NuSTAR Memo

Reflectivity investigations
and code verifications

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/r4/njw/Htex/nustar_refl_comp

Introduction

The calculations of reflectivities of the optics of NuSTAR are based on the IMD software package by David Windt[1], in particular the 'FRESNEL' function.

The distribution of angles are from raytracings performed by KKM by using 'ctrace' (ref ?) and by NJW by using 'MT_RAYOR'[2].

This is a comparison of various reflectivities for the NuSTAR flight optics based on FEC's email as of August 26, 2011, with the goal to verify the codes against each other and make sure that the conditions and assumptions are identical.

The above mentioned email gives a number a steps for this verification procedure and each of the following sections is devoted to at step.

1 Step 1 – reflectivity comparisons

KKM and NB/NJW compare reflectance vs. energy for selected graze angles. It should be done for design recipes and as-coated recipes.

1.1 NJW case

Figures 1 and 2 show the coefficients of reflection for nominal recipes. The NJW results have been folded with a gaussian with a FWHM of 0.7 keV since the KKM curves also are smoothed. The NJW roughness is the nominal one of 4.5 Åfor Pt/C and 4.3 Åfor W/Si (see table section 14, page 17).

A test of the evaluation of the reflectivities from NB's fits to the witness sample was made for the sample si5355 with a grazing angle of 0.238 deg, where NB provided the data and his fit, see figures 3 and 4.

2 Step 2

KKM and NJW should calculate the effective area for a perfect geometry using design recipes. Any discrepancies should be explained.

2.1 Comparison of raytracing codes

A test of the raytracing codes was performed by importing the reflection coefficients used by KKM into the MT_RAYOR code used by NJW and evaluate the effective area using both codes. Figure 5 shows a very good agreement.

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[1]Windt, 1998, **Computers in Physics**, 12, 360.
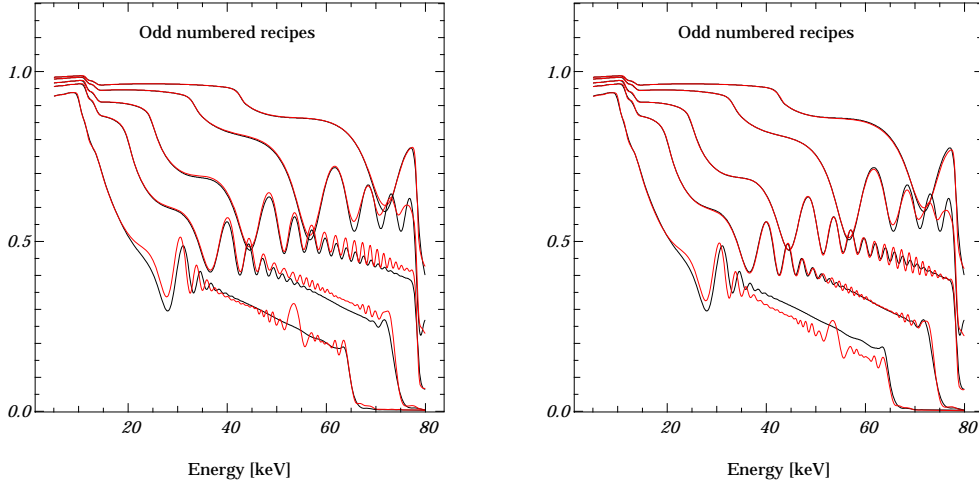[2]Westergaard, 2011, **SPIE Proceedings**, vol. 8147, 8147-64.

Figure 1: The reflection coefficients for nominal recipes 1, 3, 5, 7, and 9. Black curves are KKM results and red curves are NJW results folded with a gauss function of sigma = 0.3 keV. The angles are 1.6, 2.1, 2.6, 3.5, and 4.4 mrad resp. **Left panel** is for NJW nominal roughness. **Right panel** is for NJW roughness of 5.0 Å. In both the KKM result with roughness 5.0 Å is used.

2.2 NJW case

The effective area given here includes all photons that make it through the optic with two bounces to the focal plane. Neither the thermal foil nor the detector quantum efficiency has been taken into account.

In order to illustrate the effect of the deviations from the ideal coating as monitored by the witness samples on a layer by layer basis, a plot has been produced for each layer with four curves as exemplified in figure 6. Figures 13 through 21 go through all layers for FM1.

A similar series for the average recipes that are approximations to the as-coated detailed results is shown in figures 22 through 30.

The total effective area is the sum of all the individual ones.

The file `eff_area_FM1_A_multi.fits` holds the effective area of one flight telescope with no scatter, perfect mirror shapes, and nominal reflectivities. The statistical 1-sigma error is included. Figure 7 shows the result. So far no differences between FM1 and FM2 have been defined in the ideal case.
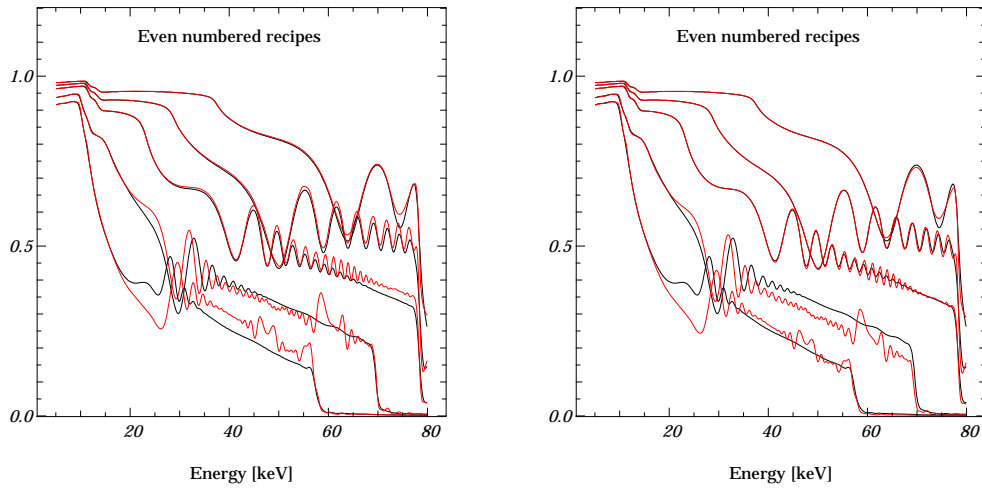
Figure 2: The reflection coefficients for nominal recipes 2, 4, 6, 8, and 10. Black curves are KKM results and red curves are NJW results folded with a gauss function of sigma = 0.3 keV. The angles are 1.6, 2.1, 2.6, 3.5, and 4.4 mrad resp. **Left panel** is for NJW nominal roughness. **Right panel** is for NJW roughness of 5.0 Å. In both the KKM result with roughness 5.0 Å is used.
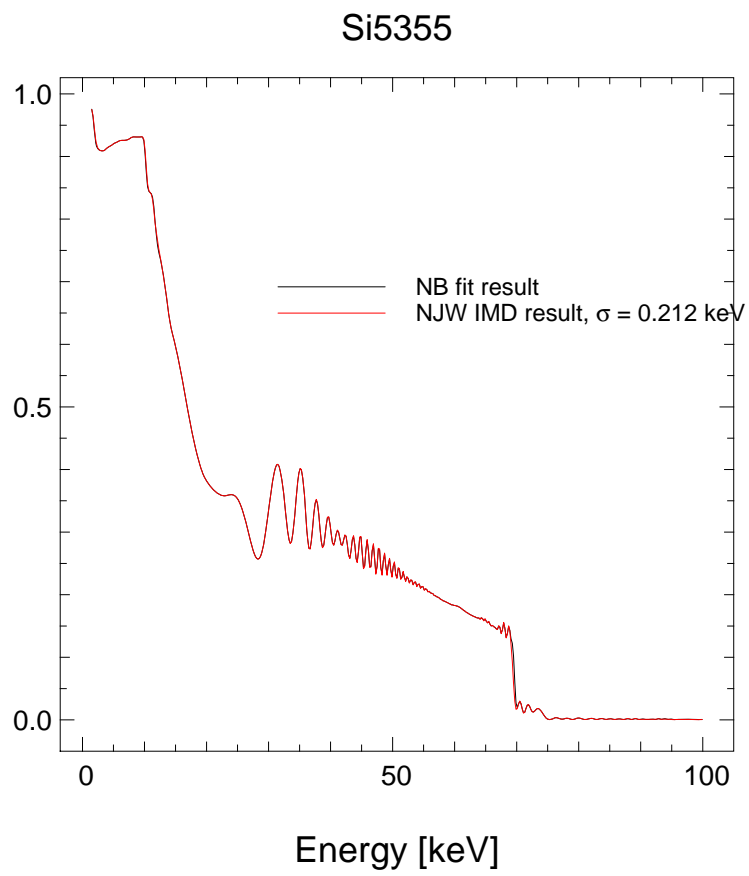
Si5355

