

Realization of the Reflection Grating Spectrometer on XMM-Newton

Jan-Willem den Herder joined the team which developed the Reflection Grating Spectrometer (RGS) for XMM-Newton in 1988. This team was led by Bert Brinkman of SRON, the Netherlands Institute of Space Research and was a collaboration between the group of Steven Kahn (who moved from the University of California, Berkeley to Columbia University and then to Stanford over the duration of the project), the group of Graziella Branduardi-Raymont (Mullard Space Science Laboratory, UCL, London, UK) and the group of Alex Zehnder and Knud Thomson (Paul Sherrer Institute, Switzerland). Each of the institutes had quite large teams on the project. The reason to recall this as first item is that the realization of complex instruments is a real team effort and can only be successfully accomplished if the teams work closely together and get satisfaction from the achieved results.

Initially den Herder was leading the calibrations of the RGS, then he became responsible for the delivery of the instrument and the commissioning. Following the commissioning he has been following the instrument with an emphasis on the performance. Below I will give my personal view of the different phases but not after describing some general aspects.

The development of the instrument took over 15 years with a group of dedicated scientists and engineers and some overarching aspects, which contributed to the final success of the instrument, included:

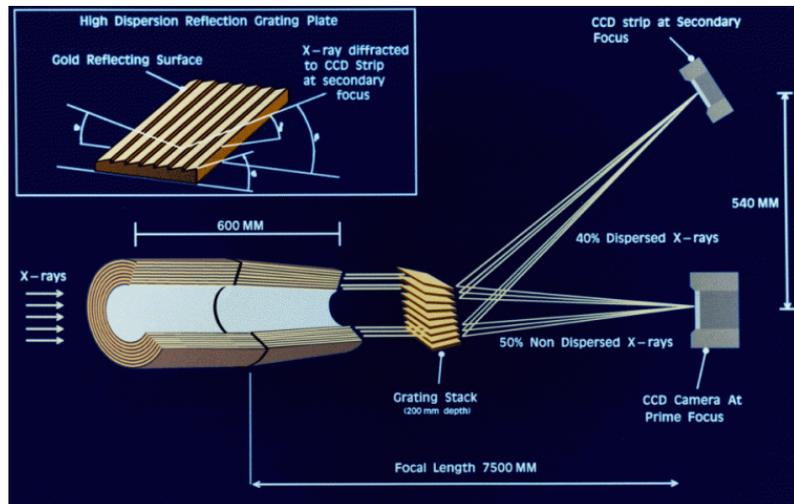
- There was a relatively small project and system engineering team and the number of partners was small with, in general, very clean interfaces. This allowed the project team to work efficiently without the overhead needed to manage larger consortia.
- There were early end-to-end tests including the optics provided by ESA, the reflection gratings and the camera at the Panter facility in Munich. This enabled us to identify issues with our instrument in an early stage and find the best possible technical solution in time. We spend months in the Munich area where dr. Heinrich Bräuninger supported our measurements in a very pragmatic and flexible way. Even during some of the many free days during May in Munich, we were able to perform tests for more than 12 hours a day.
- In case of unexpected performance (which is a euphemism for a problem) the team focused on finding the technical root causes and the best technical solutions. The programmatic issues were essentially solved once the best technical solution was defined. This was facilitated by, on one side a relatively small group but also flexibility in the team and by ESA in covering the drawbacks in the best possible technical way.
- A very focused interaction with the project team at ESA/ESTeC. Similarly to the RGS team the ESA team which interfaced with us was small (a few people). Again, in combination with a practical focus on technical solution, made our interactions very efficient.

- A similarly focused interaction with the prime contractor (Astrium Friederichshafen) where we could concentrate with the experts of the prime contractor on technical issues and any programmatic items were covered by the ESA project manager (Robert Laine) without complicating our technical discussions

XMM-Newton is now operational for 20 years with ground breaking contributions to science. In the following I describe some of my personal observations, approximately following the timeline of the mission but I first indicate the major components of our instrument. Clearly I focus on areas where issues arose which we did not expect but, by careful and dedicated analysis, managed to handle. The major reference is in two A&A articles (A&A 365, L7-L17 (2001), A&A 573, A128 (2015)) but many more instrumental papers have been presented at the SPIE conferences.

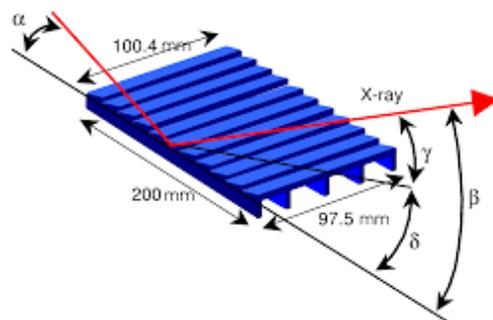
The Reflection Grating Spectrometer (RGS)

The basic diagram depicting the RGS instrument (of which there are two on XMM-Newton) is given at the right. Behind the X-ray collecting mirror a set of 182 gratings is placed which create a dispersed beam on a CCD strip at the secondary focus. Using the energy resolution of the CCDs the different orders can be separated. With this design a resolution varying between 100 and 500 has been realized.

