating the geometric parameters given above. The mechanical
557 support structure of the telescope, illustrated in Figure 1, is accounted for and perfect
558 stacking of microchannel multifibres is assumed. The on-axis effective area for the
559 MIXS-T optics (not including the detector efficiency) as a function of energy is shown in
560 Figure 10 both for rays which are truly focused (labelled “focussed”) and for all rays
561 incident in the focal plane, including those which undergo scattering or multiple
562 reflections inside the microchannels (labelled “focal plane”). Counting all rays in the
563 focal plane, both focussed and non-focussed, provides a means of maximising the

564 counting rate for any given elemental line, gaining sensitivity at the expense of spatial
 565 resolution. Raytracing indicates that the likely limiting resolution for the MIXS-T optics,
 566 assuming perfect alignment of microchannels, multifibres and sectors is ~ 1 arc minute..
 567 The formal science requirement for MIXS-T is to achieve an angular resolution better
 568 than 9 arc minutes.

569

570 The effective area of MIXS-T decreases with off-axis angle, because the X-ray
 571 reflectivity decreases with increased grazing angles to the channel walls, and the
 572 reflection geometry along the channels becomes less favourable for single reflections in
 573 both front and rear MCPs. This reduction in effective area with off-axis angle is the so-
 574 called vignetting function and is shown for four X-ray energies in Figure 11.

575 **8.4 MIXS Grasp**

576 The collecting power of both MIXS channels can be described in terms of the product of
 577 effective area and field of view - which in astronomy is known as the Grasp, $G(E)$ (units
 578 of $\text{cm}^2 \text{sr}$ - derived below for a telescope in equation 6). Where X-rays in the energy
 579 interval $E, E+dE$ are emitted from an extended source (i.e. the surface of Mercury) and
 580 are incident on the instrument aperture with a flux $I(E)$ (in photons $\text{cm}^{-2} \text{s}^{-1} \text{steradian}^{-1}$
 581 keV^{-1}) then the number of detected photons C detected in a time t is given by

$$582 \quad C = I(E)G(E)tdE . \quad (3)$$

583 The calculated $G(E)$ for MIXS-C shown in Figure 12, is the result of multiplying the
 584 field of view (0.033 steradians), by the geometrical area of the collimator (64 cm^2) while
 585 taking into account the raytraced transmission of the collimator geometry and the
 586 detector QE. Also included is the X-ray transmission of a 60 nm Al thermal filter on the

587 input face of the microchannel plates, and an additional 100nm of Al on 300nm of
 588 polyimide as an optical filter directly in front of the focal plane array. The calculated
 589 Grasp at 1 keV is $0.032 \text{ cm}^2 \text{ sr}$.

590

591 Let us consider a “focusing” collimator and planar collimator of equal aperture; a planar
 592 collimator would have a grasp of $\sim 0.096 \text{ cm}^2 \text{ sr}$, a factor of ~ 3 larger than MIXS-C,
 593 However, this requires a factor of 16 greater focal plane area, which is limited for MIXS
 594 (cooling power, cost, development time). Therefore, a planar collimator would be
 595 unsuitable for MIXS and the advantages of using a focusing collimator are clear.

596 The grasp, G , for an imaging telescope (MIXS-T) can be calculated from the on-axis
 597 effective area $A(0,E)$ and the vignetting function. For an instrument with a circular FOV
 598 the element $d\Omega$ of solid angle subtended by an angular element $d\xi$ at an off-axis angle ξ is
 599 approximated at small off-axis angles by

600

$$601 \quad d\Omega = 2\pi\xi d\xi \quad (2)$$

602

603 and the off-axis effective area $A(\xi,E)$ is

604

$$605 \quad A(\xi,E) = A(0,E)V(\xi,E), \quad (3)$$

606

607 The grasp $G(E)$ is given by

608

$$609 \quad G(E) = 2\pi\epsilon_d(E)T(E)A(0,E) \int_0^{\xi_{\max}} \xi V(\xi,E) d\xi, \quad (4)$$

610

611 where $\varepsilon_d(E)$ is the detector QE and $T(E)$ is the combined transmission of the optical and
612 thermal filters in front of the detectors.

613

614 An approximation to the vignetting function can be obtained by assuming that there is a
615 linear fall off from the peak on-axis effective area to a minimum of zero at the edge of the
616 field of view, which is defined by the 19.2×19.2 mm detector, which at a 1m focal
617 length gives an FOV of 1.1° (0.55° half angle). Using this approximation for the
618 vignetting function and assuming a perfect detector and 50cm^2 on axis effective area, G is
619 estimated to be $\sim 0.009 \text{ cm}^2 \text{ sr}$. Figure 12 shows the MIXS-T grasp ($G(E)$), incorporating a
620 more realistic vignetting function generated by Monte-Carlo raytracing software (Figure
621 11), the detector's QE and the calculated absorption of a 60 nm thick Al thermal filter on
622 the input optic surface and a 100 nm Al optical filter deposited on 300nm of polyimide.
623 The grasp is calculated for both focussed X-rays and for all rays incident in the focal
624 plane, as shown in Figure 10,.

625

626 **9 Instrument background levels and minimum detectable flux**

627 The sensitivity of a photon-detecting instrument can be quantified by the minimum
628 detectable flux I_{min} , which is the minimum signal flux from a source that can be
629 distinguished from the background B . We assume that an isotropic flux I (in units of
630 photons $\text{cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$) of fluorescent X-rays at a discrete energy (in keV) from an extended
631 source is incident on the front of an instrument with a grasp G . This instrument has a
632 focal plane detector with an area for photon detection A_{det} and energy resolution δE . The

633 detected fluorescent X-ray signal is accompanied by a background of solar X-rays which
 634 are scattered from the surface under examination, denoted by I_{scat} (in units of photons cm^{-2}
 635 $\text{s}^{-1} \text{sr}^{-1} \text{keV}^{-1}$).

636

637 Although features in the scattered continuum may contain information on surface
 638 properties and absorption features in the continuum may yield compositional information,
 639 in terms of measuring fluorescence spectra the continuum constitutes a background and is
 640 treated as such here. The detector also has a non-X-ray background component, caused
 641 by charged particle events B_p (units of events $\text{cm}^{-2} \text{s}^{-1} \text{keV}^{-1}$). For a cooled, photon-
 642 counting detector, intrinsic thermal noise is negligible and the scattered X-ray component
 643 and the particle induced background will dominate. If a signal to noise ratio R is required
 644 for the detection of an X-ray line then I_{min} may be defined as the flux that, in a given
 645 integration time, produces a count R standard deviations of B above its mean. I_{min} for a
 646 given value of R (typically taken to be 3-5) is given by

$$647 \quad I_{min} = \frac{R\sqrt{\delta E(B_p A_{det} + I_{scat} G)}}{G\sqrt{t}} \quad (5)$$

648

649 The particle-induced X-ray background B_p results from a combination of both high
 650 energy cosmic rays and lower energy (10-100 MeV) protons ejected from the Sun. To
 651 reduce B_p MIXS's detectors are shielded by 15 mm of Al, which is the Continuous
 652 Slowing Down Approximation (CSDA) range for 60 MeV protons in Al.

653

654 In the absence of direct measurements at Mercury, in order to calculate the expected
 655 instrument background, we must use data for the integrated intensities of solar X-rays and

656 protons in various energy bands, measured in geostationary orbit at 1 AU by the
657 Energetic Particle Sensor (EPS) on the GOES spacecraft (Sellers et al., 1996). EPS data
658 show a poor correlation between the flux of protons with energies > 60 MeV and X-ray
659 flux for most solar conditions, and for lower energy protons the flux can be highly
660 variable. For high (M – X) X-ray flare states, however, the flux of > 60 MeV protons may
661 increase by several orders of magnitude, with the peak in proton flux occurring some time
662 after the X-ray flux. At 1 AU the time delay between the peaks in the X-ray and proton
663 fluxes during an X-flare is typically of the order 2 hours. At Mercury the delay will be
664 between approximately 35 and 55 minutes for perihelion and aphelion, respectively. The
665 MIXS background count rates due to solar protons will typically vary by less than one
666 order of magnitude for the majority of the instrument lifetime. Very large solar flares may
667 however be followed, within an hour, by an increase in background of several orders of
668 magnitude.