Figure 3: The reflection coefficients for witness sample si5355 for the grazing angle of 0.238 deg, NB's fit as well as NJW's IMD result.
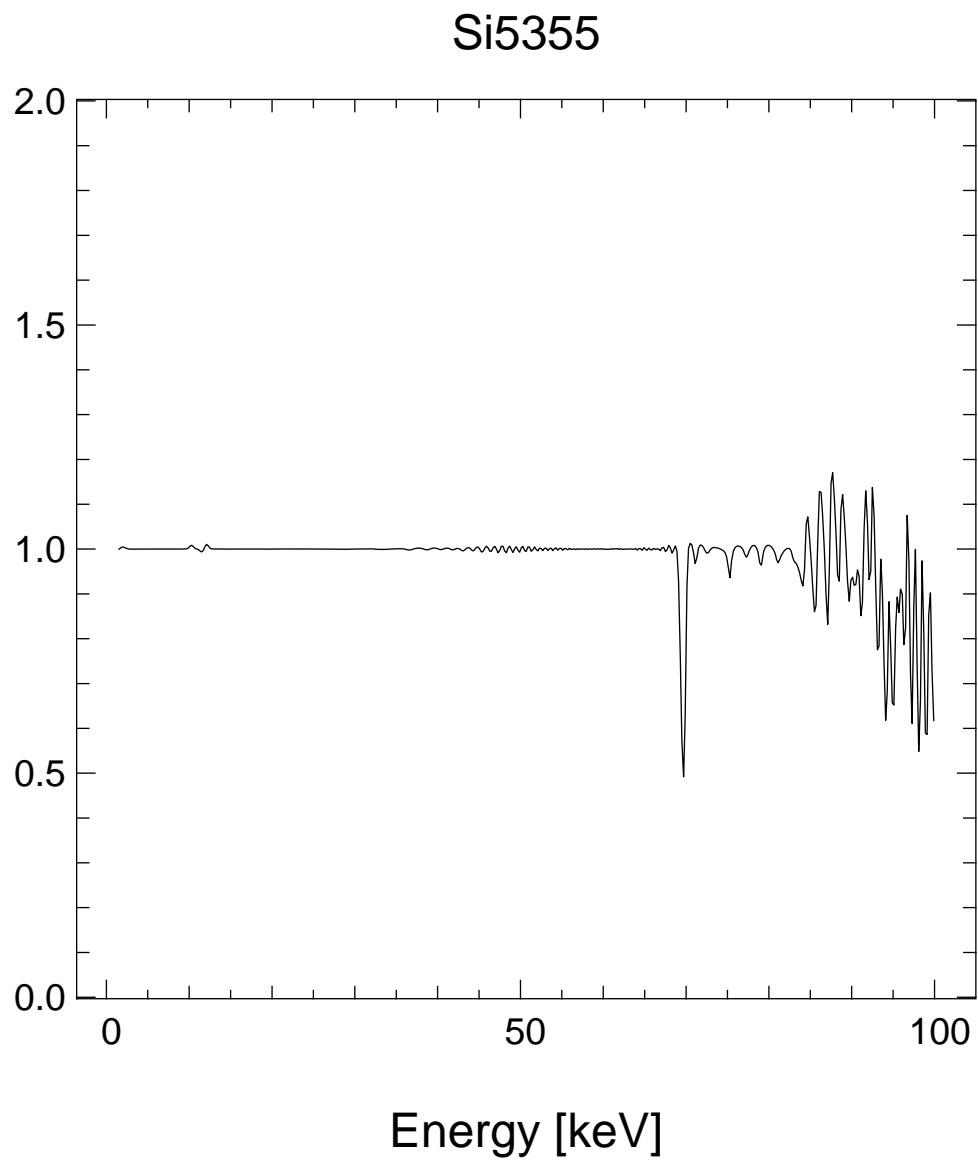
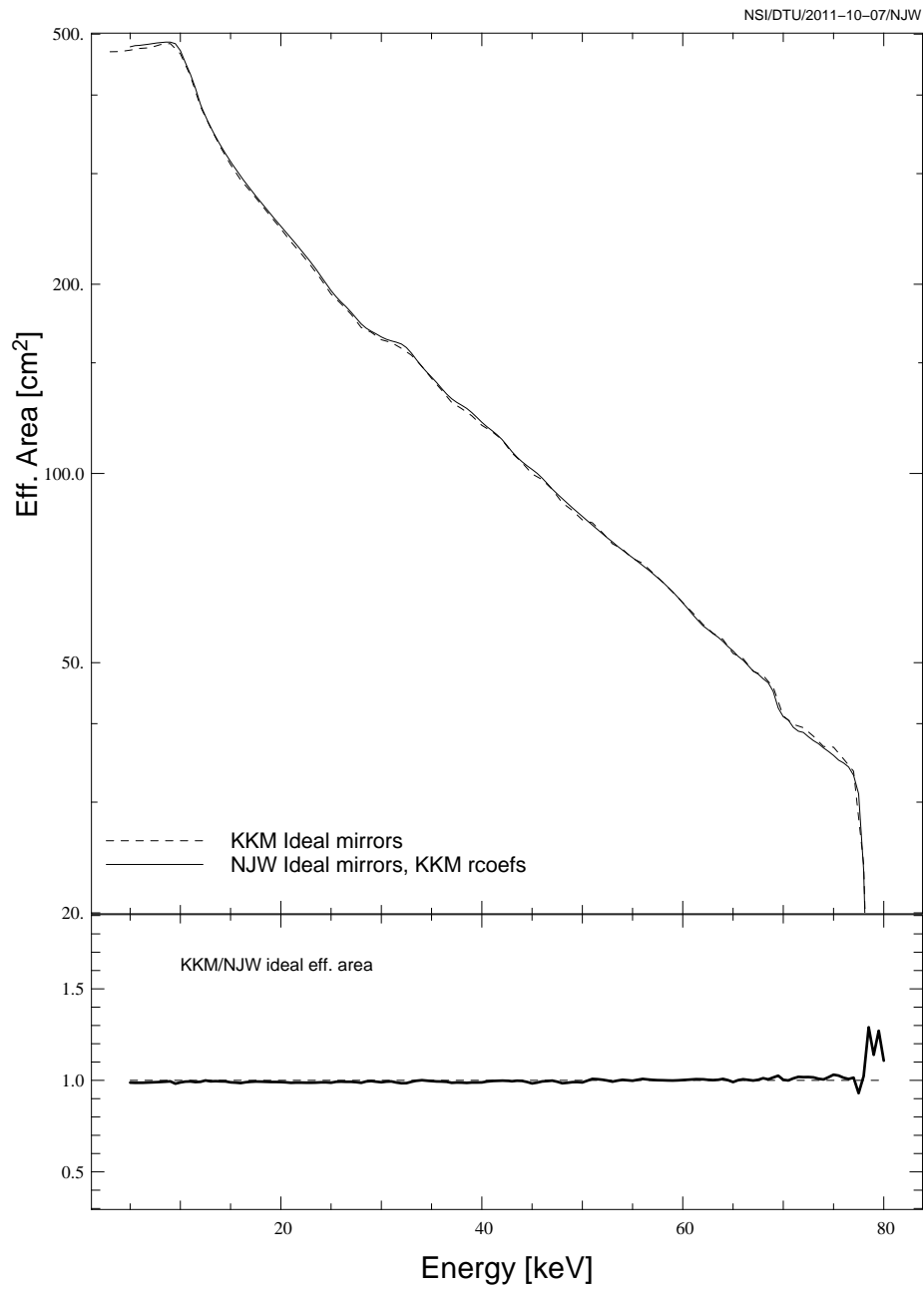Figure 4: The ratio of the reflection coefficients shown in figure 3.

Figure 5: The effective area evaluated with the two codes ('ctrace' and 'MT_RAYOR') with identical reflection coefficients, disregarding scattering and mirror deformations.
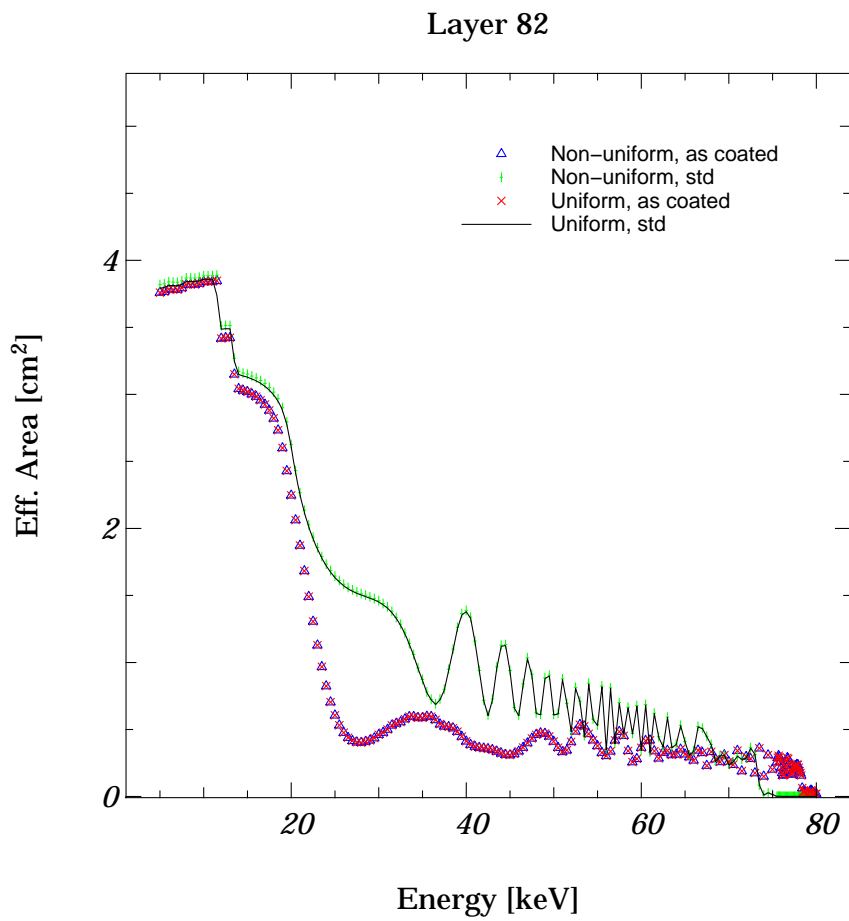
Layer 82

Figure 6: An example of the effective area for FM1 for a single layer with four different assumptions: nominal and as coated (i.e. with coatings as derived from witness samples), both with and wouthout non-uniformites incorporated.

3 Step 3

KKM and NJW should evaluate the effect of the LVDT figure using design recipes.