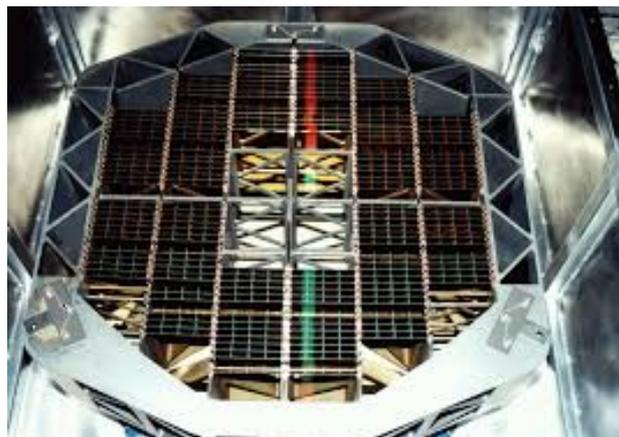


The reflection grating assembly

For the RGS instrument reflection gratings were selected as they allow to optimize the effective area with a good resolution in the energy band between 5-35 Å where K-shell transitions for low-Z elements (C, N, O, Ne, Si) and L-shell for Fe can be found. To achieve the effective area one needs to match the full exit aperture of the mirrors and this requires a large set of ultra-flat, accurate and light-weight gratings. This was feasible by placing 182, accurately flat gratings of 100 x 200 mm² in the convergent beam of the telescope. Many issues had to be overcome (our US colleagues had the lead) but to mention some:



- A variable line density was required. To get this right at the master grating an interferometrically controlled ruling machine was used
- All gratings had to be identical requiring a very repeatable process using one master grating and making replicas from this
- The gratings had to be very stiff and thin. SiC was selected as substrate and ribs were applied to enable the correct surface flatness
- Scattering from the back sides of the gratings and from the ribs had to be taken into account and to be minimized (by having a rough surface)
- The gratings needed to be mounted in a light weight structure with a very low thermal expansion (to maintain the alignment between the 182 gratings). A Beryllium structure was selected but manufacturing of such a large structure was a real challenge. Only two proto-flight units were produced
- Each grating had to be accurately positioned in the grating structure. This was done in a two-step approach: 4 rails which could fix 8 gratings were accurately glued to the Be-structure and next the gratings were hold in place by clips (see figure). However, during vibration tests these clips started to resonate and a soft glue had to be added to avoid this. One of these rails had a production error and the position was left open (explaining the difference of 182 – 181 gratings per grating box)
- An unique alignment reference for the assembly of gratings in the Be structure had to be defined as the gratings had to be aligned accurately not only with respect to each other but also with respect to the mirror. For the first grating unit the reference during the assembly process was not set as it should and this was identified during the end-to-end calibration campaign in Munich. Fortunately, the relative alignment of all gratings was correct and by a simple rotation and displacement of the full structure this issue could be largely solved. To verify this fix we had to repeat the calibration of the unit in Munich after the fixes and this was successful. Obviously, this issue could be avoided for the second reflection grating assembly. Again, showing the relevance of sufficient testing of the hardware before delivery.



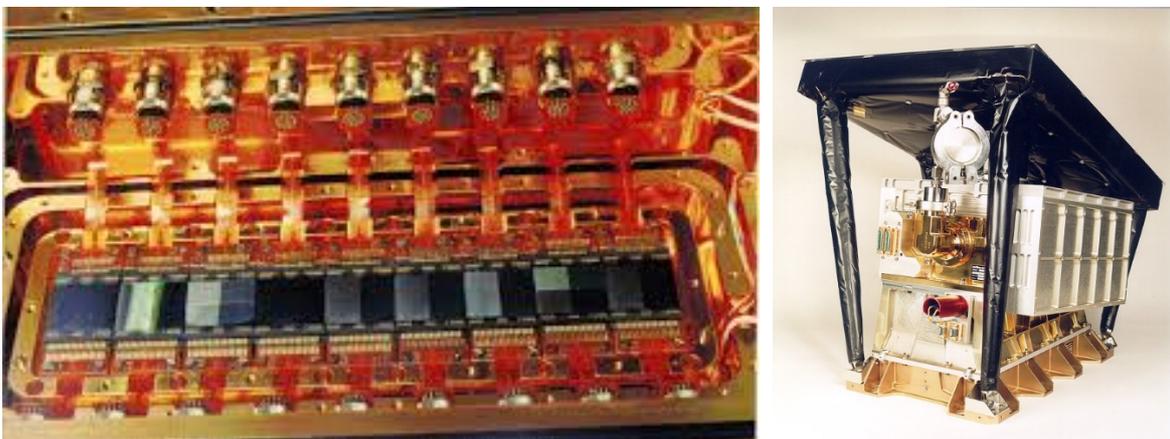
Alignment rails for the gratings (left) and an integrated Reflection grating Assembly with 182 gratings (right)

Detector development

The critical component in the camera are CCDs with good spectral resolution and high quantum efficiency in the range of RGS. High efficiency at low-energies forced us to develop back-illuminated CCD, which was a tricky development path. Development and production of CCDs was beyond the technical capability of SRON and thanks to contributions from ESA a very efficient collaboration was setup with the industry EEV in the UK (now Teledyne/E2V). In the development phase, there was a close interaction between SRON and EEV, since SRON measured the X-ray performance and other key properties of all the development CCD's. The performance of the back-illuminated CCD made by conventional ion implantation remained unsatisfactory. This forced us to find another solution. The flexibility and dedication at EEV and our good working relations made it possible to develop, test and implement Gas-immersed Laser Doping (GILD) successfully very late in the program.