669
670 We have estimated the MIXS background at Mercury by scaling that experienced by the
671 XMM Newton X-ray observatory's EPIC X-ray camera's pn-CCDs (Strüder et al., 2001)
672 which are in a highly elliptical orbit around the Earth. These are analogous to the MIXS
673 detectors and are considered useful for comparison with MIXS. . Cosmic ray and solar
674 proton events in the EPIC pn detectors are rejected on the basis of energy, or the shapes
675 of tracks left by particles as they deposit energy in adjacent pixels. The post-rejection
676 background rate for the pn-CCDs is reported to be $0.039 \text{ cm}^{-2} \text{ s}^{-1}$ in the energy band 0-10
677 keV (Lumb, 2002) giving a count rate per keV of $0.0039 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$. XMM Newton's
678 CCDs have 30mm Al shielding for the detectors which can be penetrated by particles

679 with energies > 90 MeV. The fluxes for >90 MeV protons are typically a factor 2-3 less
680 than for > 60 MeV protons (Xapsos, 2000). The proton flux at Mercury for all energies
681 can be assumed to scale relative to that at 1 AU according to an inverse square law
682 dependence on the distance from the Sun (Mukai, 2003).

683

684 The energy deposited by minimum ionising particles (MIPS) in a silicon X-ray detector is
685 a function of the distance travelled in a single detector pixel and has been simulated by
686 Strüder (2000) who shows that for a $150\mu\text{m} \times 150\mu\text{m} \times 300\mu\text{m}$ Si pixel the Landau
687 energy distribution peaks at about 40 keV. This peak corresponds with a most probable
688 distance travelled in a single pixel of $150\mu\text{m}$. Scaling this distribution to account for the
689 larger MIXS pixel size ($300 \times 300 \times 450 \mu\text{m}$) gives a peak at 80 keV and approximately
690 10% of energy deposited by MIPS will be in the energy band 0-10 keV. The MIXS
691 energy band is from 0.5-7.5 keV. The distribution varies little over the range 0-10 keV
692 and it is therefore assumed to be constant within this energy range. Consequently, a
693 background rate in the 0.5-7.5 keV energy band of $0.04 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$ is calculated.

694

695 If a three order of magnitude increase in flux is assumed after high flare states then the
696 background rate may reach values of $40 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$. The background value given for
697 the XMM-Newton detectors, however, includes galactic cosmic rays and solar protons
698 and it is inappropriate to scale the former event rate with distance from the Sun. Solar
699 protons are believed to contribute only $\sim 10\%$ of the XMM background at 1 AU on
700 average (Strüder, 2000). If only 10% of the 1 AU background value attributable to SEPs
701 is scaled to 0.31 AU then the typical MIXS background under normal conditions is

702 estimated to be $\sim 0.008 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$. We have therefore adopted $0.04 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$ as a
703 worst-case background rate.

704 **10 The detection of elements by MIXS**

705 Using Equation 7 we have calculated the time required for 3σ detection of the various
706 elemental lines of interest in different solar flare states, for which the incident solar
707 spectra are shown in Figure 2. It is assumed that a minimum of ten photons is required for
708 a significant detection. The calculated integration times for MIXS-T and -C are shown in
709 Table 3 and Table 4 respectively. A worst case value of $0.04 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$ is assumed for
710 the particle background B_p . The L shell emission lines of Ti and Cr are coincident with
711 the far more intense O-K line and therefore cannot be separated and are not included
712 here. Where the required integration times are longer than 1 year, an element is
713 considered to be undetectable and is left blank in the tables. The spatial scales on which
714 elements may be measured are defined by the required integration times, the instrument
715 FOVs and by the orbital velocity of the BepiColombo MPO. The imaging capability of
716 MIXS-T allows data to be manipulated for optimum imaging or spectroscopy. For MIXS-
717 T it is assumed initially that all photons in the focal plane are added together and the
718 imaging capability within the field of view is not applied, this optimises the measurement
719 statistics for spectroscopy. For times where the flux from Mercury is high, the imaging
720 capability of MIXS-T can be applied, by subdividing the focal plane into its imaging
721 pixels, the application of imaging to various elements is discussed below.

722

723 The number of counts from single surface elements can be maximised by combining
724 measurements made of the same surface area during multiple passes overhead (using the

725 solar spectrum, as measured by SIXS to allow normalisation between subsequent orbits).
726 The coverage time achieved as a function of position on the surface has been calculated
727 using the Satellite Tool Kit (STK) (Analytical Graphics Inc.) for illuminated segments of
728 the planet during one year of operations beginning in September 2019. The resultant
729 coverage map for MIXS-T is shown in Figure 13 and for MIXS-C in Figure 14. The
730 nodes used in the calculation are positioned on the surface at 4° latitude and longitude
731 intervals. The structure visible in the images is a combination of the node spacing and the
732 effect of including only dayside observations in the measurements. Typical accumulated
733 coverage times for near-equatorial regions of approximately hundreds of seconds increase
734 to more than three hundred seconds at high latitudes. For MIXS-C we calculate
735 accumulated coverage times of ~ 9000 seconds in near-equatorial regions, increasing to
736 almost 30000 seconds at high latitudes. Assuming a “worst case” scenario in which all
737 measurements of a surface element are made during solar quiet, the number of counts
738 expected for MIXS-T is shown in Table 5 and for MIXS-C is shown in Table 6, assuming
739 nadir viewing and normal incidence for solar X-rays. A more typical scenario would see
740 $\sim 20\%$ of the year in B-flare state during solar minimum (Huovelin et al., this volume).
741 The percentage errors shown in the tables correspond to the Poissonian errors in the
742 number of counts.
743
744 The dwell times for a surface element (the time between a point on the surface entering
745 and then leaving the FOV) during single passes by MIXS-C at apoherm and periherm are,
746 respectively, 209 and 27.9 seconds. For MIXS-T, the dwell times at apoherm and
747 periherm are 22.1 and 3.0 seconds. Measurements made in a single surface element

748 during solar flare events will contain many more counts than during solar quiet and
749 provide access to X-ray lines with higher energies than can be measured during low solar
750 flare states. Simulated spectra for single passes at apoherm (1500 km altitude) are shown
751 for MIXS-T in Figure 15 and for MIXS-C in Figure 16. The spectra assume nadir
752 pointing and normal incidence for solar X-rays at a Sun-Mercury distance of 0.39 AU.
753 The detectors have 40 eV energy bins and, for illustrative purposes, the surface is
754 assumed to have the lunar high-K basalt composition of Table 2. We assume a FWHM
755 energy resolution of 100eV at 1 keV, varying as a function of energy according to
756 Equation 3. In the period after an X-flare, the solar proton flux may (in extreme cases)
757 increase by five orders of magnitude, implying a particle-induced background in the
758 detector of $400 \text{ cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$. If X-flare intensities are maintained in the period post flare
759 then the sensitivity of the instrument to weaker K_{β} lines is reduced but does not alter the
760 sensitivity to the more intense K_{α} lines shown here, other than for P- K_{α} which can no
761 longer be detected. This is primarily because the background due to the scattered X-ray
762 continuum is typically much greater than the proton-induced background. The enhanced
763 proton flux following a flare can take several days to decay, while the X-ray flux returns
764 to typical values within hours. During these periods, the proton background may remain
765 sufficiently high relative to the X-ray signal that measurements may be compromised.

766

767 The imaging capability of MIXS-T allows measurements from surface areas smaller than
768 the surface footprint of the 1.1° FOV. For M1 and X1 flares (assuming that the incident
769 solar intensity for an X1 flare = 10 M1), Table 8 gives an estimated spatial resolution
770 achievable from apoherm for key elements which still give a statistically significant

771 measurement as described in Section 5 and summarised in Table 7. A maximum
772 resolution of 2 arc minutes is reported in the table as this is the goal of the MIXS-T
773 optics, although the formal requirement is for an angular resolution of less than 9 arc
774 minutes. The grasp values for focussed rays only are used in these calculations.

775

776 Global abundance averages for elements may be measured by integrating spectra
777 accumulated during the entire mission. Table 9 shows the total number of counts in major
778 elemental lines expected for MIXS-C in one year, assuming a worst case scenario in
779 which all measurements are made during solar quiet and assuming measurements are
780 made at 0.39 AU. A mean angle for incident solar X-rays of 45° is assumed and only
781 dayside measurements are considered.