3.1 NJW case

The result of using design recipes together with the unchanged LVDT data is shown in figure 7.
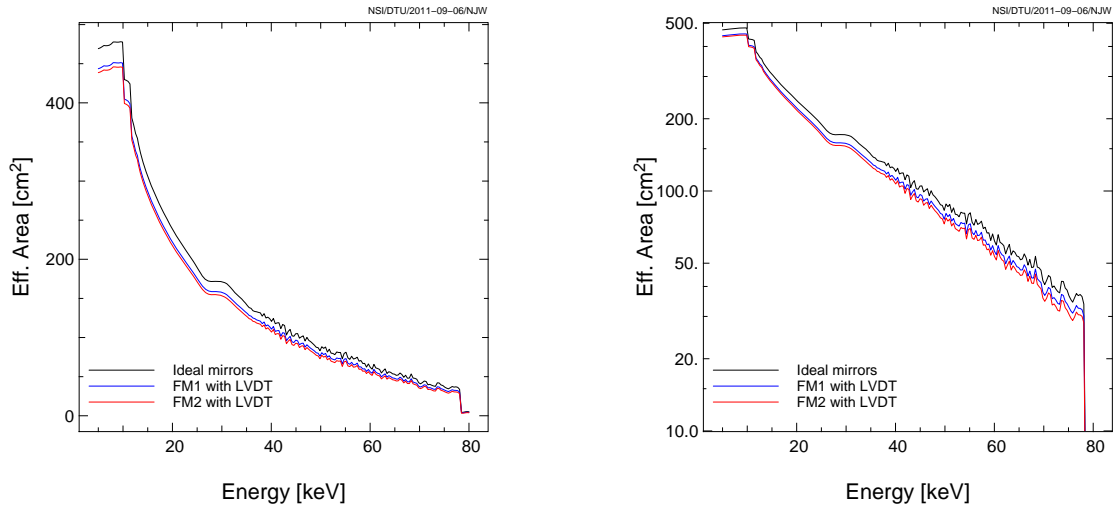

Figure 7: **Left panel:** The effective area in linear scale. **Right panel:** The effective are in log scale.

4 Step 3a

A comparison between the average recipes for FM1 and the as-coated case including the first approach to evaluating the effect of non-uniformities was done and the effective areas are shown in figure 8 and their ratio in figure 9.

5 Step 4

Once the above is established evaluate the effect of the as-coated recipes while using the measured average roughnesses for each recipe as opposed to the design recipes.

6 Step 5

Evaluate the effect of the higher roughnesses of the glass relative to our design by taking the as coated average roughnesses for each recipe and assume 5.1 Å for Pt/C and 4.7 Å for W/Si for the glass. Higher values should also be tested.
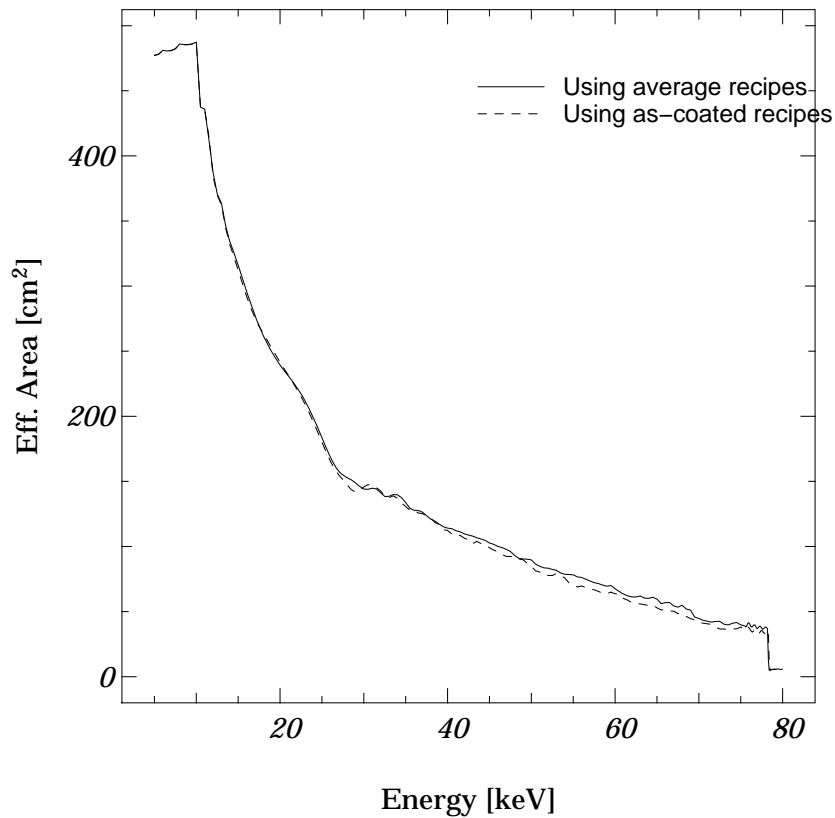
Figure 8: Effective areas.

7   Step 6

Evaluate the effect of edge shadowing by adding in a realistic continuation of the LVDT figure to the edge of the mirrors based on input from Kaya Mori.

8   Step 7

NJW should add in the measured non-uniformities (i.e. coating variations across the individual mirror surfaces) and evaluate the effect of those.

9   Step 8

Get a synchrotron measurement done fo the flight mirror scatter. Can be obtained from Mike Pivovaroff's beam time or from a new application supported by Fiona Harrison.
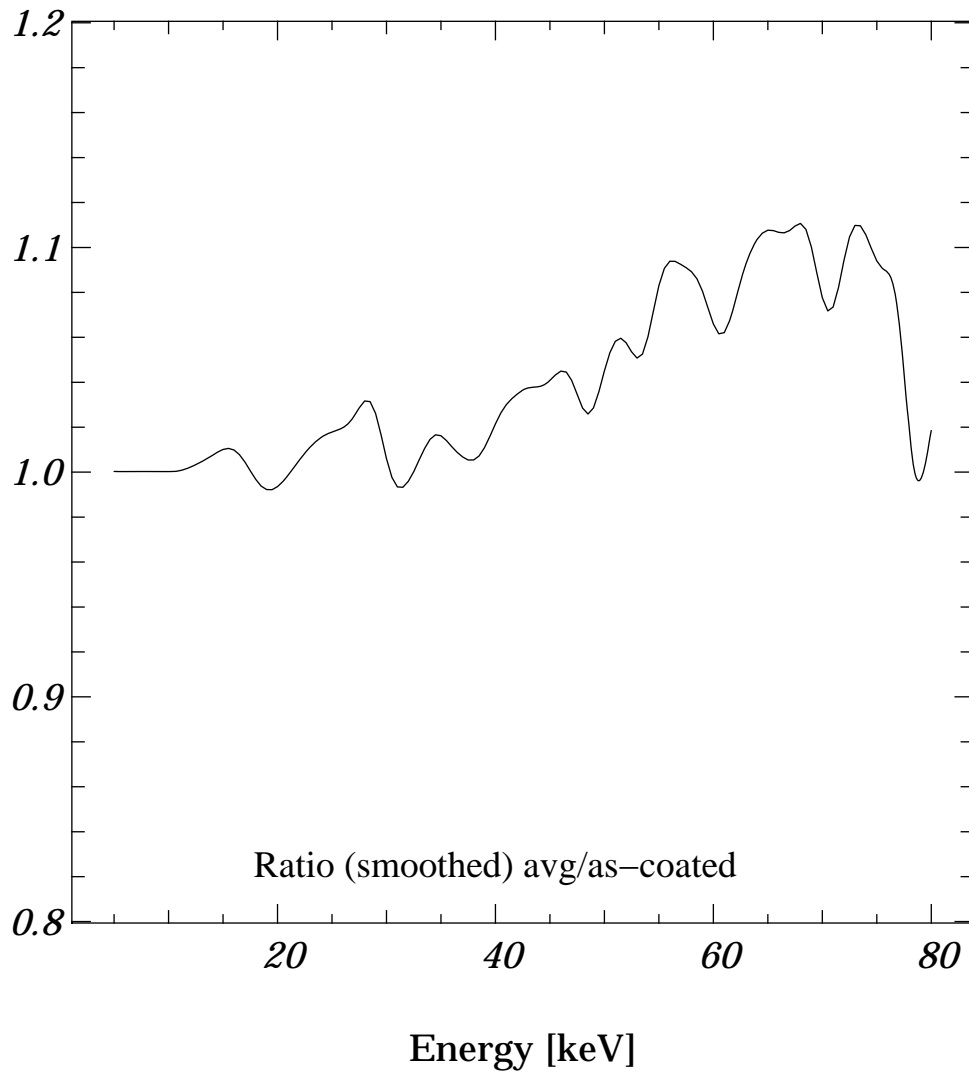
Figure 9: Ratio of effective areas in figure 8.

10   Step 9

Generate a theoretical scatter model, compare to the results obtained above, adjust and fold into the raytrace on top of the LVDT.

11   Step 10

Do a detailed comparison with all the results from steps 1 through 9 to the actual calibration measurements.

12   Step X

See effect of LVDT mirror deformations. Figure 10 gives the relative decrease in effective area as a result of the deformations. The NJW curve for FM2 is lower than the KKM one, probably indicating a difference in how the edge effects are handled. These are more pronounced for FM2 relative to FM1.
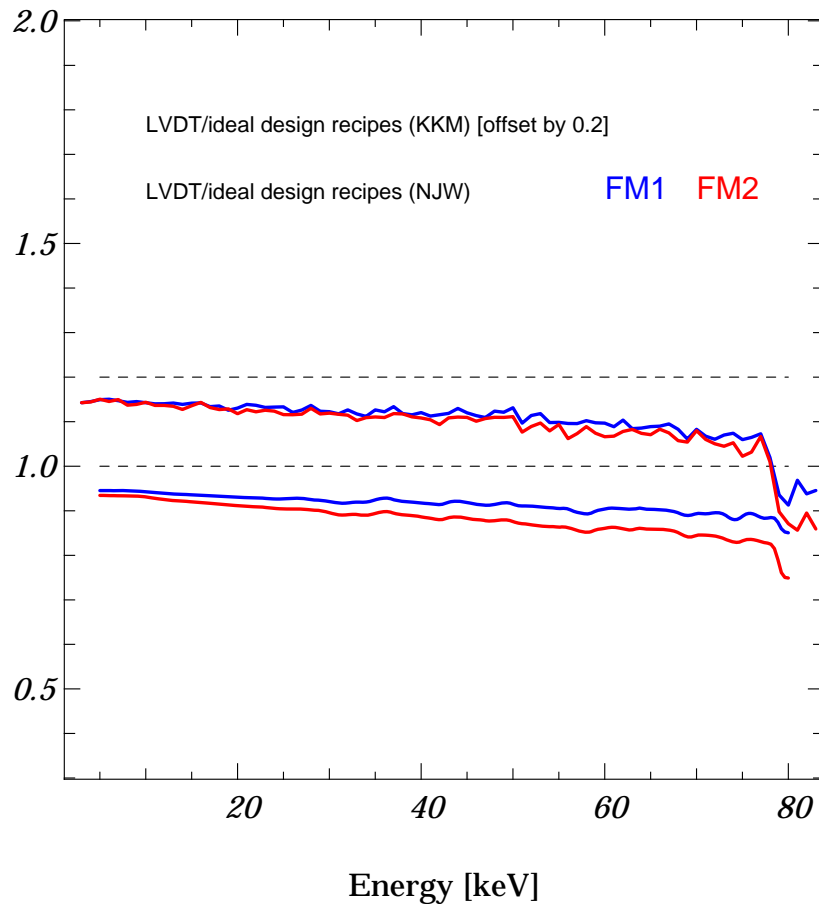

Figure 10: The ratios between the KKM and NJW effective area evaluated include the LVDT mirror deformations and the case for ideal mirror shapes.

