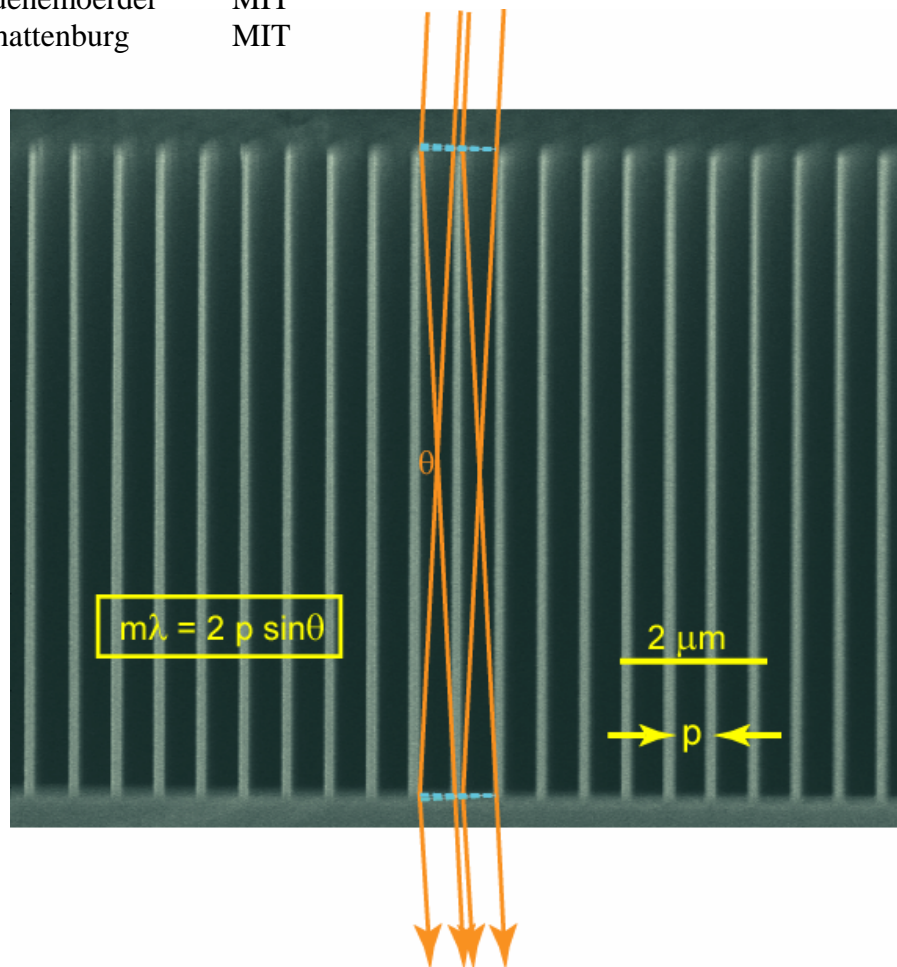


The Importance of General Technology Development: The Example of the Critical-Angle Transmission Grating

A White Paper submitted to the Discipline Program Panel on Electromagnetic Observations from Space (EOS) in response to the Astro2010 Call for White Papers on Technology Development

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Abstract:

We argue for support of university-based technology development in the areas of basic grating and detector research that enables improved detection and spectroscopy. We use the recent development of blazed transmission grating for the soft x-ray to EUV band as a case study to show how universities can provide a high return on investment, and how fundamental technology development can provide benefits beyond its initial goals and the confines of NASA.

I. Introduction

The expression “spectroscopy puts the ‘physics’ into astrophysics” nicely sums up the tantamount importance of spectroscopy for the quantitative modeling of many astrophysical theories [1]. The main ingredients for good useful spectroscopic data are high signal-to-noise, high spectral resolution R , and usually accurate wavelength or energy calibration. Spectroscopy not only is a very rich area in the science of astronomy and astrophysics, but also in the realm of technology. This, of course, is due to the fact that astrophysics practically covers the whole electromagnetic spectrum, within which the properties of interactions between photons and matter vary widely. This has led to a large variety of spectroscopic techniques that cover different parts of the electromagnetic spectrum.

In this White Paper we argue for support of university-based technology development in the areas of basic grating and detector research that enables improved detection and spectroscopy. We use the recent development of blazed transmission grating for the soft x-ray to EUV band as a case study to show how universities can provide a high return on investment, and how fundamental technology development can provide benefits beyond its initial goals and the confines of NASA.