782

783 However, unless Mercury has only one widespread type of crust, combining
784 measurements to give global averages may obscure important variations and result in
785 geologically uninformative results. Because of the divergent formation mechanisms for
786 primary and secondary crust (Section 4), it will be more useful to make separate
787 calculations of average element abundances in primary and secondary crust. To separate
788 the two sets of measurements, we will use data from other BepiColombo experiments
789 (notably SIMBIO-SYS and MERTIS) to help to map the extent of each crustal type.

790 **10.1 Validation of the fluorescence model**

791 To validate our X-ray spectral calculations, we compare X-ray spectra of the Moon, made
792 by the Chandra X-ray observatory ACIS instrument and presented by Wargelin et al.
793 (2004), with synthetic spectra generated using the fluorescence model presented above.

794 The Chandra observations were made in July 2001 using the I2 and I3 front illuminated
795 chips of the Advanced CCD for Imaging Spectroscopy (ACIS) focal plane instrument
796 (Garmire et al, 2003).

797

798 The GOES X-ray data sets for the period of the Chandra observations of the Moon
799 typically show a mid B-flare state. In the following simulations, a B2 flare state is
800 modelled as a B1 flare, as in Figure 2, multiplied by two, independent of energy. The
801 composition of the large areas of the lunar surface observed by Chandra is unknown; the
802 modelled spectra represent the two possible lunar soil compositions given by Clark and
803 Trombka (1997); Apollo 16 Highlands and Apollo 12 mare basalt. The calculations
804 assume that the illuminated lunar surface is perfectly smooth. The illumination angle θ
805 and the observation angle ϕ are taken to be 45° , approximating the geometry illustrated
806 by Wargelin et al. (2004). The I2 and I3 effective area as a function of energy for the
807 ACIS-I instrument was determined from the Chandra Science Data Center
808 (<http://asc.harvard.edu/proposer/POG/>). The FWHM energy resolution of the measured
809 spectrum presented by Wargelin et al., (2004) is ~ 111 eV at the O-K line (0.525 keV) and
810 is scaled to other energies here according to Equation 3. The aperture of a single ACIS-I
811 CCD is 5.9×10^{-6} steradians and the combined I2 and I3 integration time is 8063 s
812 (Wargelin et al, 2004). The simulated spectra are shown in Figure 17 along with the
813 measured peak count rates for O-K, Fe-L and Si-K.. There is good agreement between
814 measurement and model; in particular, this comparison demonstrates the feasibility of
815 detecting iron in planetary regoliths at all solar states via the L-shell emission.

816

817 The correct interpretation of X-ray measurements from the surface of Mercury will
818 require a detailed understanding of the processes that generate X-rays and the effects of
819 observing a real planetary surface as opposed to an idealised surface as modelled herein.
820 Theoretical and experimental investigations are proceeding to investigate the effects of
821 surface and regolith properties on emission spectra. Investigations are also ongoing into
822 the likely properties of the Mercurian magnetosphere and the X-ray emission that may
823 result from its interaction with the surface and exosphere as well as the solar wind. The
824 results of these investigations will be reported in future papers.

825 **11 MIXS at Mercury**

826 By accumulating data globally and/or for regions representing primary and secondary
827 crust, we expect to be able to measure at least Na, Mg, Al, Si, P, K, Ca, Ti, Fe and Ni
828 (although separation of the Ni-L line from the much more intense O-K line may prove
829 challenging), all to a high statistical precision. These data can be subdivided into data
830 from the various, large scale, Mercurian terrains. If Mercury has exposed primary crust as
831 well as secondary crust, subsets of data, representing areas dominated by primary crust
832 and areas dominated by secondary crust, will be more informative than global averages.

833 Under typical solar conditions MIXS-T will determine Na, Mg, Al, Si and Fe abundances
834 on scales of some tens of km, and MIXS-C will achieve scales of hundreds of km with
835 greater numbers of counts to provide increased statistical certainty for the spectral lines.
836 During solar flares, MIXS-C will have the capability to measure P, K, Ca, Ti, Cr, while
837 Na, Mg, Al, Si and Fe will be measured with increased statistical certainty. Spatial scales
838 of hundreds of km are sufficient to subdivide the surface of Mercury into the individual
839 terrains identified on Mariner-10 images; for example heavily cratered terrain and

840 intercrater plains (possibly both primary crust), smooth plains (probably secondary crust)
841 and ‘hilly and lineated terrain’ and ‘hummocky plains’ (probably impact-modified
842 versions of other terrain units) (e.g. Trask and Guest, 1975; Strom, 1997; Strom and
843 Sprague, 2003). It may be possible to distinguish differences in composition between
844 individual lava flows in compound flow fields to indicate the fractionation history of
845 magma chambers or the time-related depth of magma sources.

846

847 Highest spatial resolution measurements of just a few km will be achieved by MIXS-T
848 during solar flares for the major elements Na, Mg, Al, Si, P, K, Ca, Ti, Fe. These
849 measurements will provide access to a wide range of landforms including possible
850 volcanic constructs, craters of various diameters and depths as well as their central peaks.
851 The latter are uplifted material from the middle or lower crust and so may expose strata
852 formed during various eras in Mercury’s history (including primary crust, which will be
853 important if it is not widespread at the surface) and/or bodies of magma intruded into the
854 crust. The youngest craters and their ejecta may also provide information on the rate and
855 nature of space weathering.

856

857 MIXS observations of X-ray emission from Mercury will allow the determination of
858 elemental abundances with unprecedented spatial resolution for a range of elements of
859 key importance for understanding the geology, evolution and formation of the planet. X-
860 ray emission will also provide a mechanism for investigating the unique surface-
861 magnetosphere interactions at Mercury.

862

863 Since preparation of this paper, the Messenger flyby data from the Gamma-ray
864 spectrometer has been able to place a 0.5 wt % upper limit on the potassium content of
865 the equatorial regions of Mercury. This is shown to rule out formation models which
866 include k-rich feldspar. Future observations of this kind will be used to inform and
867 improve the performance predictions for MIXS at Mercury. To date, a number of
868 assumptions about the nature of the planet's surface have been made which were
869 constrained only by our knowledge of the properties of the regolith and the superficial
870 resemblance of Mercury to the Moon.

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Accepted manuscript

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1121 **Figure 1. A Schematic illustration of MIXS showing the adjacent MIXS-T and MIXS-C channels.**

1122

1123 **Figure 2. Polynomial approximations to the solar X-ray spectrum in M1, C1 and B1 flare states**
1124 **derived from various sources as described in the text together with measured solar X-ray spectra**
1125 **from the X-ray Solar Monitor (XSM) instrument on SMART 1. Also shown is the predicted**
1126 **magnitude of the diffuse X-ray background (DXB) measured by XSM between 3 keV and 7 keV.**

1127

1128 **Figure 3. Simulated fluorescence emission spectrum from a lunar basalt surface at 0.39 AU, under**
1129 **various solar flare conditions calculated using Equation 1. Lines are shown with a 2 eV width.**

1130

1131 **Figure 4. Scanning electron microscope image showing the Ir coated, square microchannel structure**
1132 **of an MCP X-ray optic.**

1133

1134 **Figure 5. Calculated quantum efficiency of the MIXS FPA detectors.**

1135

1136 **Figure 6. Geometry of the MIXS-C slumped collimator. The side length of the collimator is 80mm**
1137 **and the 550 mm separation of the MCP collimator and the detector is equal to the collimator's**
1138 **spherical slump radius. The acceptance half angle for a single channel is defined by its aspect ratio**
1139 **(L:d).**

1140

1141 **Figure 7. Raytraced effective area as a function of off axis angle for the Ir coated MIXS-C optics at 1**
1142 **keV.**

1143

1144 **Figure 8. Illustration of the path of an X-ray through sections of the front and rear slumped MCP**
1145 **optic microchannels, which together are a conical approximation to a true Wolter type I optic. The**
1146 **three channel lengths shown correspond to the inner, middle and outer rings of the MIXS-T optic.**

1147 The channel side length in each case is $20\mu\text{m}$ and the thickness of the septal wall between
1148 microchannels is $6\mu\text{m}$.