12.1   KKM case

1. Use the average roughness of the actual witness samples.

2. Replace all roughness with 5.0 Å

3. Replace all roughness with 6.0 Å

LVDT data for FM2 have been used with check for "curled" edges, see figure 11.

Comments:

- The "as coated" recipes are responsible for the drop in effective area between 20 and 50 keV.

- The witness sample roughnesses are too good (compared with the mirror substrate) which leads to the rise above baseline at 50 keV.

- The roughness can easily account for the high energy area deficit.

- Changing spacer width for inner layers has little effect on the numbers.

12.2 NJW case

See figure 12. The reference effective area is for ideal mirrors and nominal recipes and a roughnes of 4.5 Å. The red curve is obtained by replacing the reflectivity by the one from NB's witness sample fitting results whereever the data are available (see section 15).
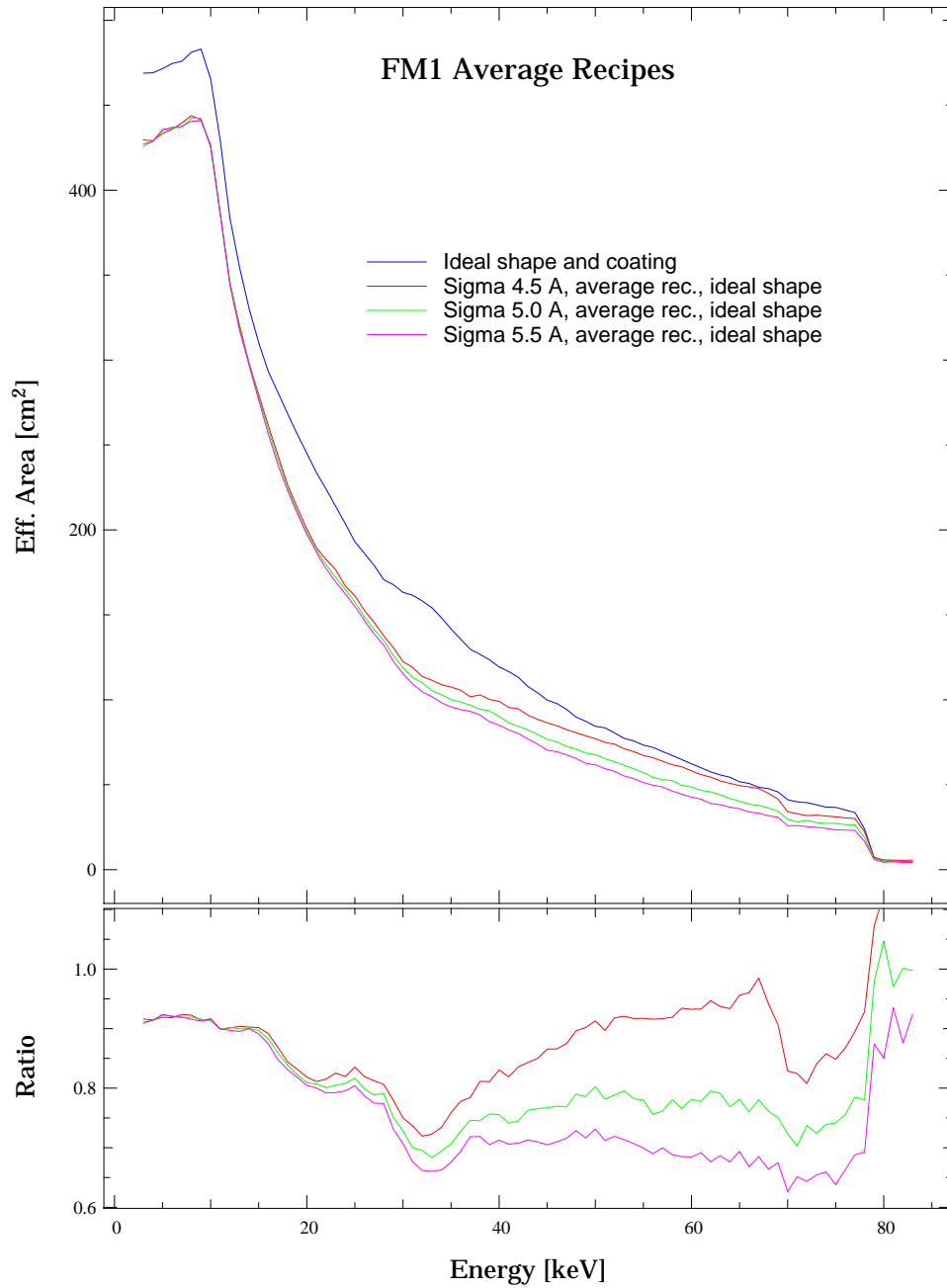
Figure 11: KKM evaluations of the FM1 effective area for the design coatings and the average recipes for three different roughnesses.
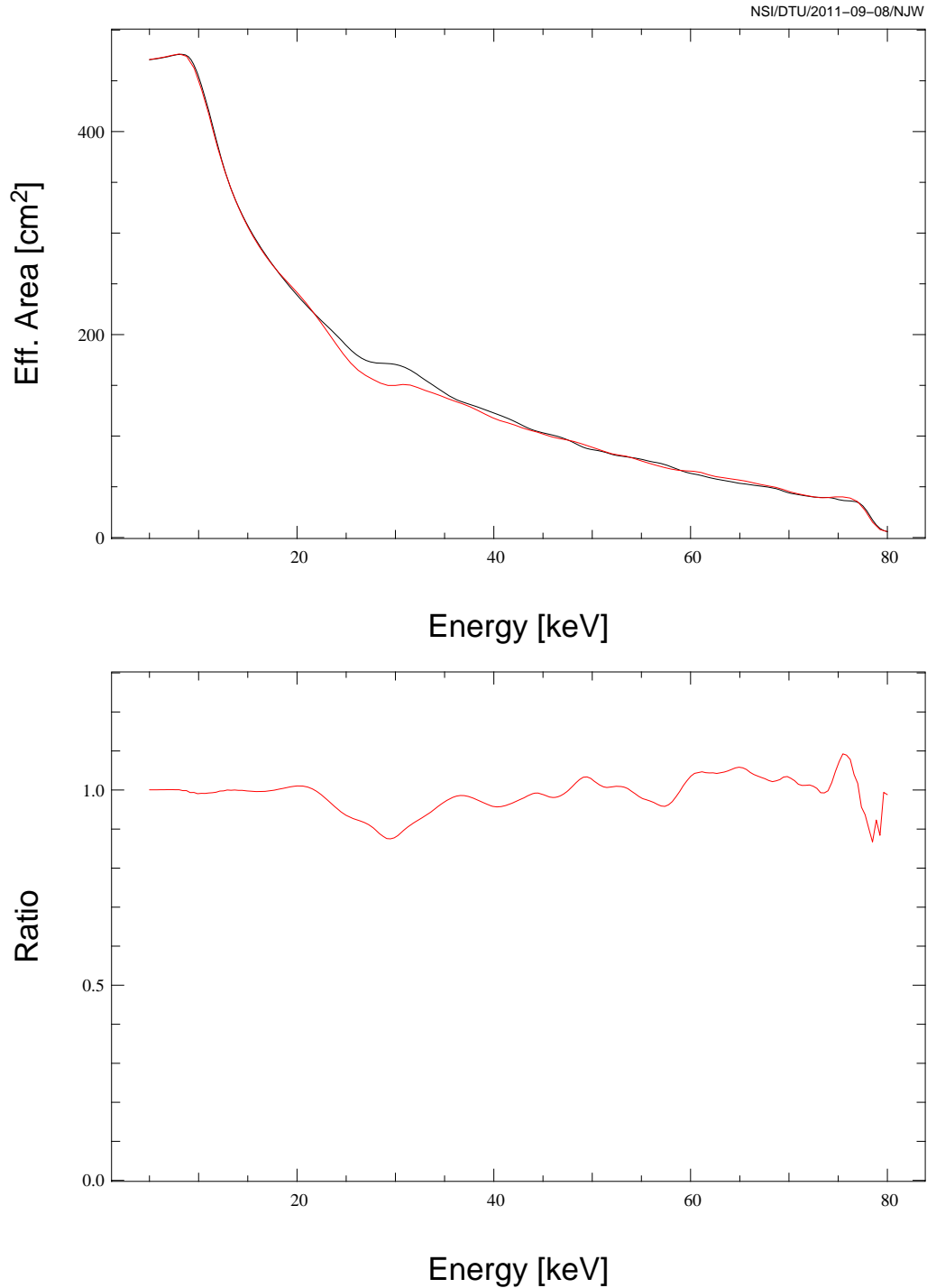
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Figure 12: Black curve: NJW effective area for ideal mirrors and nominal recipes with roughness 4.5 and 4.3 Å. Red curve: Using as-cated recipes where the information is available. **Lower panel** The ratio between the two curves.

13   Appendix: The MT_RAYOR raytracing

The reflectivities are obtained from an interpolation in a two-dimensional table in angle and energy and there is a table for each mirror group that is supposed to have identical coatings. This approach implies that some of the oscillations found in the reflection coefficients as a function of energy are not always accurately represented in the actual determination of reflectivities. Once all contributions are added together from all the mirror this has very little importance.

The alternative approach that can be used is to save all the reflection angles and positions of mirror impact in table of all succesful photons. This information can under various assumptions be used to calculate the effective area of the optic. As long as the scattering process is nearly energy independent this works well. If energy dependencies become stronger then a number of such 'photon files', each with an assigned energy range, must be produced.