II. Spectroscopy in the Soft X-Ray and EUV Bands

A technologically interesting situation exists in the spectral region between harder x rays (several keV) and the vacuum ultraviolet (VUV). On the higher energy (E) side fine energy resolution (fixed $\Delta E \sim 2$ eV, $R \sim E$) can be achieved with non-dispersive imaging detectors such as CCDs or x-ray microcalorimeters, while towards longer wavelengths (λ) dispersive spectrometers (utilizing crystals, gratings, fixed $\Delta\lambda$, $R \sim \lambda \sim 1/E$) give higher resolution (see Fig. 1).

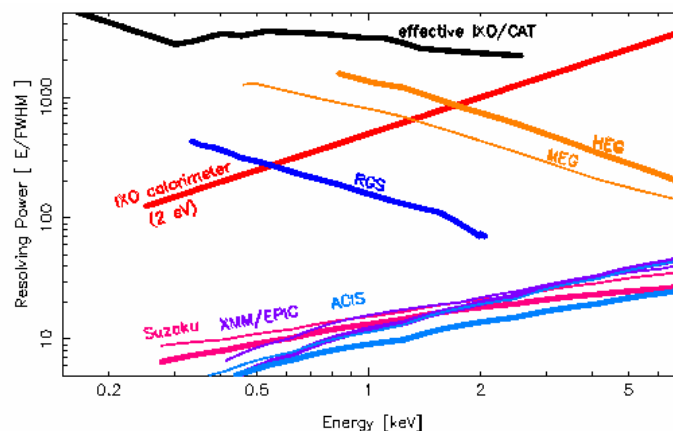


Fig. 1: Resolving power comparison between instruments on different missions [2].

Astronomers are interested in this spectral region for many reasons, and the International X-ray Observatory (IXO) as well as Generation X (Gen-X) are designed with high spectral resolution and high effective area soft x-ray spectroscopy in mind. Areas of

research to be addressed range from the large scale structure of the universe to the detailed structure of individual stars. They all have in common the need to resolve the absorption and emission signatures of atomic ions which reveal the temperatures, compositions, and dynamics of the plasmas involved. Some of this work was begun with Chandra and XMM-Newton grating instruments, but often, the resolving power and area do not provide enough sensitivity, or only allow access to the extreme cases. We briefly list a few areas where a grating spectrometer (as envisioned on IXO) can enable breakthrough discoveries. Details of some of these areas can be found in various Science White Papers submitted to the Decadal Survey:

Detection of the warm/hot intergalactic medium (WHIM) - the "missing baryons", detectable only in x rays - can be done through absorption line studies toward distant galaxies [3]. Cosmological models predict the number, temperature, and composition of this matter. On a more local scale, similar studies of nearby galaxies can reveal the structure of galactic haloes and relation to dark matter, and the relative importance of abundances, temperatures, and flows in the galactic and inter-galactic media, using absorption features of the abundant elements from carbon to nickel [4]. High resolution is crucial for progress in understanding the evolution of young stars. Chandra grating spectra showed that there are large temperature and composition anomalies in some stars, which are probably signatures of x rays from accretion [5]. However, only a few bright stars are available to Chandra; the relevance as a process in formation of stars and planetary systems is an important ongoing study. Probing material between the stars - the Interstellar Medium (ISM) - is also done in x rays by detecting the details of absorption edge structure due to gas and dust in the ISM on the line-of-sight to a bright object [6]. The composition and distribution of gas and dust has wide significance, from nucleosynthesis to planet formation.

In general the transition-rich soft x-ray and extreme ultraviolet (EUV) band contains many resonances for low to intermediate atomic number elements. On the one hand it provides many useful spectral diagnostics, but on the other hand this also leads to strong photon absorption, which is responsible for the relatively low diffraction efficiency of the gold phase-shifting transmission gratings on board of the Chandra X-Ray Observatory at energies below 1 keV [7]. Such transmission gratings could be optimized for a different wavelength through the use of other materials, but not for a broader band of wavelengths that is often demanded for an observatory-type spectrometer.