1149

1150 Figure 9. Schematic diagram of the MIXS-T MCP Wolter optics in cross section (not to scale). The
1151 front MCPs are slumped to a radius of 4m . The rear MCPs are slumped to a radius of 1.33m . The
1152 mosaics of MCPs are arranged in three rings of differing thicknesses which approximate an ideal $1/r$
1153 profile in channel thickness (see text). Rays are reflected from the internal surfaces of both front and
1154 rear microchannels and are focussed at a distance of 1m from the optic. The MIXS-T optic as viewed
1155 from the front and showing the arrangement of the sectors and rings is shown in Figure 1. The
1156 middle section in the pattern does not contain an MCP optic – this area is masked by the telescope
1157 structure.

1158

1159 Figure 10. On-axis effective area for the MIXS-T MCP optics. Focused rays are those that arrive at
1160 the focus of the telescope. The focus of the telescope is defined by the FWHM of the peak generated
1161 on a detector by parallel rays entering the aperture, the effective area is calculated for all rays that
1162 are truly focused by the optics (one reflection in each MCP). Focal plane in the figure refers to all
1163 rays arriving in the focal plane, including non-focussed rays that have been scattered or undergone
1164 multiple reflections in the optics.

1165

1166 Figure 11. The reduction in effective area with off axis incident angle, relative to the on-axis value
1167 (vignetting) for MIXS-T at four different X-ray energies.

1168

1168

1169 **Figure 12. Grasp G as a function of energy for MIXS-T and MIXS-C. The structure indicated is the**
1170 **result of X-ray absorption by the Ir coating.**

1171

1172 **Figure 13. Hammer-Aitoff projection of Mercury showing the predicted day side coverage time as a**
1173 **function of latitude and longitude on Mercury for MIXS-T during one year of operations beginning**
1174 **in September 2019. Craters shown are major craters observed by Mariner 10.**

1175

1176 **Figure 14. Hammer-Aitoff projection of Mercury showing the predicted day side coverage time as a**
1177 **function of latitude and longitude on Mercury for MIXS-C during one year of operations beginning**
1178 **in September 2019. Craters shown are major craters observed by Mariner 10.**

1179

1180 **Figure 15. Simulated X-ray spectra for MIXS-T during a single 22.1 s pass at apoherm in various**
1181 **solar flare states and assuming normal solar illumination and a nadir viewing angle at 0.39 AU. The**
1182 **spectra have 100 eV FWHM energy resolution at 1keV and the bin width is 40 eV.**

1183

1184 **Figure 16. Simulated X-ray spectra for MIXS-C during a single 209 s pass at apoherm in various**
1185 **solar flare states and assuming normal solar illumination and a nadir viewing angle at 0.39 AU. The**
1186 **spectra have 100 eV FWHM energy resolution at 1keV and the bin width is 40 eV.**

1187

1188 **Figure 17. Simulated Chandra ACIS X-ray spectra of the Moon for highland and Mare lunar soil**
1189 **compositions. Also shown are peak values for the Chandra ACIS lunar X-ray spectrum presented by**
1190 **Wargelin et al. (2004). The energy bin width shown here is 30 eV.**

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1193

1194 **Table 1 Percentage by mass of some major elements in Mercury's bulk silicate fraction for nine**
1195 **models of Mercury's formation, ¹Morgan and Anders, 1980; ²Chapter 4, Basaltic Volcanism on the**
1196 **Terrestrial Planets, 1980; ³ models 3 of 4 of Fegley and Cameron, 1987; ⁴Goettel, 1988).**

1197

1198 **Table 2. Compositions of rocks (% by mass for the main elements) in the lunar crust, to give an**
1199 **indication of the possible variability of composition that might be encountered during study of**
1200 **Mercury's crust. Also shown are the line energies for X-rays in the MIXS 0.5-7.5 keV energy band.**
1201 **The compositional data is derived from % mass oxides data from Taylor (1975). The mass fraction**
1202 **not shown is O.**

1203

1204 **Table 3. Integration times in seconds required for MIXS-T to detect various elements in different**
1205 **solar flare states assuming a high K lunar basalt surface composition.**

1206

1207 **Table 4. Integration times in seconds required for MIXS-C to detect various elements in different**
1208 **solar flare states assuming a high K lunar basalt surface composition.**

1209

1210 **Table 5. Counts detected by MIXS-T in 100s during solar quiet.**

1211

1212 **Table 6. Counts detected by MIXS-C in 9000 s during solar quiet.**

1213

1214 **Table 7. The minimum precision required to allow for significant interpretation of measurements for**
1215 **possible minimum % mass values of various elements at Mercury. The table condenses the**
1216 **requirements from Section 5. A failure to meet one of these requirements does not necessarily detract**
1217 **significantly from the science as other elemental measurements may be sufficient. The % mass values**
1218 **are speculative minima based primarily on measurements of lunar rocks.**

1219

1219

1220 **Table 8. Estimated spatial resolution achievable by MIXS-T in M1 and X1 flares to make “useful**
1221 **scientific measurements” as defined in Table 7.**

1222

1223 **Table 9. Predicted number of counts for major elemental lines detected by MIXS-C in 1 year of**
1224 **operations.**

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Model	Element % mass						
	Na	Mg	Al	Si	Ca	Ti	Fe
Chondritic formation ¹	0.03	20	3.4	22	3.7	0.2	5.8
Equilibrium condensation (EC) ²		24	5.1	19	6.1	0.29	0.078
EC with usage of feeding zones ²		25	3.8	21	4.7	0.22	0.06
Dynamically mixed ²		29	2.5	20	2.9	0	0
Collisionally differentiated ²		33	0	20	1.3	0	0
Vapourisation ³		25	9	12	4.1	0.5	0.62
Refractory-rich ⁴	0	21	8.8	15	11	0.43	0
Intermediate preferred ⁴	0.074 - 0.37	19 - 22.9	1.9 - 3.7	16 - 22.4	2.5 - 5.0	0.090 - 0.18	0.78 - 7.8
Volatile-rich ⁴	0.5	19	1.7	21	2.2	0.084	23.4

1226

1227

Table 1

1228

1228 **Table 2:**

Element	X-ray Energies and emission lines(keV)	Anorthosite	Troctolite	Low-K Fra Mauro basalt	Medium-K Fra Mauro basalt	Apollo 15 green glass	Apollo 15 Quartz basalt	High-K Apollo 11 basalt
Si	1.74 (K)	20.7	20.5	21.8	22.5	21.4	22.9	19.0
Ti	4.51 (K)	0.04	0.10	0.7	1.3	0.17	0.9	7.1
Al	1.49 (K)	18.6	12.0	10.0	9.3	4.04	4.9	4.6
Fe	0.71 (L) 6.40 (K α) 7.07 (K β)	0.52	3.81	7.5	8.5	15.3	14.5	14.8
Mn	5.91 (K)	0	0.05	0.0	0.0	0.16	0.2	0.2
Mg	1.25 (K)	0.48	8.86	6.6	5.2	10.0	5.7	4.6
Ca	3.70(K α) 4.02(K β)	13.4	9.36	8.3	7.6	6.23	7.7	7.3
Na	1.04 (K)	0.59	0.29	0.3	0.5	0.09	0.2	0.4
K	3.35 (K)	0	0.00	0.2	0.7	0.03	0.0	0.4
P	2.02 (K)	0	0.00	0.0	0.0	0.00	0.0	0.1
Cr	5.41 (K α) 5.95 (K β)	0	0.07	0.2	0.1	0.34	0.5	0.3
Ni	7.47 (K α)	0	0.03	0.2	0.37		0.01	0.002

1229

1230

1230 Table 3:

Element	Line	Quiet Sun	B1 Flare	C1 Flare	M1 Flare
O	K	0.04	0.05	0.08	0.007
Na	K	66	64	20	2.0
Mg	K	14	8.2	1.9	0.23
Al	K	58	17	3.2	0.42
Si	K	53	7.2	1.1	0.16
P	K	2.1×10^7	1.1×10^5	2000	170
K	K		2.5×10^5	270	61
Ca	K α	3.2×10^6	3900	18	4.3
Ca	K β		2.3×10^5	140	32
Ti	K α		2.57×10^5	58	12
Ti	K β		1.55×10^7	440	93
Cr	K α			4.3×10^4	980
Cr	K β			2.3×10^6	6.1×10^4
Fe	K α		1.5×10^7	440	40
Fe	K β			2.2×10^4	300
Fe	L α	0.46	0.68	0.51	0.05
Fe	L β	0.50	0.74	0.53	0.05
Ni	L α	3.9×10^5	5.0×10^5	1.9×10^5	1.8×10^4
Ni	L β	4.3×10^5	5.5×10^5	2.0×10^5	1.9×10^4