14   Appendix: Flight optic multilayer design

Group	Material	Angle [mrad]	Layer range	D_{min} [Å]	D_{max} [Å]	N	c	σ [Å]	Γ_{top}	Γ_{stack}	D_{stack} [μm]
1	Pt/C	1.52	1 - 12	29.0	133.7	145	0.245	4.5	0.7	0.45	0.558
2	Pt/C	1.73	13 - 24	29.0	131.6	145	0.228	4.5	0.7	0.45	0.547
3	Pt/C	1.96	25 - 36	29.0	129.6	145	0.234	4.5	0.7	0.45	0.551
4	Pt/C	2.22	37 - 49	29.0	121.8	145	0.214	4.5	0.7	0.45	0.537
5	Pt/C	2.52	50 - 62	29.0	109.5	145	0.225	4.5	0.7	0.45	0.541
6	Pt/C	2.85	63 - 76	29.0	107.5	145	0.225	4.5	0.7	0.45	0.541
7	Pt/C	3.23	77 - 89	29.0	102.8	145	0.212	4.5	0.7	0.45	0.534
8	W/Si	3.67	90 - 104	25.0	95.2	291	0.238	4.3	0.8	0.38	0.955
9	W/Si	4.16	105 - 118	25.0	83.9	291	0.220	4.3	0.8	0.38	0.934
10	W/Si	4.72	119 - 133	25.0	74.5	291	0.190	4.3	0.8	0.38	0.902

15   Appendix: The witness sample information accessible

The following tables give the positions where the fits to the measured witness sample reflection data are available and are of good quality, meaning that the reduced χ^2 is smaller than 2.5. A 'U' or an 'L' tells that data are available for the twelftant given by the position counting in the reading direction. Layer numbers are given as the left column. A hyphen '-' means that data were not taken or that the fitting quality was too bad.
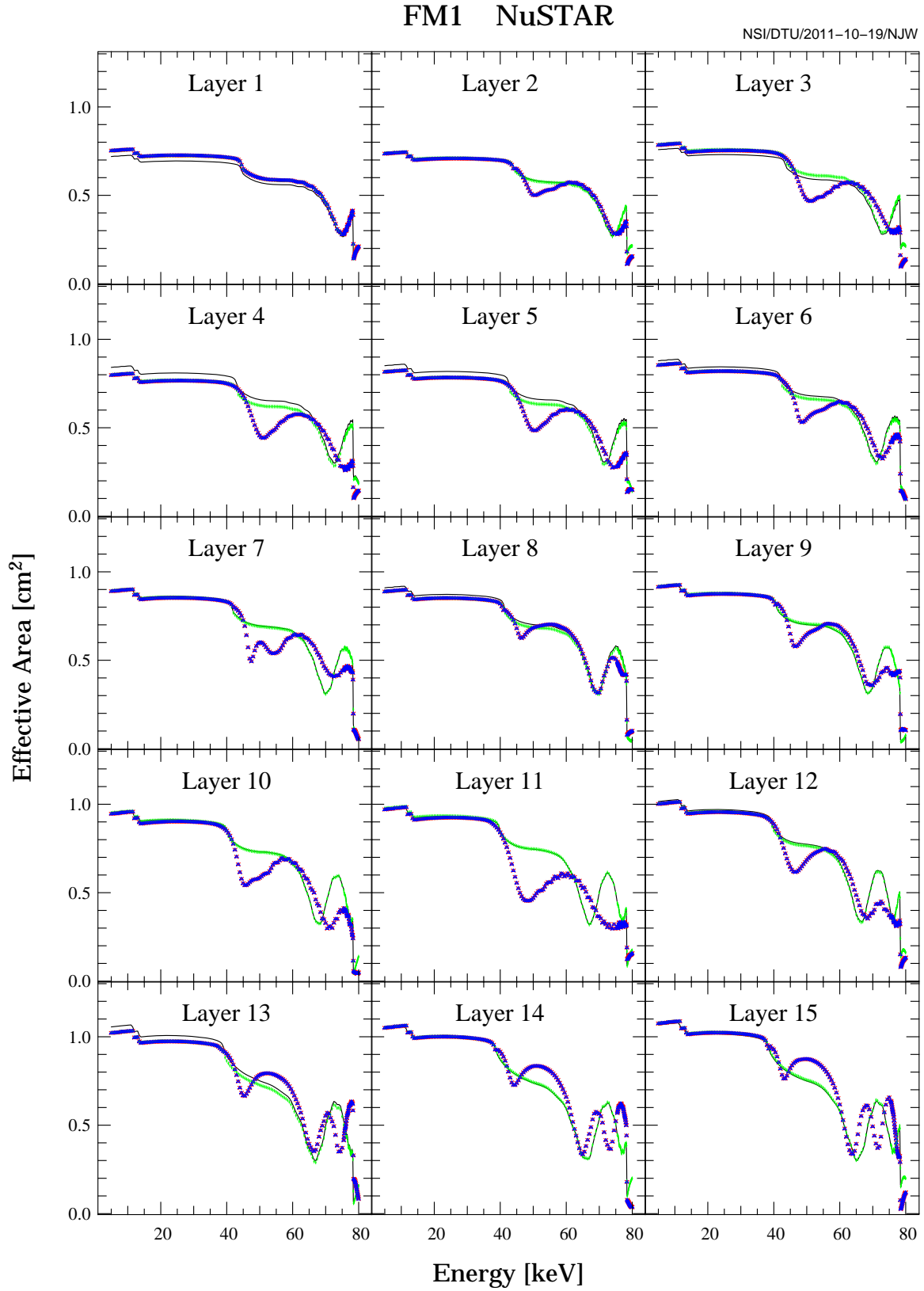
16   Appendix: The detailed plots

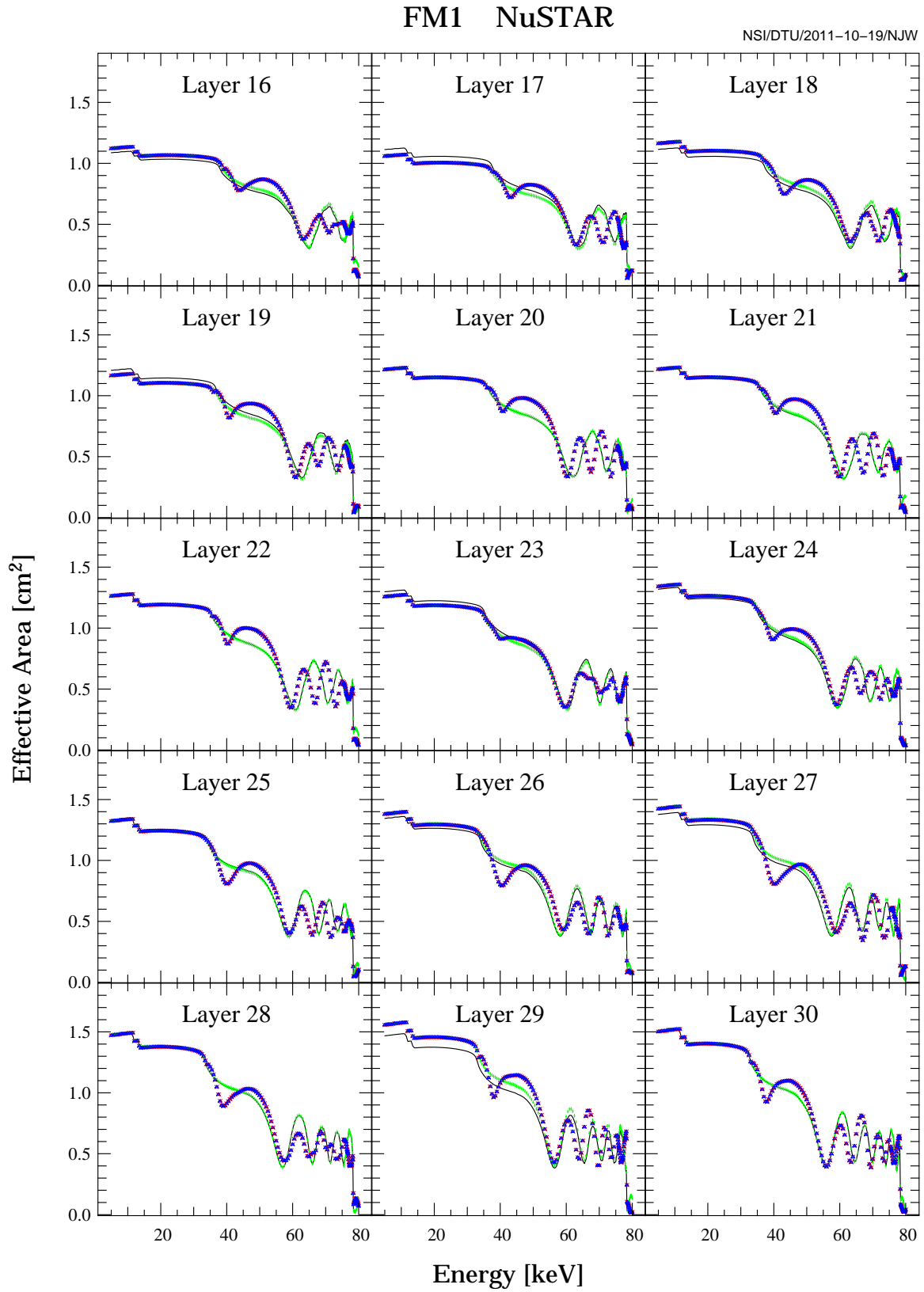**FM1   NuSTAR**

Figure 13: See figure 6 for explanation.

FM1   NuSTAR

Figure 14: See figure 6 for explanation.