One, not uncommon, problem is that the very high resistivity wafers needed for our application, could only be produced in short periods at the wafer manufacturer and we (even ESA) was a very small client to this firm (Wacker). Thanks to the willingness of the manufacturer just a sufficient set of wafers was available.

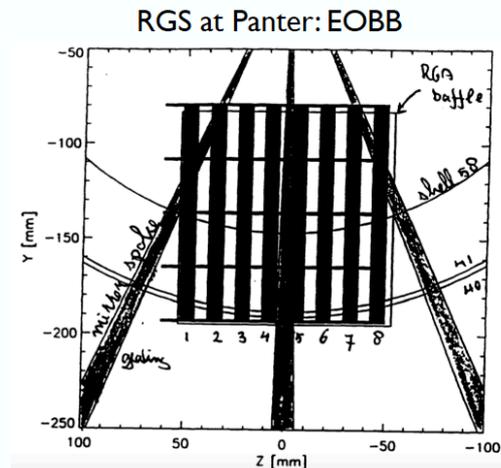
The CCD bench is shown below where 9 CCDs are placed on the Rowland circle with a minimal gap between them. Vacuum feedthroughs are also visible to allow the camera to stay closed on the ground. At the right side the integrated camera is shown with its radiator (to enable passive cooling to -120°C). The temperature is controlled by heaters on the CCD bench. Also seen is a part of the ground support equipment to enable the purging of the camera with dry Nitrogen.



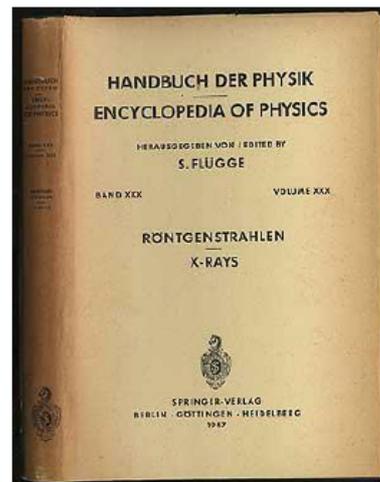
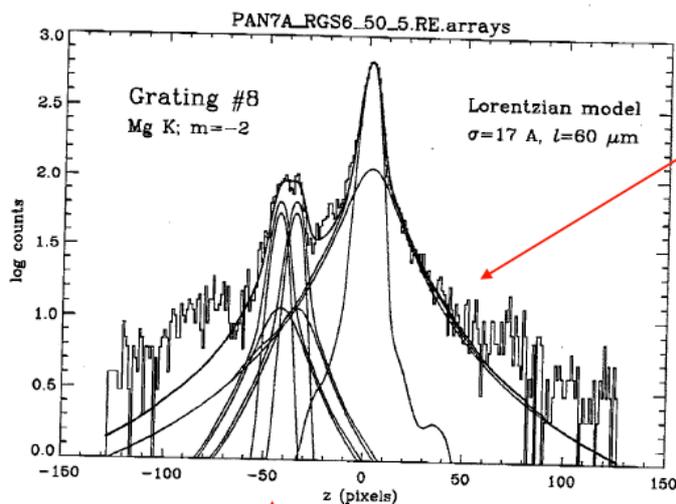
The CCD bench with 9 frame transfer CCDs and the integrated camera clearly showing the passive radiator

Calibrations

The calibrations and verifications were performed very early in the development cycle. Early testing of a system is always a very beneficial exercise. Any problem found early can be relatively cheaply solved. For RGS we performed an early test in the so-called Electro-Optical Breadboard (EOB) where we combined a set of 8 properly aligned gratings with a model of the mirror with 4 shells in place. Due to the relative orientation of the optical layout, the resolution is much better than for a fully populated RGS ($R \sim 3000$). At the right we show this layout as seen from the camera.



To our surprise, the width of the emission lines (the resolution) measured in the EOB was not as we expected. At shorter wavelength a second peak appeared which we could not explain. Where these reflections from the ribs which support each grating or could this be a kink in the grating surface? Colleague Heinrich Bräuninger alerted us to satellite lines listed in the *Handbuch der Physik* (1957) indicating that satellite lines will appear at longer wavelength than their 'parent line' in highly ionized plasmas. With new instrumentation we do not only push the limits of our knowledge about astrophysical sources but one can expect also to push the limits of the experimental setup at the ground facilities. A similar situation occurred when we placed our grating box in an apparently non-divergent UV beam in the Liège test facility and after a tedious effort we could conclude that there was a small divergence in the beam (less than 1 arcsec).



A measured line spread function for the EOBB at the Panter facility and the Handbuch de physic in which this effect is described

Having understood this basic physics effect we now could turn to the end-to-end testing of our two grating units. One should, however, be aware that this is not in the final flight

configuration. Due to the non-infinite beamline in Panter (120 m long) the grating units had to be placed 500 mm further from the optics than for an infinite beam. Essentially this limited the calibration in two ways: (a) the final geometry could not be tested which implies that the final alignment, if not done correctly, would result in an additional degradation of the energy resolution in the flight configuration and (b) not the full mirror was illuminated due to shadowing effects of the very densely packed mirrors for a divergent beam. This limits the accuracy of the measurements of the mirror point spread function (the entrance edges of the reflecting mirror surfaces are not illuminated) and the accuracy of the effective area (as only part of the mirror is illuminated).