1231

1232

1232 Table 4:

Element	Line	Quiet Sun	B1 Flare	C1 Flare	M1 Flare
O	K	0.01	0.01	0.02	0.0018
Na	K	13	12	3.8	0.42
Mg	K	2.7	1.53	0.36	0.04
Al	K	10	3.05	0.57	0.07
Si	K	8.4	1.15	0.17	0.03
P	K	1.3×10^5	960	80	13
K	K	1.9×10^6	1600	21	4.8
Ca	K α	1.5×10^4	110	1.2	0.29
Ca	K β	7.1×10^5	900	8.5	2.0
Ti	K α	1.8×10^5	750	3.1	0.66
Ti	K β	8.1×10^6	3.4×10^4	21	4.4
Cr	K α		5.1×10^6	200	29
Cr	K β			3700	200
Fe	K α	2.6×10^6	1.5×10^4	14	1.3
Fe	K β		7.2×10^5	95	8.6
Fe	L α	0.09	0.13	0.09	0.01
Fe	L β	0.10	0.14	0.10	0.01
Ni	K α				1.2×10^6
Ni	L α	6.6×10^4	8.2×10^4	3.3×10^4	3400
Ni	L β	7.2×10^4	8.9×10^4	3.4×10^4	3600

1233
1234

1234 Table 5:

Element	Line	Number of counts	% error
O	K	1.3×10^4	0.6
Na	K	14	30
Mg	K	70	10
Al	K	17	20
Si	K	19	20
Fe	L α	1500	2
Fe	L β	1500	2

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1236 Table 6:

Element	Line	Number of counts	% error
O	K	6.1×10^6	0.03
Na	K	6500	1
Mg	K	3.4×10^4	0.5
Al	K	8700	1
Si	K	1.1×10^4	1
Fe	L α	7.6×10^5	0.1
Fe	L β	6.6×10^5	0.1

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1238 Table 7:

Element	Possible minimum % mass	Minimum Precision required (%)
Si	20	5
Ti	1	20
Al	1	20
Fe	2	50
Mg	2	25
Ca	18	20
Na	0.4	Detection
K	0.1	Detection
Cr	0.05	Detection
Ni	0.04	Detection
S	0.1 (at poles)	Detection

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1240 Table 8:

Flare State	X1	M1
Element	Spatial resolution (km)	Spatial resolution (km)
Na	3	9
Mg	1	4
Al	2	6
Si	5	15
P	25	
K	15	
Ca	6	20
Ti	10	
Fe	1	1

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1242 Table 9:

Element	Line	Counts	error (%)
O	K	7.6×10^9	0.00081
Na	K	8.0×10^6	0.034
Mg	K	4.2×10^7	0.015
Al	K	1.1×10^7	0.031
Si	K	1.3×10^7	0.027
P	K	12000	0.91
K	K	3200	1.77
Ca	K α	37000	0.52
Ca	K β	5400	1.38
Ti	K α	10000	0.96
Fe	K α	3000	1.8
Fe	L α	9.0×10^8	0.0028
Fe	L β	5.7×10^8	0.0029
Ni	L α	98000	0.32
Ni	L β	90000	0.33

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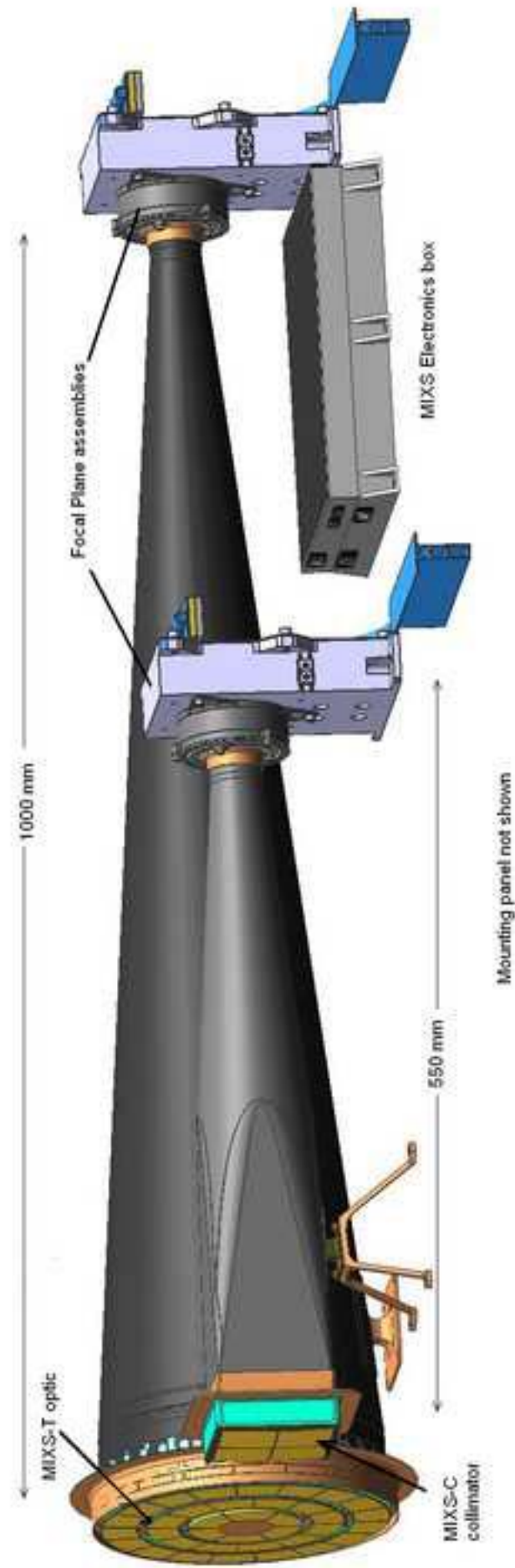
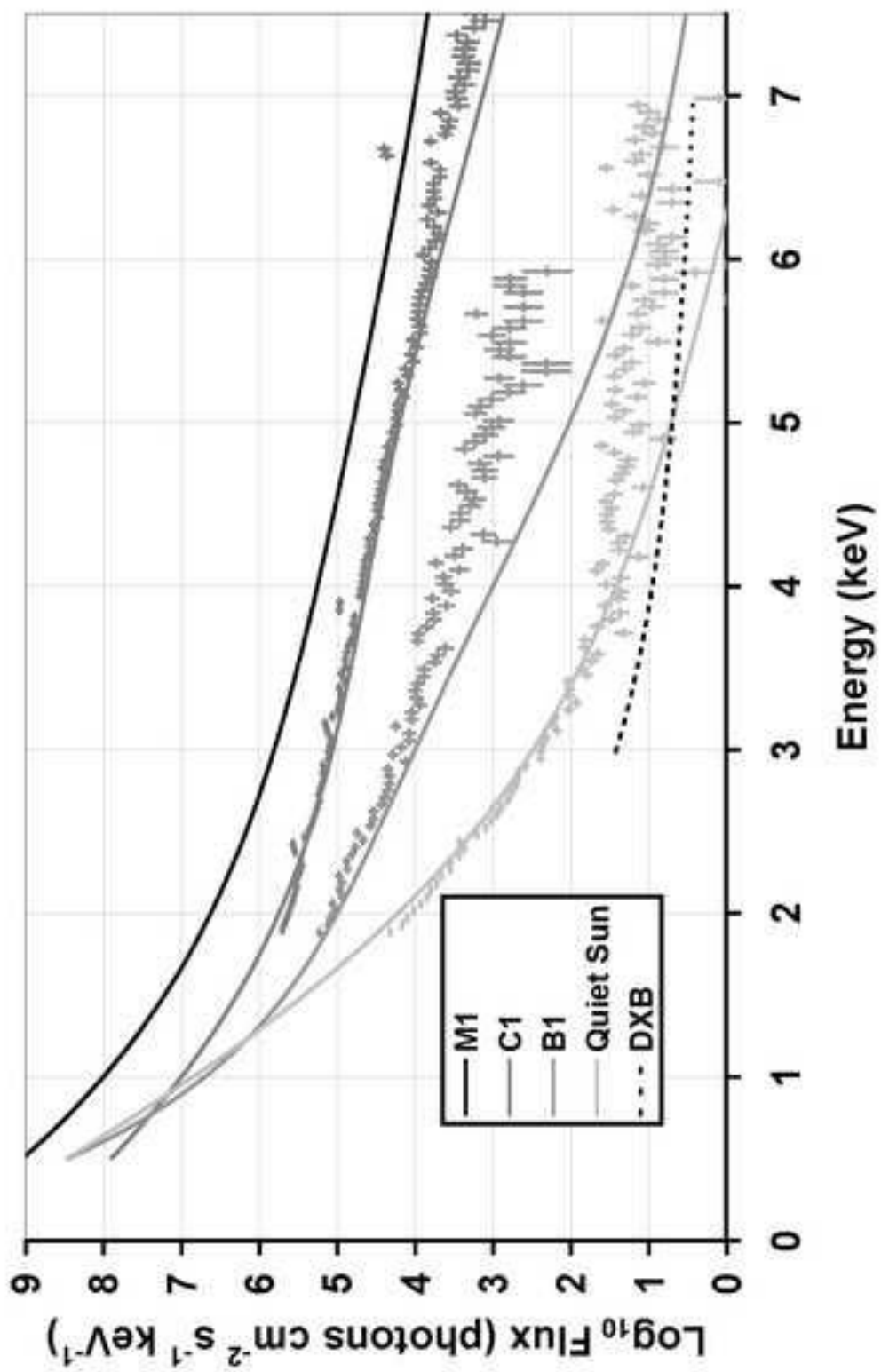