FM1 NuSTAR

NSI/DTU/2011−10−19/NJW
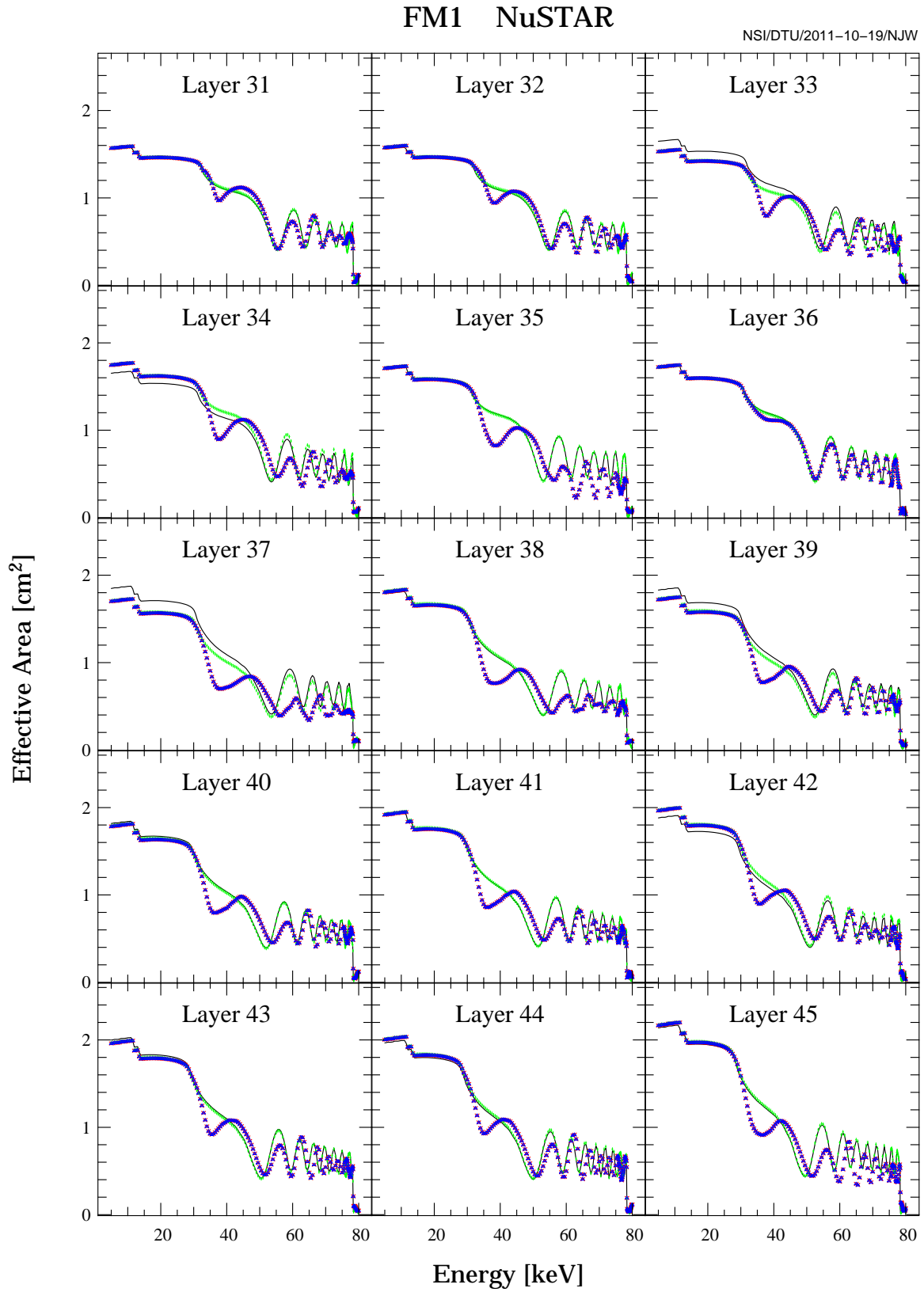
Figure 15: See figure 6 for explanation.

FM1   NuSTAR

NSI/DTU/2011–10–19/NJW
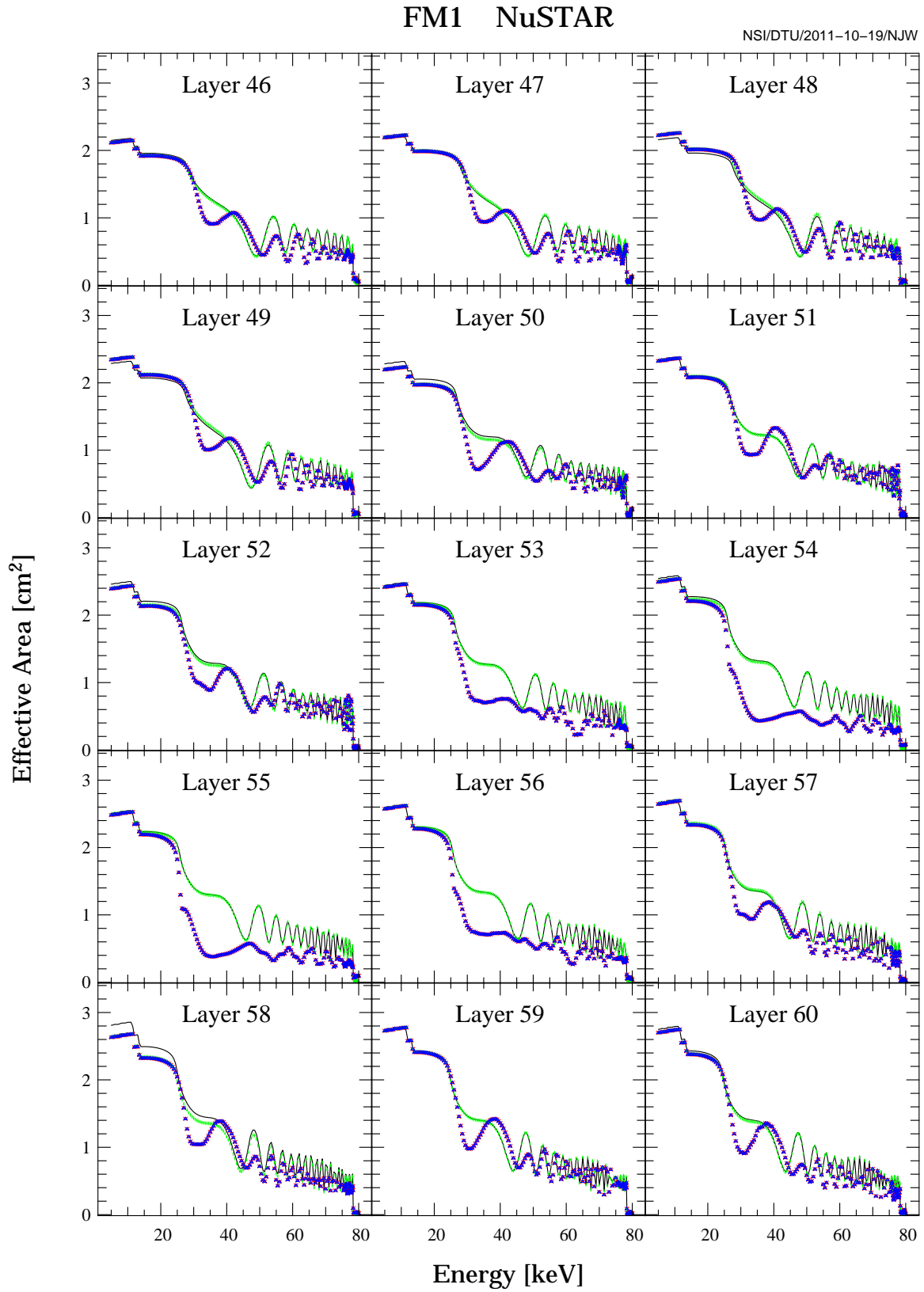
Figure 16: See figure 6 for explanation.

FM1   NuSTAR

NSI/DTU/2011−10−19/NJW
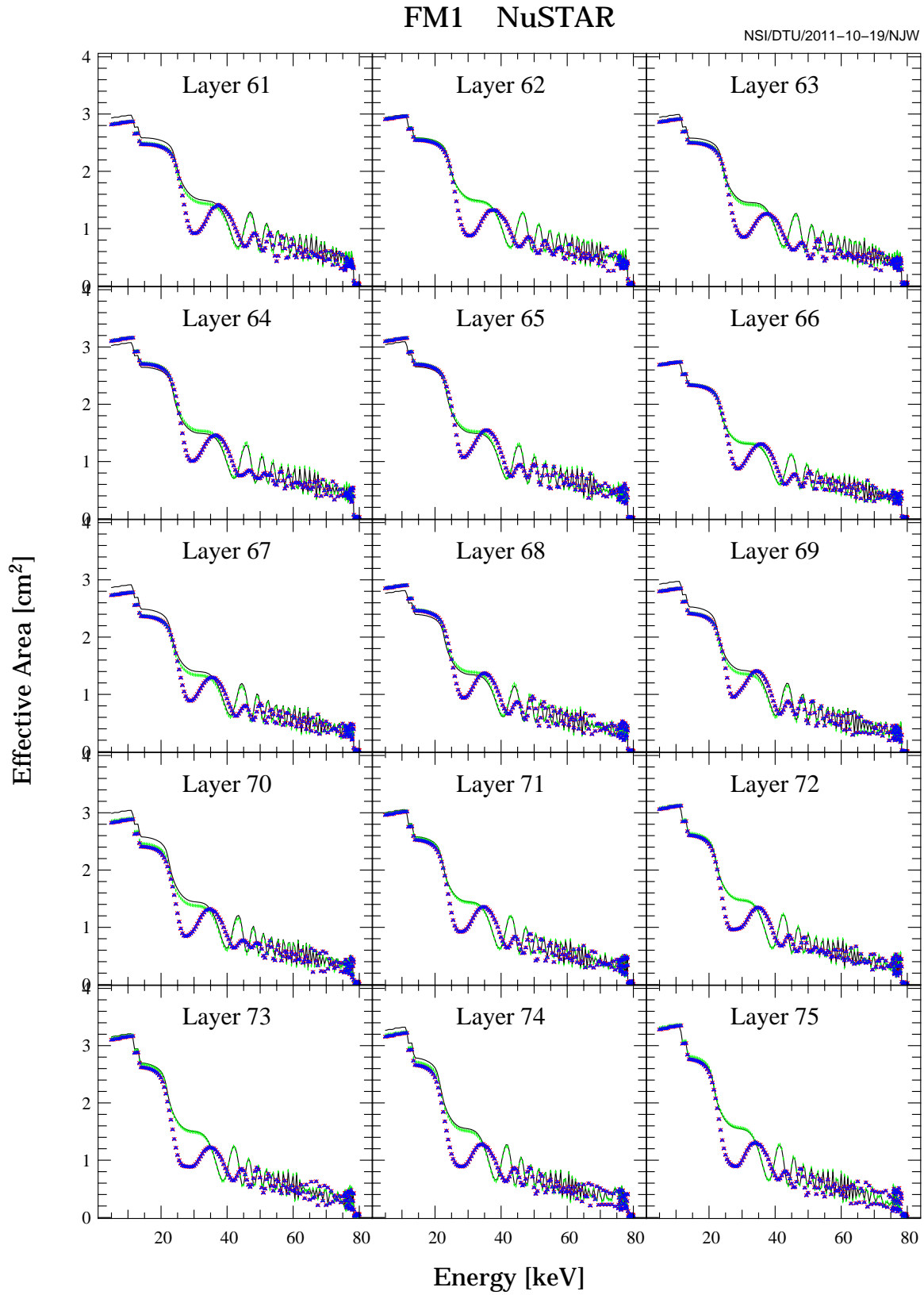
Figure 17: See figure 6 for explanation.