Absorption is less of a problem for reflection gratings. They can be blazed for reflection at grazing angles of incidence ($90 \text{ deg} - \alpha - \gamma$, Fig. 2) below the angle of total external reflection, which leads to relatively high diffraction efficiencies ($> 20\text{-}40\%$) for wavelengths longer than a certain value. For example, for x rays incident at a graze angle of $\theta = 3 \text{ deg}$ onto the smooth facet of a gold covered reflection grating good diffraction efficiency ($> 20\%$) could be achieved for $\lambda > \lambda_c(\theta, n(\text{Au})) = 0.9 \text{ nm}$. ($n(\text{Au})$ = index of refraction of Au.) Examples for soft x-ray reflection grating spectrometers are the RGS on XMM-Newton, and an off-plane grating spectrometer proposed for IXO [8].

However, reflection gratings have two main drawbacks. First, the small angles of incidence require gratings that are long along the direction of photon propagation in order to cover the telescope aperture. Second, the reflection geometry demands high optical figure and alignment precision to prevent broadening of the telescope point spread function (PSF) in the direction of dispersion, and thus loss of spectral resolution. Both requirements lead to a mass disadvantage (long, relatively thick grating substrates) compared to transmission gratings, which are extremely alignment and figure tolerant, and only need to be a few micrometers thick along the optical axis. Another interesting feature of soft x-ray transmission gratings is that they become increasingly transparent towards higher energies, allowing those photons to –for example - continue towards a non-dispersive imaging detector at the telescope focus that provides higher spectral resolution at those higher energies. This way collecting area and resolution would be optimized for simultaneous spectroscopy over a wide band pass, covered by dispersive and non-dispersive spectrometers.

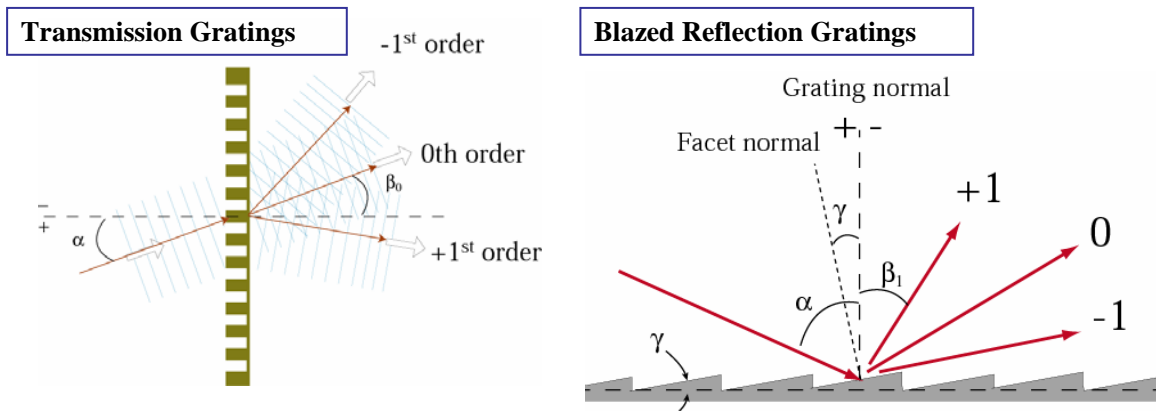


Fig. 2: Comparison of transmission gratings and blazed reflection gratings.

Against this background we describe a recent approach that combines the advantages of transmission (relaxed figure and alignment tolerances, low weight, synergy with non-dispersive spectrometers) and blazed reflection gratings (high diffraction efficiency for wavelengths $\lambda > \lambda_c$).

II. The Critical-Angle Transmission (CAT) Grating

The CAT grating is a blazed transmission grating [9]. Blazing is achieved in analogy to blazed reflection gratings through incidence onto a smooth grating surface at a small angle of grazing incidence. The main difference lies in the fact that the reflecting surfaces in the CAT grating are the sidewalls of the thin, high-aspect-ratio grating bars that are freely suspended at their narrow sides by support structures from within the plane of the grating (see Fig. 3). The geometrical parameters of the grating bars are given by the small angles of grazing incidence, the desire to have each photon incident on the gap between two bars undergo a single “reflection” (in a geometrical optics approximation), and minimum grating duty cycle (ratio of bar thickness to grating period) for maximum

throughput. The resulting geometrical parameters might look a little “crazy”, even for people who have a certain familiarity with modern nanofabrication technology. For a soft x-ray spectrometer an example set of parameters would be $p = 200 \text{ nm}$, $b = 40 \text{ nm}$, $\theta = 1.5 \text{ deg}$, and $d = a/\tan\theta = 6.11 \text{ }\mu\text{m}$. This means that the grating bar aspect ratio b/d is on the order of 150. Until recently similarly high aspect ratios have been achieved in unrelated work through anisotropic etching of silicon by several groups, albeit not on such a small scale and without a supporting substrate.