Figure 1



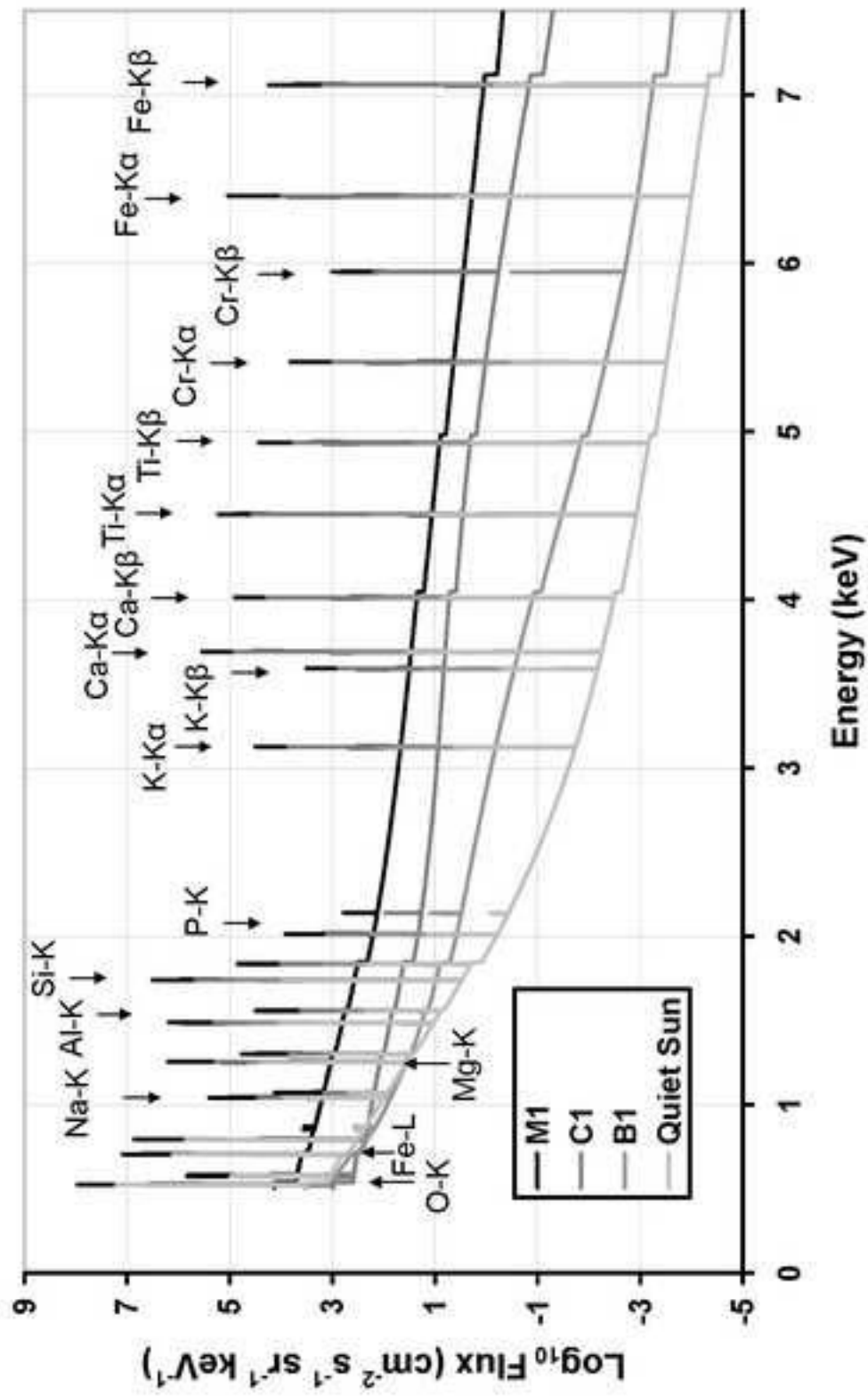


Figure 3

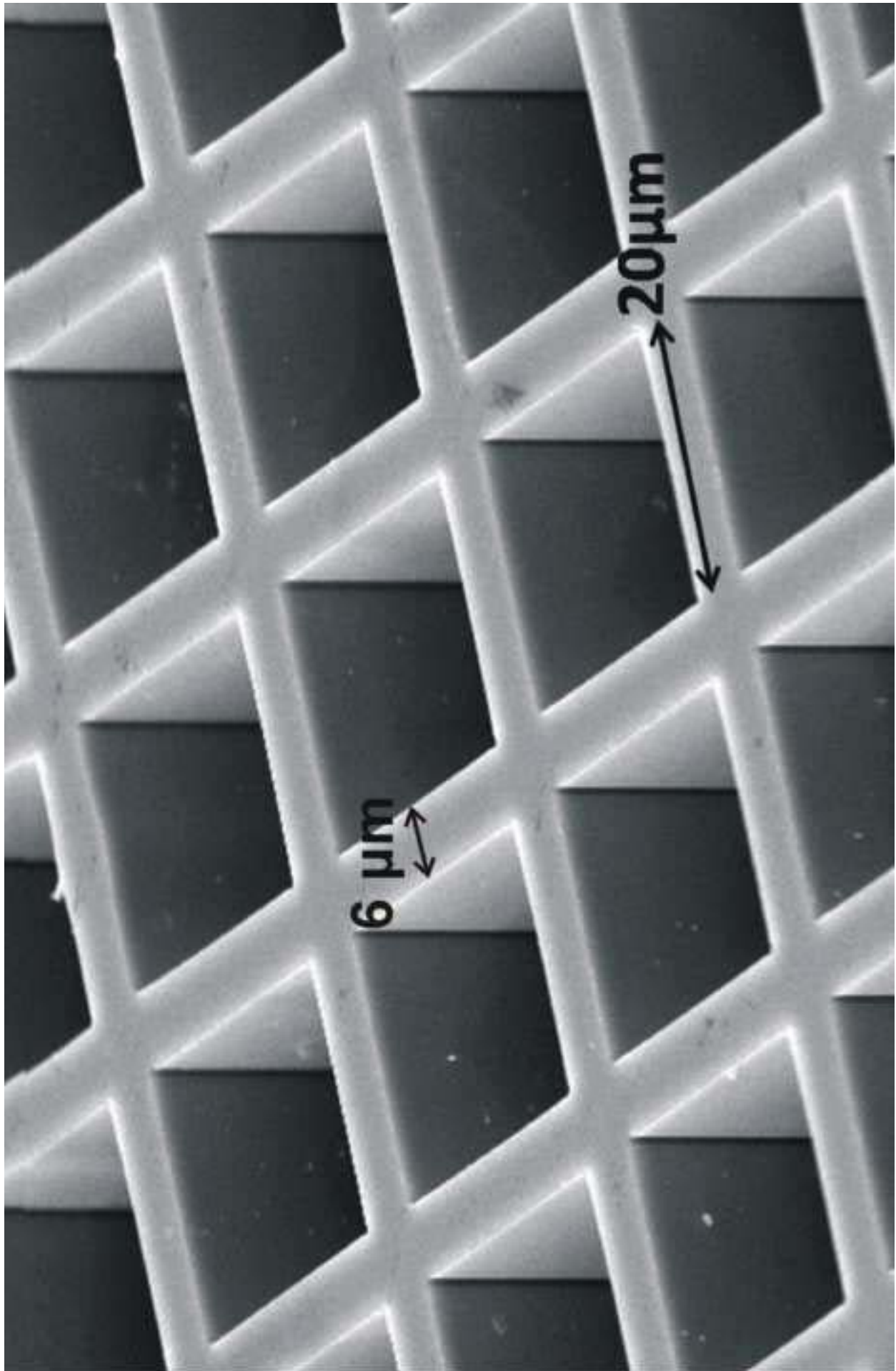