FM1   NuSTAR
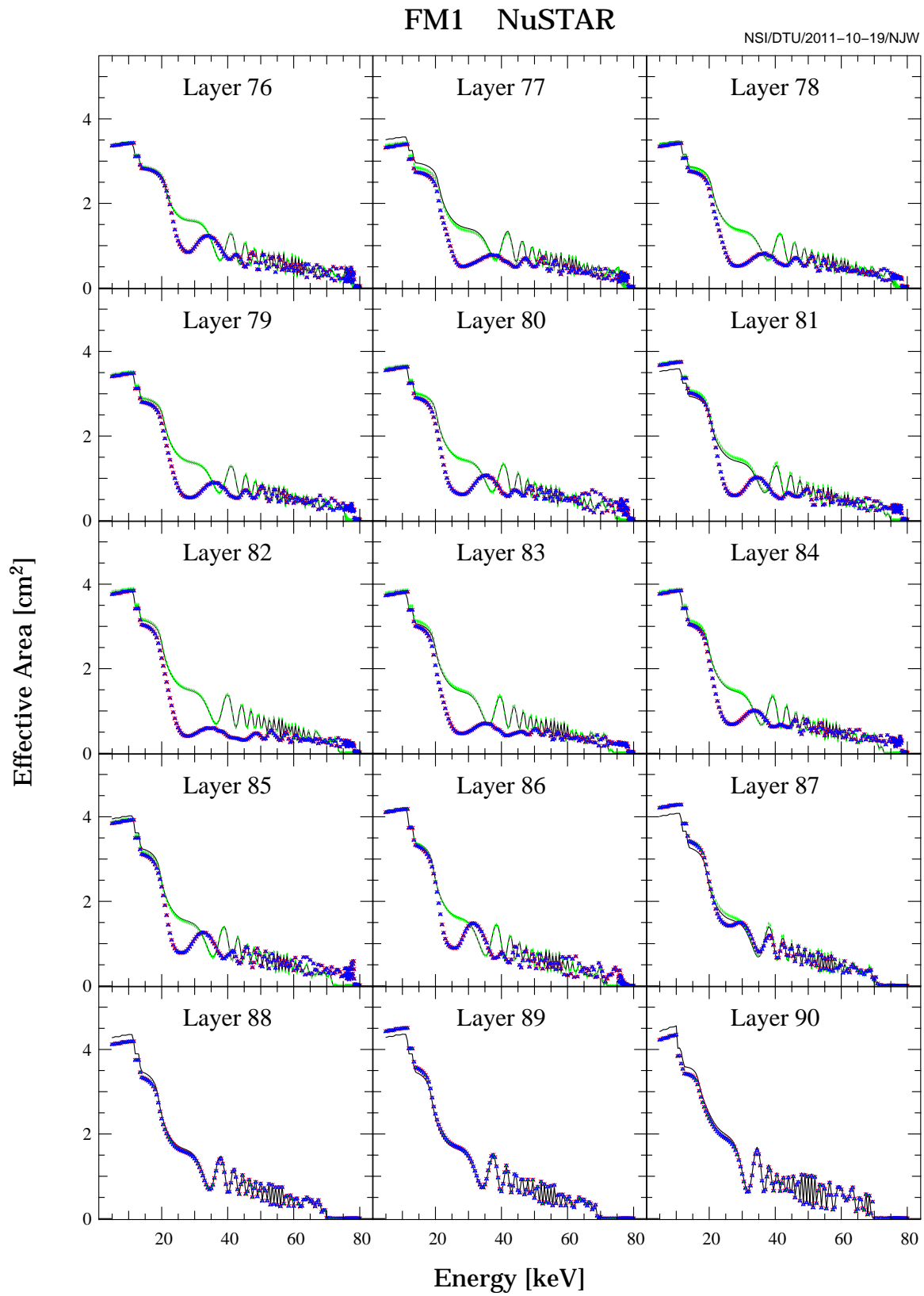
Figure 18: See figure 6 for explanation.

FM1   NuSTAR
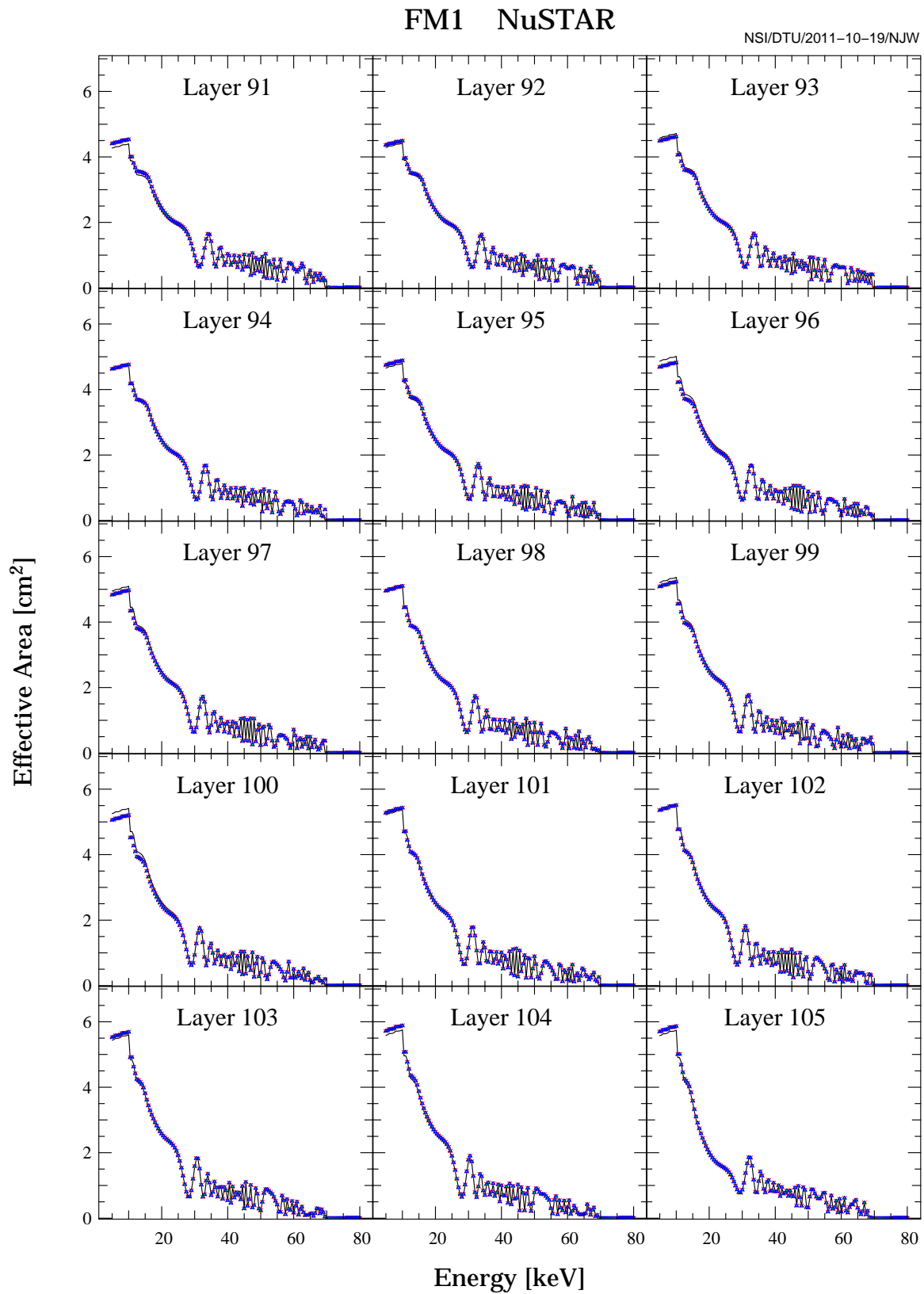
Figure 19: See figure 6 for explanation.