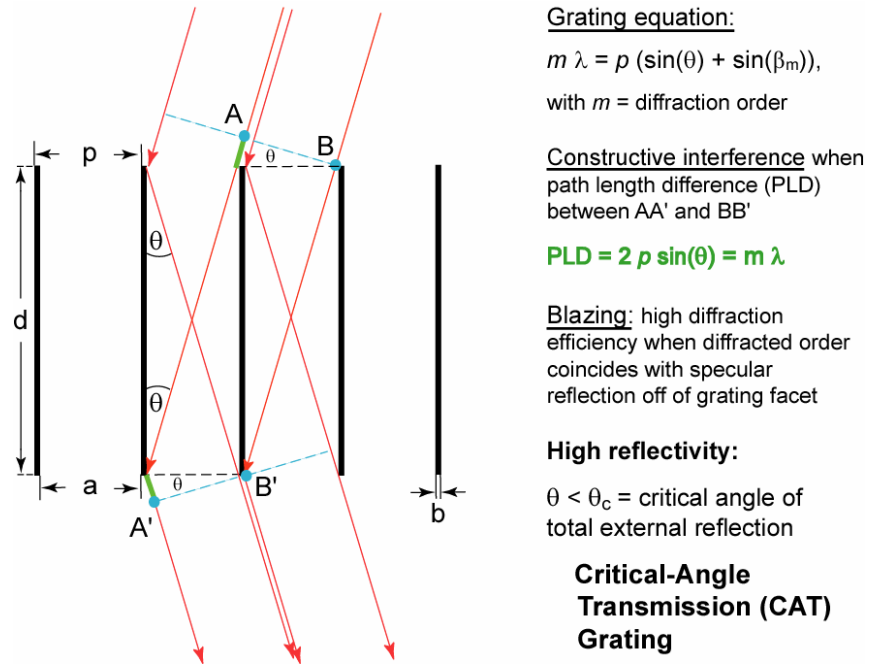


Fig. 3: Schematic of the basic CAT grating concept.

Simulation of the diffraction efficiency of such ideal CAT gratings through rigorous coupled-wave analysis gives very promising results that make it worthwhile to attempt fabrication of such structures (see Fig. 4) [10,11]. Most of the efficiency would end up in a small number of (either positive or negative) diffraction orders under a “blaze envelope”, which is centered at an angle 2θ from the path of photons transmitted in 0^{th} order. If gratings are placed in the converging beam of a telescope similar to the case of the HETGS on Chandra, the resolution can simply be estimated by dividing the distance of a given diffraction order from focus by the width of the telescope PSF (this does not take the effects of sub-aperturing into account). This distance is proportional to 2θ at the peak of the blaze and has the effect that the efficiency-weighted resolution is fairly constant across the band pass (shorter wavelengths contribute in higher orders, longer wavelengths contribute in lower orders) [10,11].

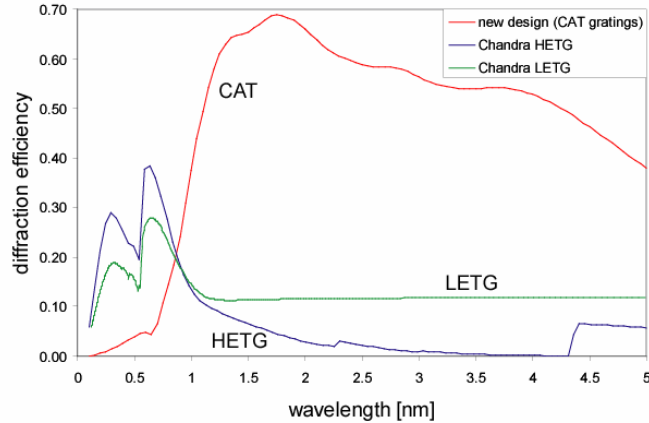


Fig. 4: Comparison of theoretical diffraction efficiency for a CAT grating design (sum over blazed orders) and measured efficiencies for Chandra transmission gratings.