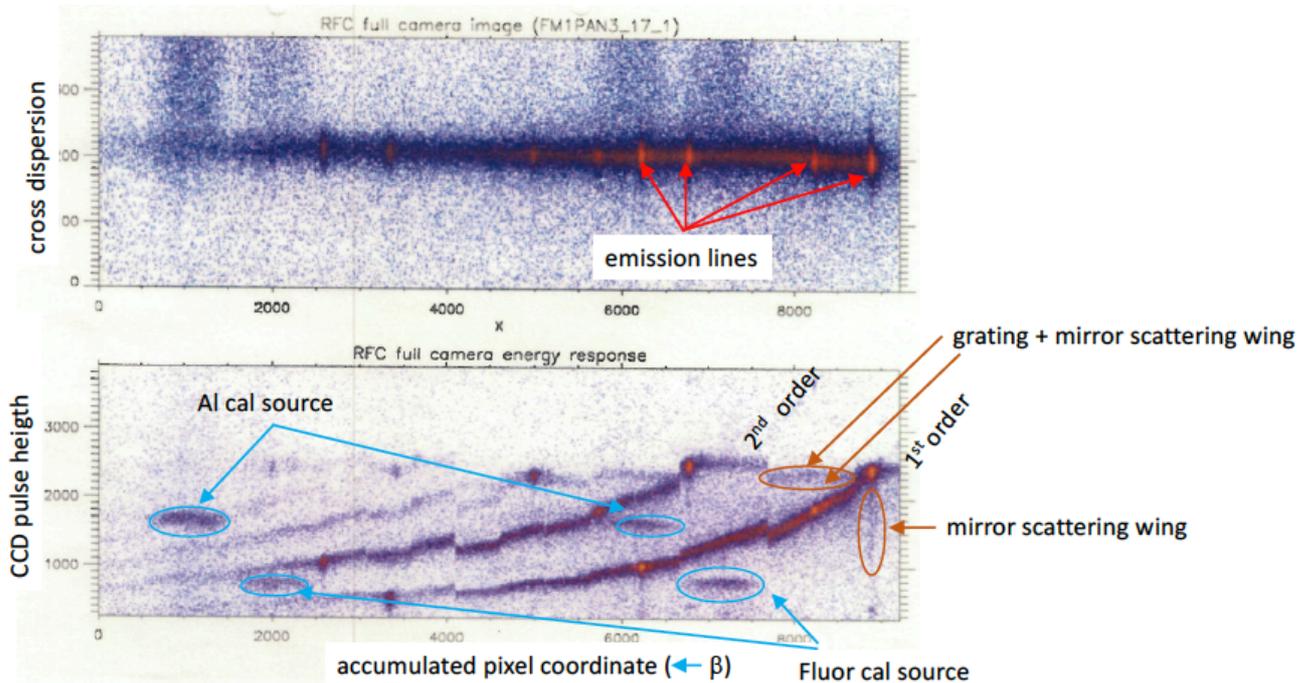
A real spectrum

As one of the last steps during the calibrations at Panter we have used a Au source with multiple lines and the results look similar to what one can expect for flight data. These measurements were performed in August 1997, more than two years before launch. For illustration we show the raw, uncorrected data as this nicely displays a number of key features. At the top panel of the figure below the Image for the source is shown (vertical cross dispersion, horizontal the dispersion in terms of accumulated pixel coordinates). At the bottom panel the corresponding CCD spectra are shown. Clearly the ‘banana-like’ representations follow the dispersion equation (note that contrary to the usual representation where the scattering angle increases to the right, in this case the scattering angle decreases to the right).

We can identify a number of components which are all taken into account in the data processing:

- In this raw data clearly the effect of the gain per CCD-half is visible (step function in the vertical direction between the different CCDs)
- the scattering wings of the mirrors is shown by the vertical extension of the spots near bright emission lines
- The combined scattering wings from the gratings and the mirror in the horizontal direction. Already this raw data shows that the gratings have a significant contribution to the scattering
- Two sets of 2 calibration sources which are mounted inside the camera and consist of an Am²⁴⁴ source (alpha emitter with a Teflon or Al target). The purpose was to use these sources as energy calibrator (which indeed works as expected) and as contamination monitor (monitoring the relative changes in the ratio of the F/Al lines as function of time). The latter function turned out to be more complex as one needs to include also the contamination on top of the Am source itself (e.g. an ice layer stops very efficiently the alpha particles) creating an additional free parameter

All these aspects had to be included in the calibrations of the instrument and having some data looking flight-like before the launch allows verification of the pipeline processing in a relatively early stage. Whereas our calibrations were concentrated on single, narrow, emission lines as this enabled us to determine efficiencies as well, at the end of the calibration campaigns we used a continuum source where clearly the lines and the bremsstrahlung is visible. We show this below.



A continuum spectrum using an Au target collected during the calibration campaign in August 1997

Delivery and satellite testing

After the instrument was delivered we participated in a limited set of tests at spacecraft level. This included two end-to-end tests with the instruments, satellite and the ground stations where we had to check the proper response of our instrument. More challenging was the thermal vacuum test at ESTeC where only half of the satellite with the instruments was tested at the time. As part of these tests we needed to verify the proper performance of the cameras and, with detector closed with a single shot door this was not obvious (as closing the door after tests was practically not feasible). At the end a solution was found by connecting a remotely controlled valve to the purging port of the camera.