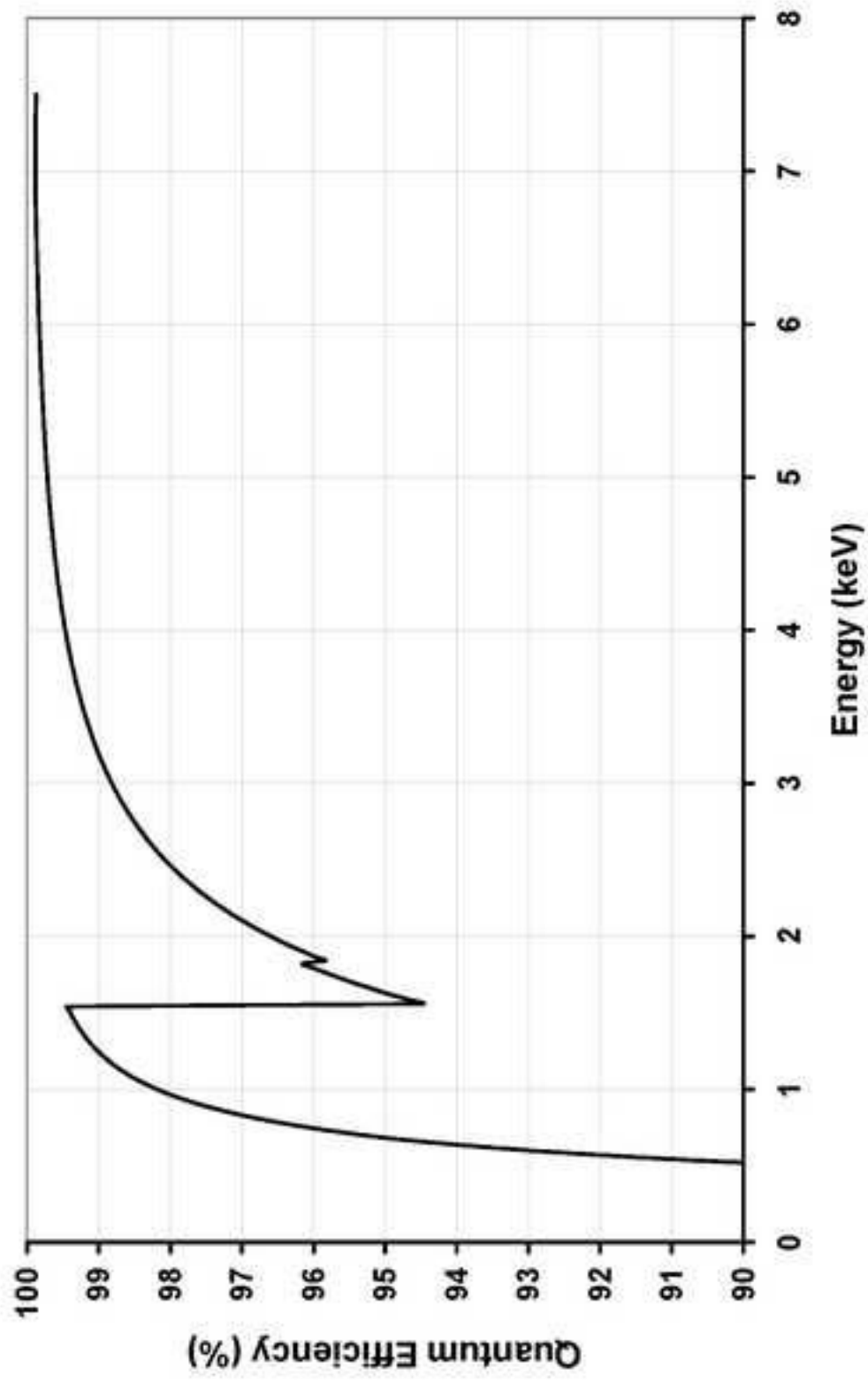
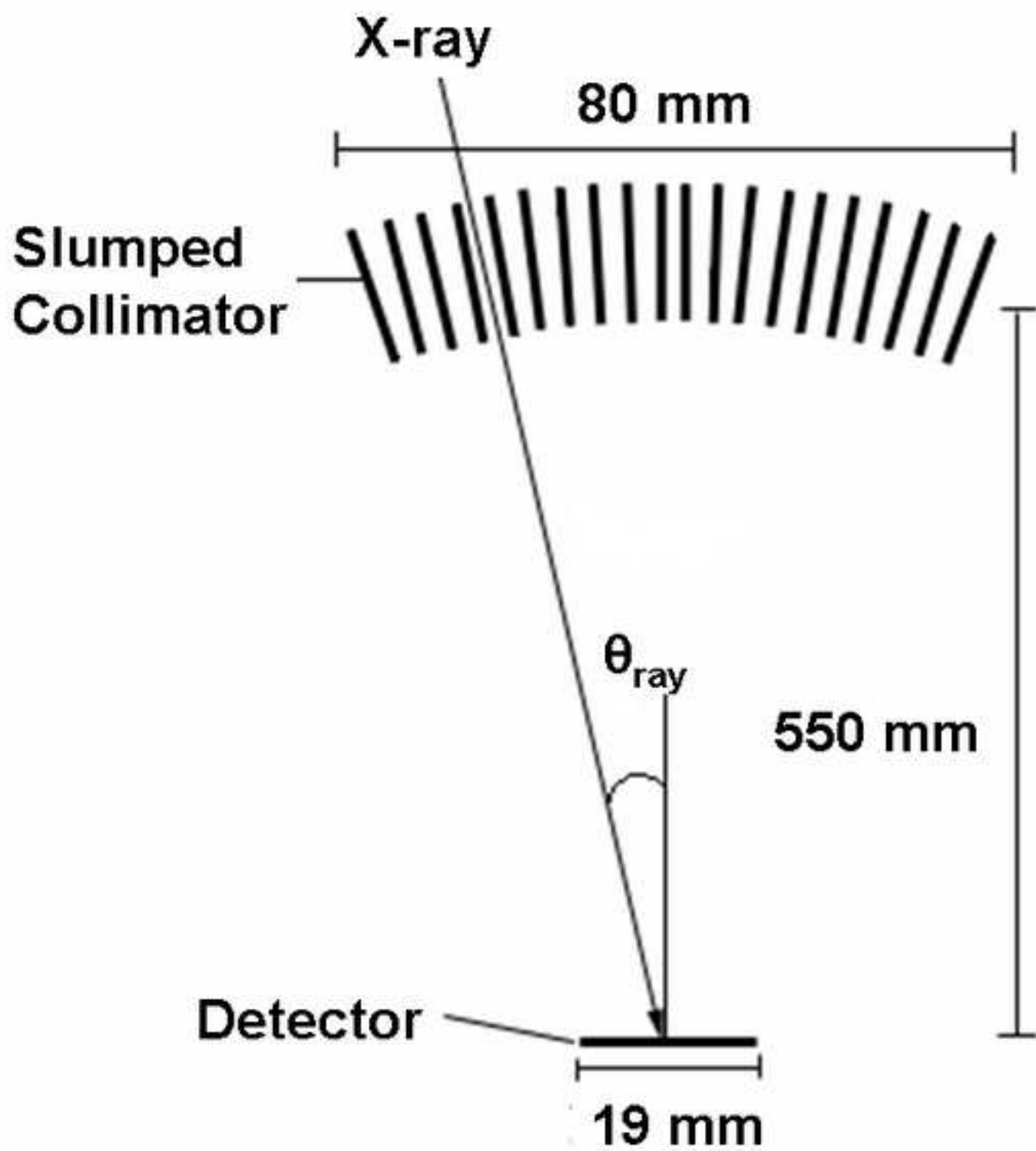
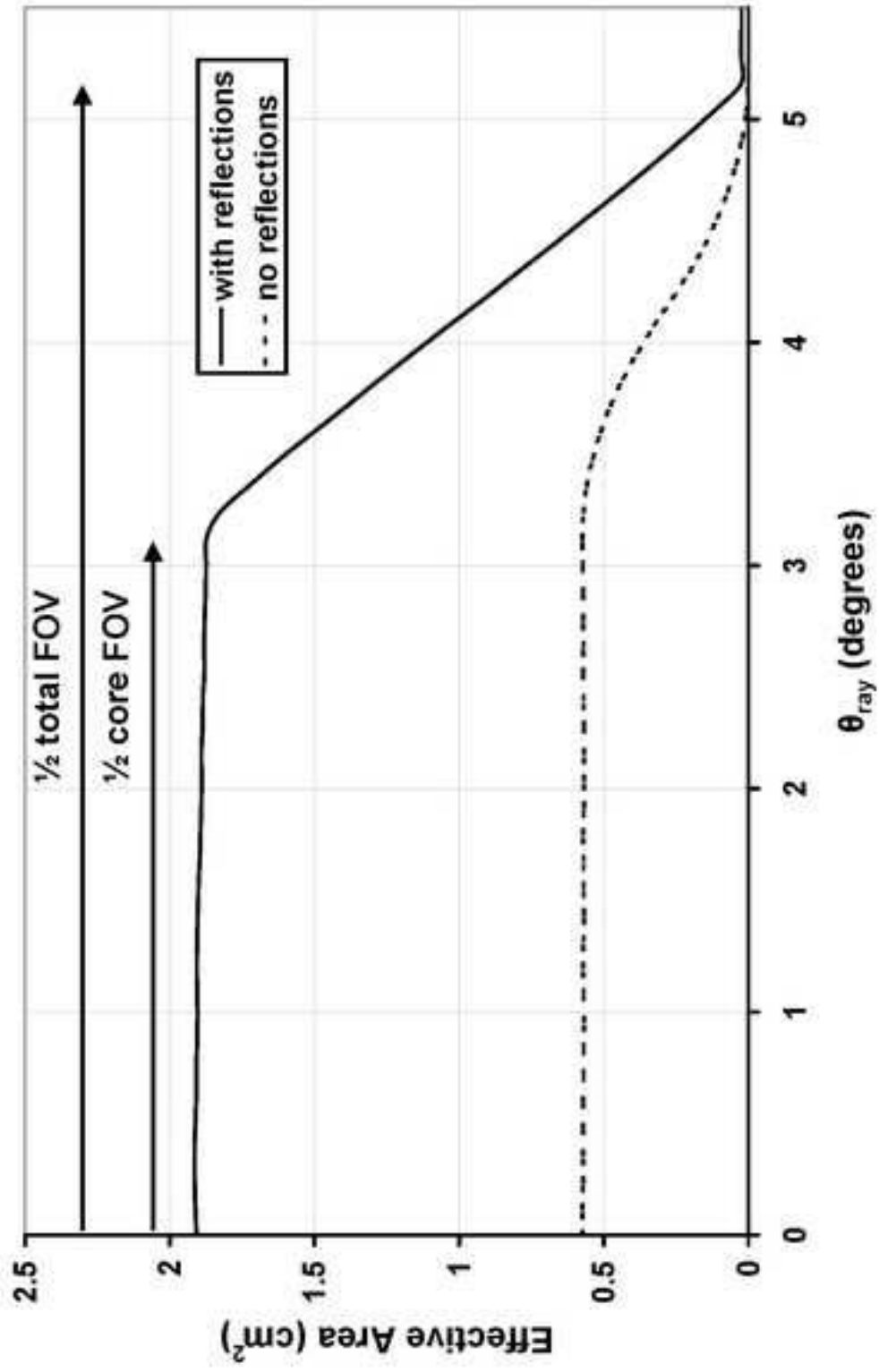