Back in 2006 we started an initially unfunded effort to fabricate such gratings. Minseung Ahn, an outstanding graduate student at MIT, systematically developed and improved the grating fabrication process, starting with a 574 nm-period prototype with lower-aspect ratio and little space between integrated support structures [9,12], and finally arriving at a 200 nm-period, 3 mm x 3 mm grating prototype of almost 50% CAT grating area [13]. Just before graduating he succeeded in fabricating a few silicon CAT grating samples with the above grating bar parameters ($p = 200 \text{ nm}$, $\langle b \rangle = 40 \text{ nm}$, $d = 6 \mu\text{m}$) [14]. Grating facets have been tested for diffraction efficiency at a synchrotron. Earlier samples with easily visible structural defects showed diffraction efficiencies in the range 60-85% of theoretical predictions for a perfect grating [9], while more recent samples seem to be in the 80-100%-of-theory range (data analysis still ongoing) [11,14].

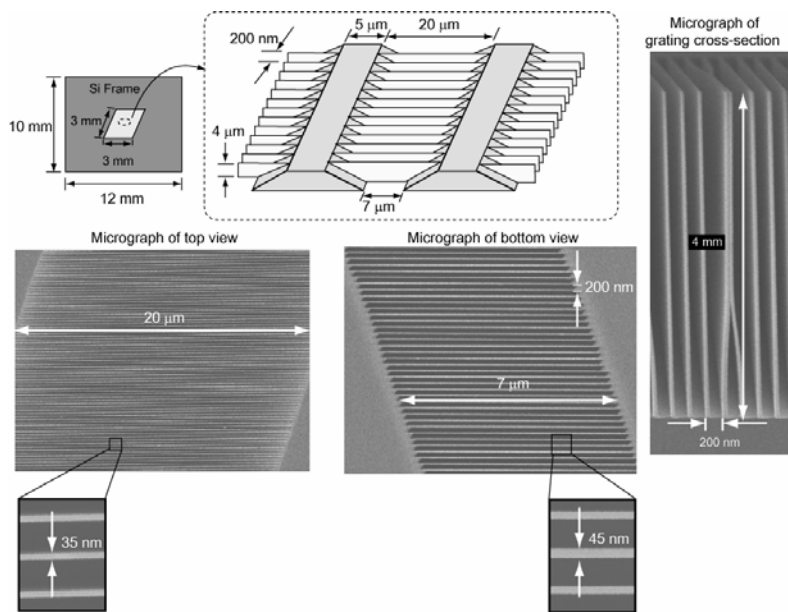


Fig. 5: Schematics and scanning electron micrographs of some intermediate-stage 200 nm-period CAT gratings.

III. Future Work

The work on CAT grating fabrication, which currently is funded only through the ROSES-APRA program, has made tremendous progress, going from conception of the idea to achievement of several goal fabrication parameters with x-ray verification in only three years with only a roughly 1.5 person/year effort. This rapid progress has allowed a CAT grating based spectrometer [10,11] to become a viable candidate for the IXO and Gen-X missions and shows the benefits of a program that is willing to support high-risk research. However, while we consider these results to be a tremendous return on a very small investment by NASA and the American taxpayer, much work remains to be done to lift this technology to a higher Technology Readiness Level (TRL). The grating area needs to be increased, which requires the development of one or two additional, coarser levels of structural supports (similar to gratings on IMAGE and TWINS [15,16]). And the fractional area of the current integrated support structures needs to be reduced. This kind of development is less suited for (the relatively inexpensive) graduate work that leads to a Ph.D. than the initial, groundbreaking work done by Ahn. Instead it requires full-time engineering work, supported by technician-level staff. Unfortunately such labor- and staff-intensive work is impossible to fund through the small ROSES APRA program. The obvious source for further development funds would be the IXO project, but IXO is currently not able to fund any technology development besides some barebones mirror and microcalorimeter efforts. This situation is not expected to improve for at least another two years. We therefore perceive a gap in funding mechanisms that would move innovative, small-scale, high risk (with potential for high reward) projects (ROSES APRA size) beyond the basic demonstration to a more mature technology level. Having to wait for a mission to be ready for ramp-up seems like a waste of time that could be better used to move technology forward instead (see also Ref. [17] for other partially related thoughts), especially if a technology is not limited to a single mission.