An even more critical item was the proper alignment of the mirrors, gratings and cameras. Whereas the mirrors and gratings are directly mounted to each other, the cameras were placed at 10 m distance and were only integrated in the ESA clean room. With dedicated alignment setup, using theodolites, autocollimation and corner cubes we managed to do so while looking through a central lens from underneath the integrated XMM-Newton. Contrary to our expectation, the alignment was not as we expected for one of the RGS cameras and needed to be corrected by about 1 cm (not impossible but larger than initially expected). Knowing the experience with the Hubble Space Telescope, we were all nervous. Fortunately we had two completely independent methods to calculate the alignment (one by our team and the other by Astrium) and they agreed with each other. Thus we decided to change the inserts and move the camera but we would not know if we did it right till we had first light in orbit.



Launch

After integration and complete testing of the satellite the Chandra mission, a NASA mission launched in August 1999, experienced a much faster degradation of the CCD detectors than anticipated. Although this information was considered sensitive from the perspective of the national security (ITAR, USA), sufficient information could be exchanged to identify the cause, estimate the risks for XMM-Newton and perform some critical tests. The actual cause is the damage due to the absorption of low-energy protons, focused by the mirrors on the detector while passing through the radiation belts. These low energy protons cause lattice damage in the detectors close to the layer where the charge is shifted through the device, creating a charge loss for each transfer. As the charge is the measure for the energy, a charge loss translates directly in a reduction of the CCD energy resolution. Once this was identified a simple solution for Chandra was in place as these protons can also be stopped by the 'closed' position in the filter wheel (shutter) with which the cameras in the mirror focus are equipped. A similar solution could be adopted for the imaging detectors of XMM-Newton (EPIC) but the RGS camera had no such shutter. To assess the risks for the RGS two actions were mandatory: to measure the proton reflectivity of the gratings at larger incident angles and to measure the damage caused by low energy protons on the RGS detectors. These detectors differed to some of the Chandra CCD detectors as they were all illuminated from the backside. These activities had to be performed between the time the Chandra problem was understood and the flight acceptance review of XMM-Newton in October in Kourou (French Guyana). Thanks to a dedicated effort of many people these tests could be completed in time to conclude that the RGS could be safely operated despite the fact that it has no 'closed' position (shutter). Simply the extra reflection reduces the fluence of the soft protons and in the back-side illuminated CCDs these low energy protons are stopped in the top layer of the Si and not close to the gate structure where the charge is transferred from one pixel to the next.

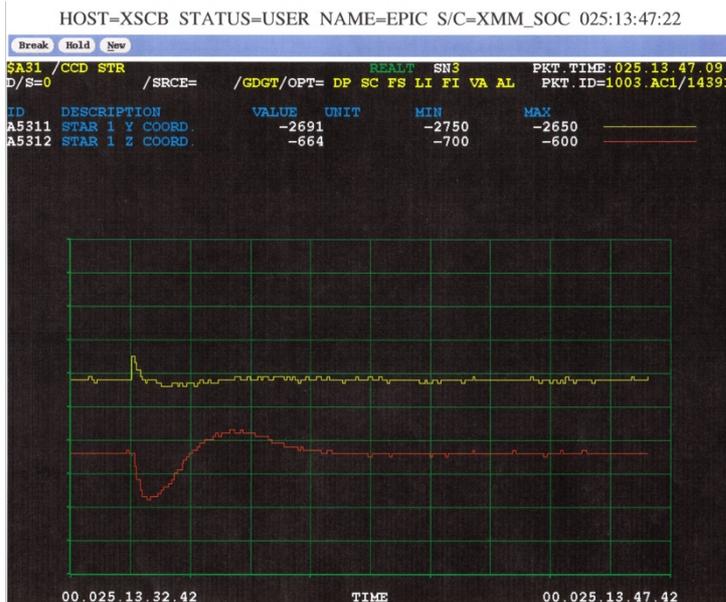
The launch was impressive and it was really great to be there. Whereas for some spectators a successful launch was enough to make them happy, we, as instrument team needed many more steps. The report on the deployment of the solar panels was important but the real stuff, commissioning and operating our instrument, was still ahead of us but would only start in the new year, allowing the team to relax a bit between launch and the next year.