Figure 4







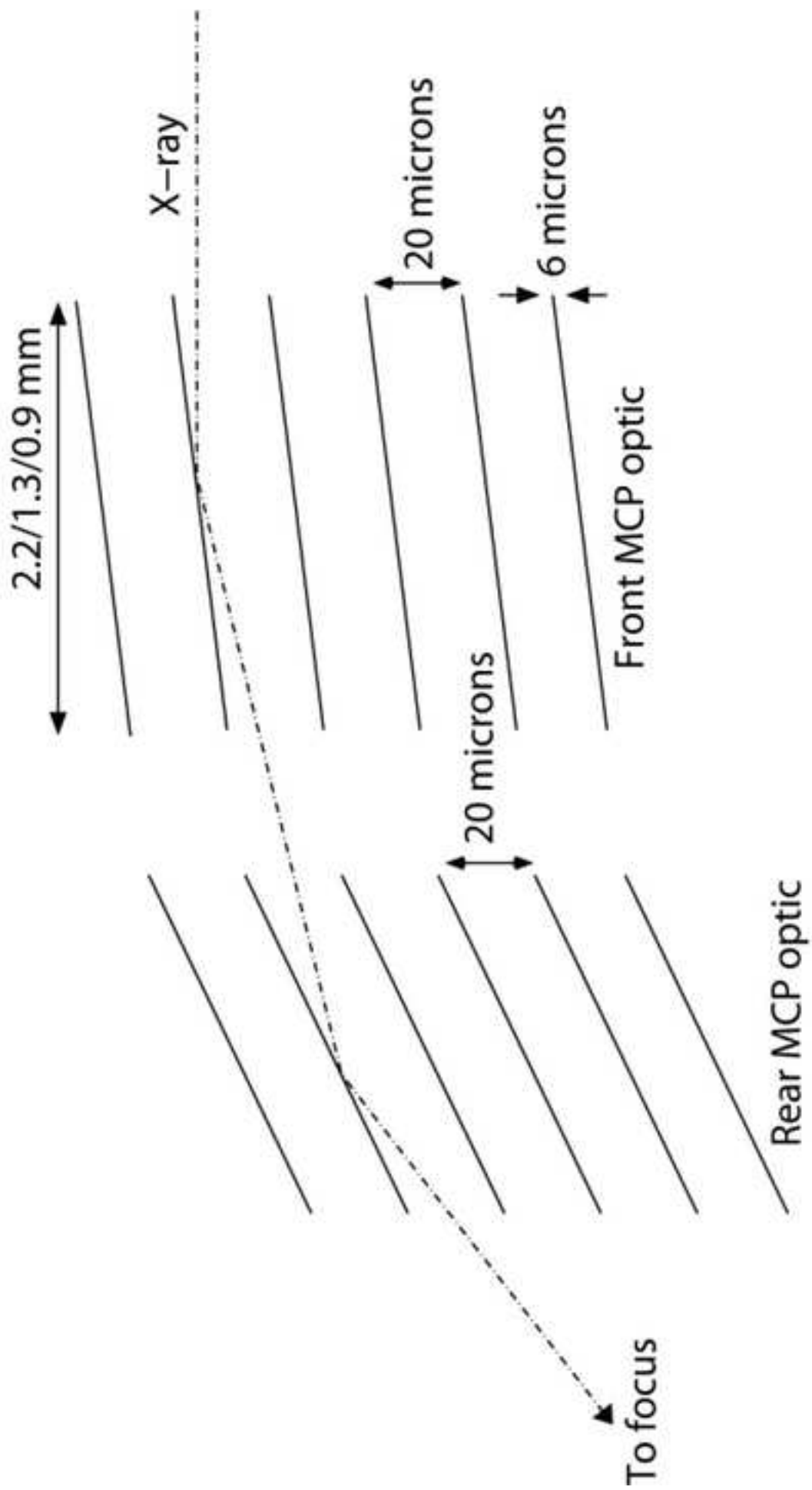


Figure 8