Beyond the immediate technology development requirements for missions that are currently being reviewed by the Astro2010 Committee there are many avenues of development that could take this young technology beyond its current straw man designs. For example, CAT grating fabrication so far has relied on the ability to etch silicon crystals in highly anisotropic fashion to achieve ultra-high aspect ratio grating bars with sub-nm smooth sidewalls. Relying on silicon for grazing incidence reflection directly couples the critical angle for a given wavelength to the reflectivity of silicon, and determines the maximum allowed angle of incidence for a desired band pass. (Example: If the desired band pass is $\lambda > 1$ nm, then θ should not be much greater than 1.5 deg.) It would be highly advantageous if the grating bar sidewalls could be made out of a higher-Z material, such as tungsten or ruthenium for example. This could be achieved through the decades-old technique of Atomic Layer Deposition (ALD) [18]. For Ru θ could be increased to 2.5 – 3.0 deg for 1 keV photons [19], resulting in increased blaze angles/dispersion/resolution and lower grating bar aspect ratios, which are easier to fabricate. Alternatively one could stay at 1.5 deg. and expand the band pass to higher energies ($E \sim 2.4$ keV), where gratings can still supply higher resolution than a microcalorimeter with $\Delta E = 2$ eV (see Fig. 1).

Of course CAT grating technology is not limited to observatory class missions, but due to its low weight, small geometrical footprint, and relaxed alignment tolerances could be an attractive candidate in smaller spectroscopy missions anywhere in the 6 Å to ~ 100 nm wavelength band. In the EUV normal incidence optics can only achieve high efficiencies with narrow-band multilayer coatings, typically limiting compact (i.e. non-grazing incidence) optical setups to quasi monochromatic applications. Introduction of a dispersive broadband CAT grating could be used in conjunction with laterally-graded multilayer-coated normal-incidence optics to build compact broadband EUV and soft x-ray spectrometers [20]. The list of examples could be continued.

Many technologies that have proven themselves useful in astronomy instrumentation have not been developed initially with astronomy and astrophysics in mind (who in their right mind would have ever developed a transition-edge sensor for astrophysics, knowing that it would require to fly a 250 kg dewar?). In contrast, CAT grating-related technology is an example where technology development based on the needs of astronomers can have a positive impact on technology and science outside of astrophysics. The small-period, high aspect-ratio structures pioneered during this work could find application in earth-based plasma diagnostics, neutron scattering and instrumentation, basic research in atom physics, the interaction between electrons and surfaces, soft x-ray microscopy, and EUV lithography (see Ref. [9] for further discussion), and it might inspire other ideas that we have not thought of ourselves.

IV. Summary

We hope that our example of CAT grating technology development to date demonstrates the types of potential payoffs that NASA could obtain through strategically placed increased funding of general technology development. Especially in the area of detection and spectroscopy it is easy to see how new developments can be of use outside of specific mission designs. We also believe that the best chance for groundbreaking results from basic research with relatively low resources comes from university research performed by motivated graduate students under experienced guidance. However, most grating and detector technologies can not move beyond a certain level on the cheap, which is why NASA should significantly increase funding for its technology development programs in these areas.

By supporting these kinds of technologies NASA can continue to argue that the benefits to society in exchange for funding NASA extend beyond the agencies' core mission. We were surprised about NASA's conspicuous absence when the American Competitiveness Initiative was announced a few years ago. This neglect by Congress might have been rooted in a perception that NASA's contribution to technological progress, education of our workforce, and American competitiveness is second rate or ineffective. If true, this would be a perception that NASA would be well advised to shed.

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Some Astro2010 Science White Papers relevant to soft x-ray spectroscopy:

Bregman et al: "The Cosmic Web of Baryons"

Bregmen et al: "The Missing Baryons in the Milky Way and Local Group"

Lee et al: "Solid State Astrophysics: Probing Interstellar Dust and Gas Properties with X-rays"

Mukai et al: "Observational Studies of Potential Progenitors of Type Ia Supernovae"

Osten et al: "Mass-loss and Magnetic Fields as Revealed Through Stellar X-ray Spectroscopy"

Schulz et al: "Distribution and Structure of Matter in and around Galaxies"

Schulz et al: "Structure and Evolution of Pre-Main Sequence Stars"