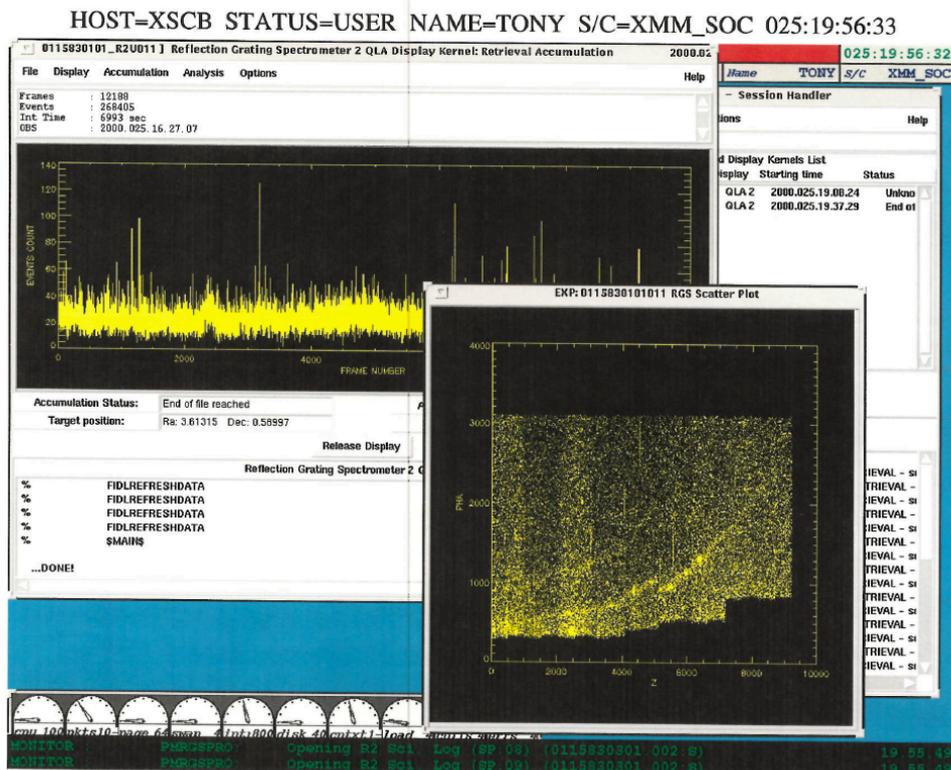
Commissioning

After the launch the critical satellite functions were, of course, commissioned but thanks to the ESA project manager the instrument commissioning started on Jan 2nd, 2000. For this I participated in the switch on of our instrument in Darmstadt and the thrill to see the first bits of our instrument (in our case this was a packet containing 'FF') was great. Before opening the door in the camera we could perform a number of tests using electronic test pulses. These test pulses injected variable charge at the output amplifiers of the CCDs and were used during ground testing to perform functional testing in the absence of X-rays. All the cameras were performing nominally but we also recognized that the cameras were all cooled to -50°C early January. We did not fully realized the fact that any water enclosed in the system with the closed door, was frozen on the detector and hence we ended up with a stronger instrumental edge near the O-line than foreseen. Once we fully understood this, the system was already down to -80° C and the additional edge was acceptable. Although the heating up of the CCD was feasible, we did not do so at that time and we never did afterwards.

Having two working cameras the remaining critical step was the opening of the doors (on 25 January and 6 February respectively). During the design phase it was decided that we did not need a separate sensor as the data of the camera would tell us if the opening was successful or not. To our pleasant surprise we could clearly see the opening in the display of the star tracker position where the impact is larger in one direction than the other but where the desired pointing is acquired a few seconds after the opening of the door (I did not think about the momentum induced by the spring when opening the door). Although we did not yet had seen X-rays, the door was OPEN!

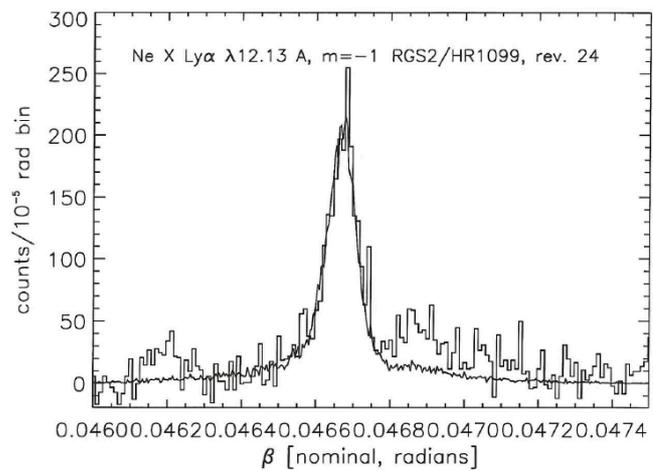


Of course, the next step was to see if X-rays were detected. In this phase the ESAC Quick Look facility could almost immediately process the data. This is shown below where it is clearly seen that these data are completely uncalibrated (e.g. the 9 CCDs with their own gain are visible). Nevertheless the 'banana like' plot was seen including the intensity variations corresponding to emission lines in HR1099.

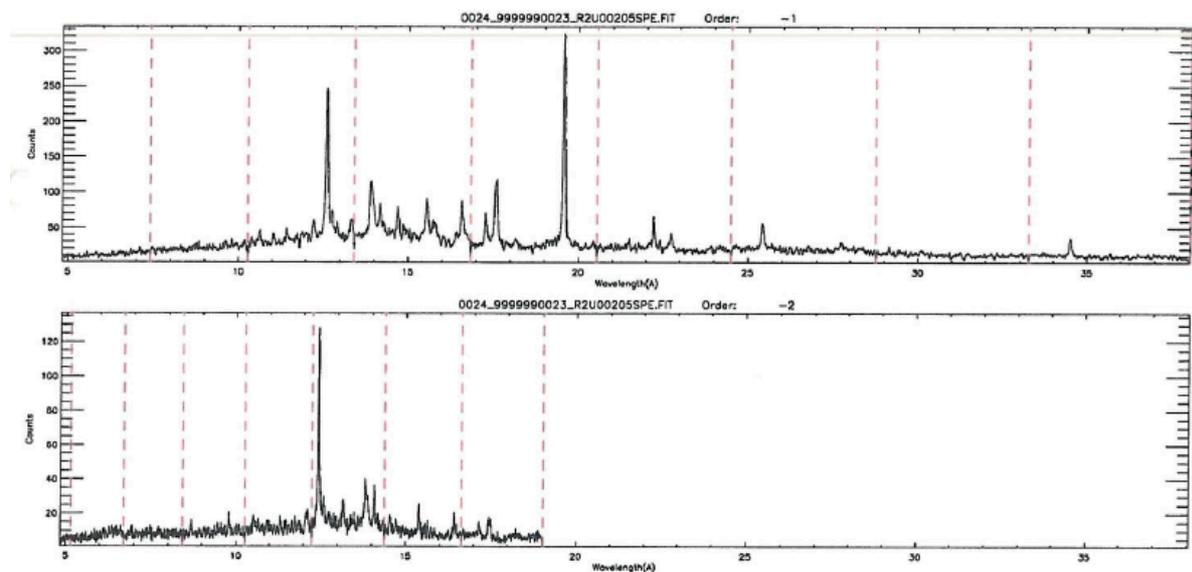


First data with the Quick Look Analysis at ESAC

Now we knew that we detected X-rays and could clearly identify the emission lines in first and second order. The next question was whether or not we got the alignment right. Using two sets of independent data reduction programs from the instrument team it was clear that the experimental resolution matched our predicted resolution perfectly. We had the alignment right! It was also reassuring to see that both reduction software systems gave an equivalent result. The formal pipeline of the software took more time but this was not critical for the instrument team.



First full spectrum of HR1099 2 days after the data were taken is shown below.



First HR1099 spectrum observed with RGS2

However, on 30 January RGS2 was switched off due to the current in one of the electronic boxes exceeding its limits. It took about 9 hours before this condition was recognized and a more prompt switch off of the camera would have been safer. Fortunately the problem was related to CCD4 only and could be traced

back to a spontaneous failure of an HI303 analogue switch. Performing tests on the flight spare on the ground showed us that with a faster reaction time we could have limited the failure but, once this CCD would again be switched on in space, the failure would have occurred in any case. Detailed testing of this switch including radiation tests indicated that this was not intrinsic to the switch. The lesson to learn is to switch off as soon as a problem is defined but at the same time, the possibilities to circumvent a failing component is always limited. After 2 days we decided to switch RGS2 on again and since then the instrument has been operational.

One other item we observed was that our telemetry rate was largely filled with background events. The cause was easily identified: Pixels with a maximum ADC value due to charged particles were rejected before the event pattern recognition was applied. The adjacent pixels with lower ADC values were not identified as part of the charged particle but were seen as genuine X-rays. We simply did not thought properly about the effect of particles on the event processing and this was also never tested. Fortunately the fix was simple (changing the sequence of pattern recognition and applying an upper threshold). Having unloadable (and thus flexible) software was crucial and thanks to the fact that we could fix this during the commissioning phase, these changes could be realized within one day (having the experts on the ESA side and instrument side still responsible. Once the satellite is handed over to the operational team, more strict procedures apply (correctly) and such change would have taken more time resulting in a reduced return of the instruments in this early phase.

Performance verification and operational phase

The cameras were working and data taking could start. The ESA software pipeline was not yet available (and it was a conscious decision to launch while the data analysis software was not yet ready). Fortunately we had our own software running and could collect tons of exciting data. Following LMC X-3 we observed many target during the initial phase: PKS-0312, Omega Centauri, PSR 0540, EXO 0748-67, Abell 3195, Crab, PKS 0558, Capella.



To: John Credland/estec/ESA@ESA, Dina Bauer/esahq/ESA@ESA
cc: Fred Jansen/estec/ESA@ESA, Howard Nye/esoc/ESA@ESA, Fabio Giannini/estec/ESA@ESA
Subject: XMM RGS2 CCD4 end

Over night the PI team in Utrecht has determined that the cause for the anomalous current drain associated with CCD4 operation is likely to be due to the failure in the bias electronic controlling one of the clock of the CCD. This circuit feeds only CCD4, it is likely to be a random component failure. The follow up action is to analyse the precise cause of this anomaly.

For continuation of operations it means that CCD4 will not be activated for the time being. RGS commissioning will resume today with the remaining 8 CCDs.

The opening of RGS1 is planned for Sunday night.

Regards

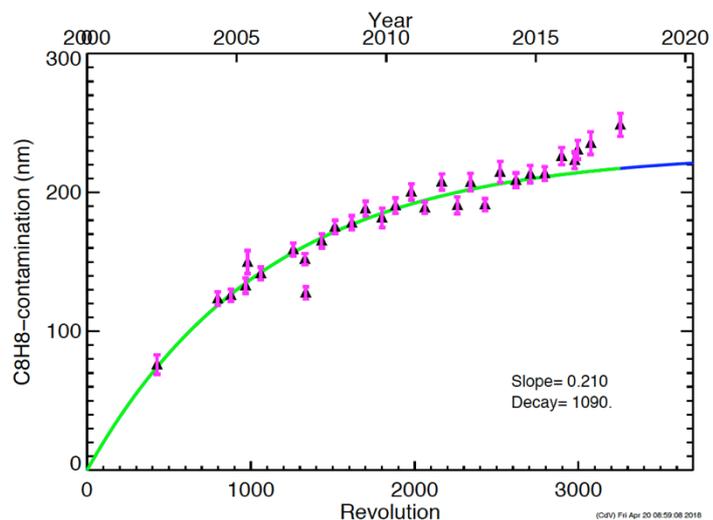
Since 8 February the two RGS instruments were fully operational. Hence, we were very surprised and concerned when on September 4th 2000 a similar problem appeared with the current limits on RGS1 (16 V current) and detailed analysis pointed to CCD7 while all other CCDs were unaffected. Comparison of this event with the event on January 30th showed that it could have the same cause (the analogue switch) but could also be caused by a failure intrinsic to other components including the CCD proper. Following this event we decided to switch off a significant part of the electronics during perigee passage and lower some clocking voltages to reduce the load on the electronics. We resumed operations of RGS1 again on 4 October as we needed sufficient time to analyse this event in detail. Although most likely the operational changes are not a critical, the instrument has been operational since then. The only adjustment we had to made is that on 16 August 2007 one readout node of RGS2 was hitting its hardware current limits due to aging of components and we had to read-out this camera through one of its output nodes only, resulting in a slower read-out by a factor two for this camera. The science impact is minimal (slightly higher fraction of pile-up events for bright sources).

Fortunately, no other problems occurred since then and the operations are running very smooth and to some extent are boring. We are lucky to have a very good and dedicated operational team which monitors all information from the instruments carefully and our team can concentrate on inflight calibrations.

Inflight calibrations

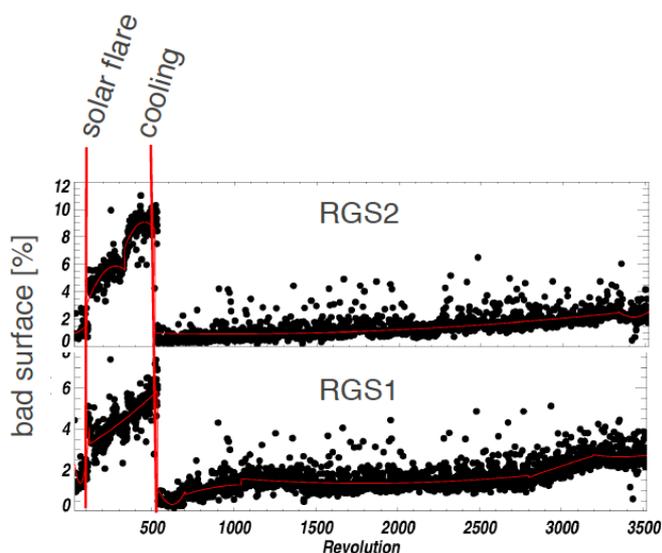
Over the operational life time of XMM-Newton a large set of calibration data has been collected and some of the relevant results are given below.

There has been a gradual increase in the collection of hydro-carbons on our cooled detectors. The evolution over time is globally as expected but there are some unexplained changes (e.g. the deviation after orbit 3000) for which no physical realistic cause could be found (such as a change in the CCD redistribution function or an additional contamination component). To some degree this has been observed for more parameters: the relative changes



in the effective area between RGS1 and RGS2 differ slightly more than we can easily justify. However, in all these cases the data tell you what the truth is and you better update your instrument models to match reality and not to match your physical understanding.

Another example is the fraction of bad surface of the CCDs caused by lattice displacement in the CCD due to charged particle hits. It was known that it increases as function of time due to radiation damage (and strong solar flares such as the one early in orbit will accelerate this). At the same time we knew that cooling from -80°C to -110°C would reduce the impact of this damage dramatically. Having reached a level of $\sim 2\%$ of the area after 20 years tells us that we can handle this far beyond the potential operational life time. Detailed analysis also shows that not all damage is persistent, after a period some of the damage will disappear.



Detailed analysis also shows that not all damage is persistent, after a period some of the damage will disappear.

Finally, there are a number of tests we like to perform before the mission ends. The CCD detectors have been operational for more than 20 years at temperatures of -80°C and -110°C . Radiation damage and contamination of the detector have been built up over the years and heating up the detectors to room temperature for around 100 hours, followed by a cool down, should repair the damage and release some of the contaminants. The confirmation of this expectation could be very helpful for future missions.

Acknowledgments

These contributions were only feasible thanks to a large team of excellent colleagues and friends which should be included. With the risk of overlooking someone these include:

The RGS team: Henri Aarts, Khalid Al Janabi, Marc Audard, Graziella Branduardi-Raymont, Jay Bixler, Bert Brinkman, Jean Cottam, Piet de Korte, Ton den Boggende, Todd Decker, Tricia Dobson, Luc Dubbeldam, Christian Erd, Hans Goulooze, Manuel Gudel, Phil Guttridge, Chuck Hailey, Fred Jansen, Steve Kahn, Bert-Joost van Leeuwen, Paul Lowes, Chris Mauche, Alec McCalden, Rolf Mewe, Albert Naber, Frits Paerels, John Peterson, Andy Rasmussen, Kevin Rees, Irini Sakelliou, John Spodek, Michaela Stern, Taka Tamura, Knud Thomson, Peter Verhoeve, Cor de Vries, Steve Welch, Alex Zehnder

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The Astrium team (Reinhard Schricke and colleagues)

The MPE-Panter colleagues (Heinrich Bräuninger, Wolfgang Burkert)

The EEV colleagues (David Burt, Peter Poole, Phil Bailey, Ralph Holton, Tim Eaton)

And in addition many technicians and other people without who we could not have realized the RGS. I am grateful to some of my colleagues (Cor de Vries, Piet de Korte) who cross checked my memories with theirs and if not all details are correct, it is my fault as I could not trace everything back in the over 100 (sometimes well) organized folders I collected in all these years.

Jan-Willem den Herder, 24 November 2019