FM1   NuSTAR
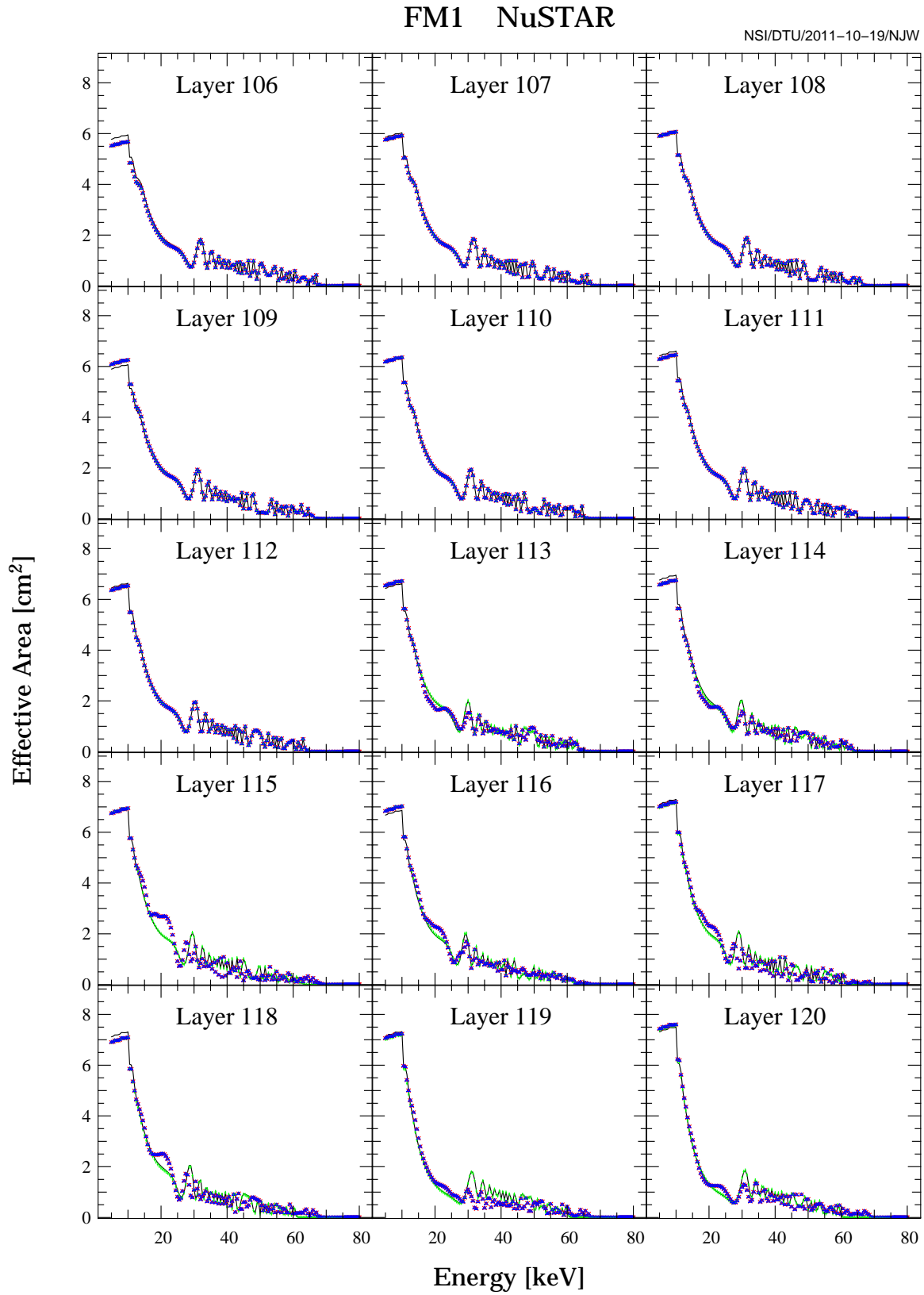
Figure 20: See figure 6 for explanation.

FM1   NuSTAR

NSI/DTU/2011−10−19/NJW
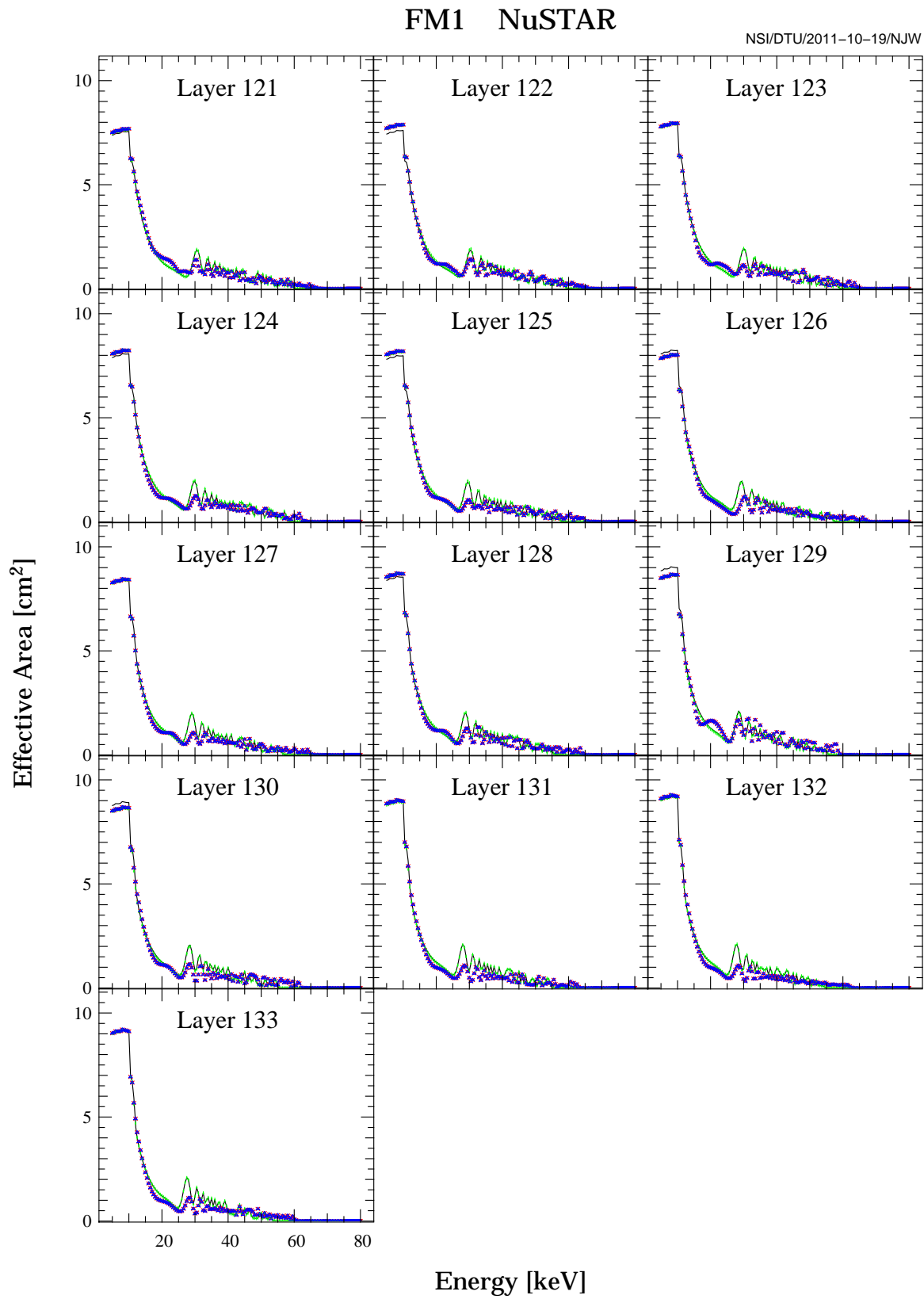
Figure 21: See figure 6 for explanation.

FM1   NuSTAR
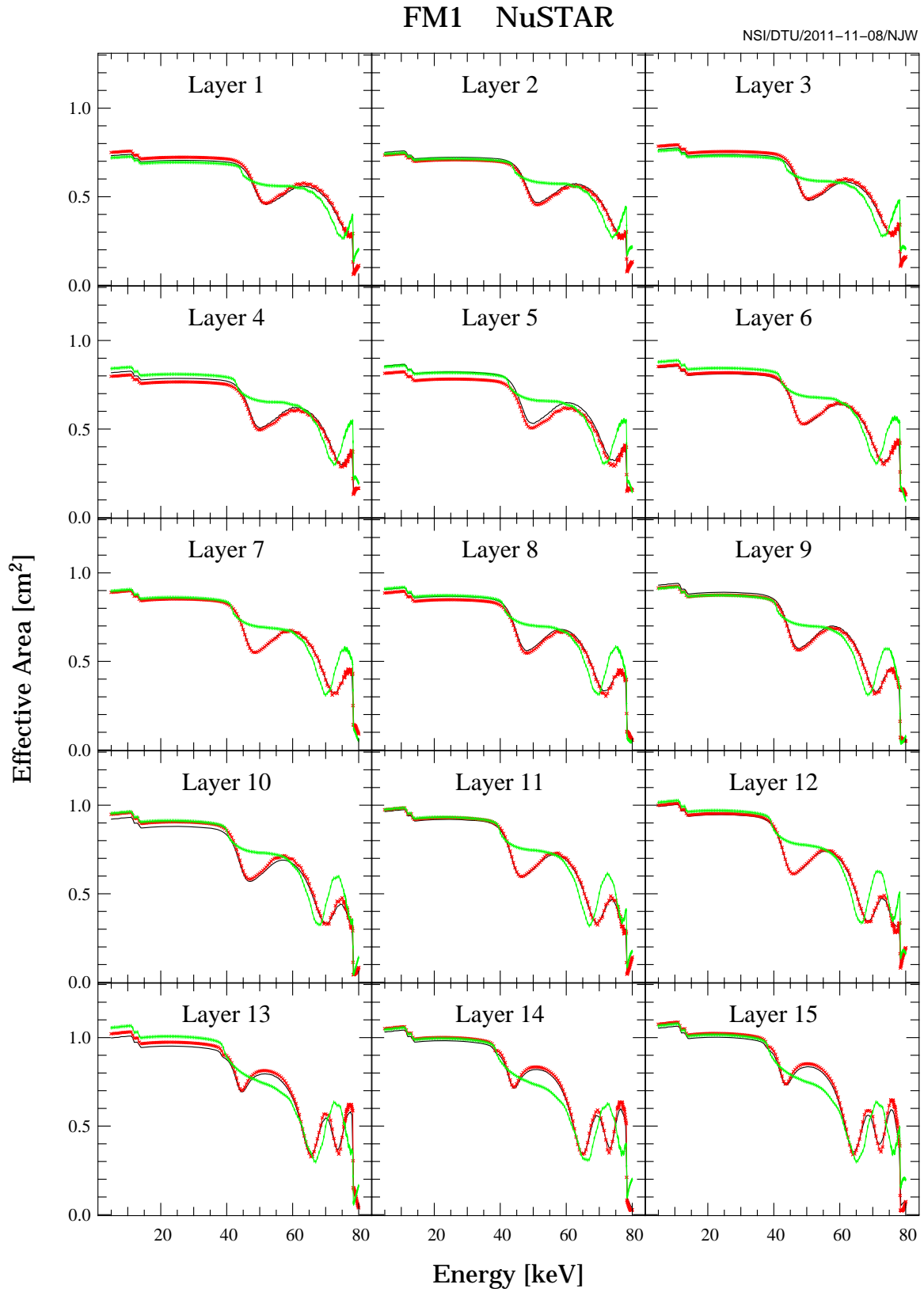
Figure 22: Comparing nominal and average recipe.

FM1   NuSTAR
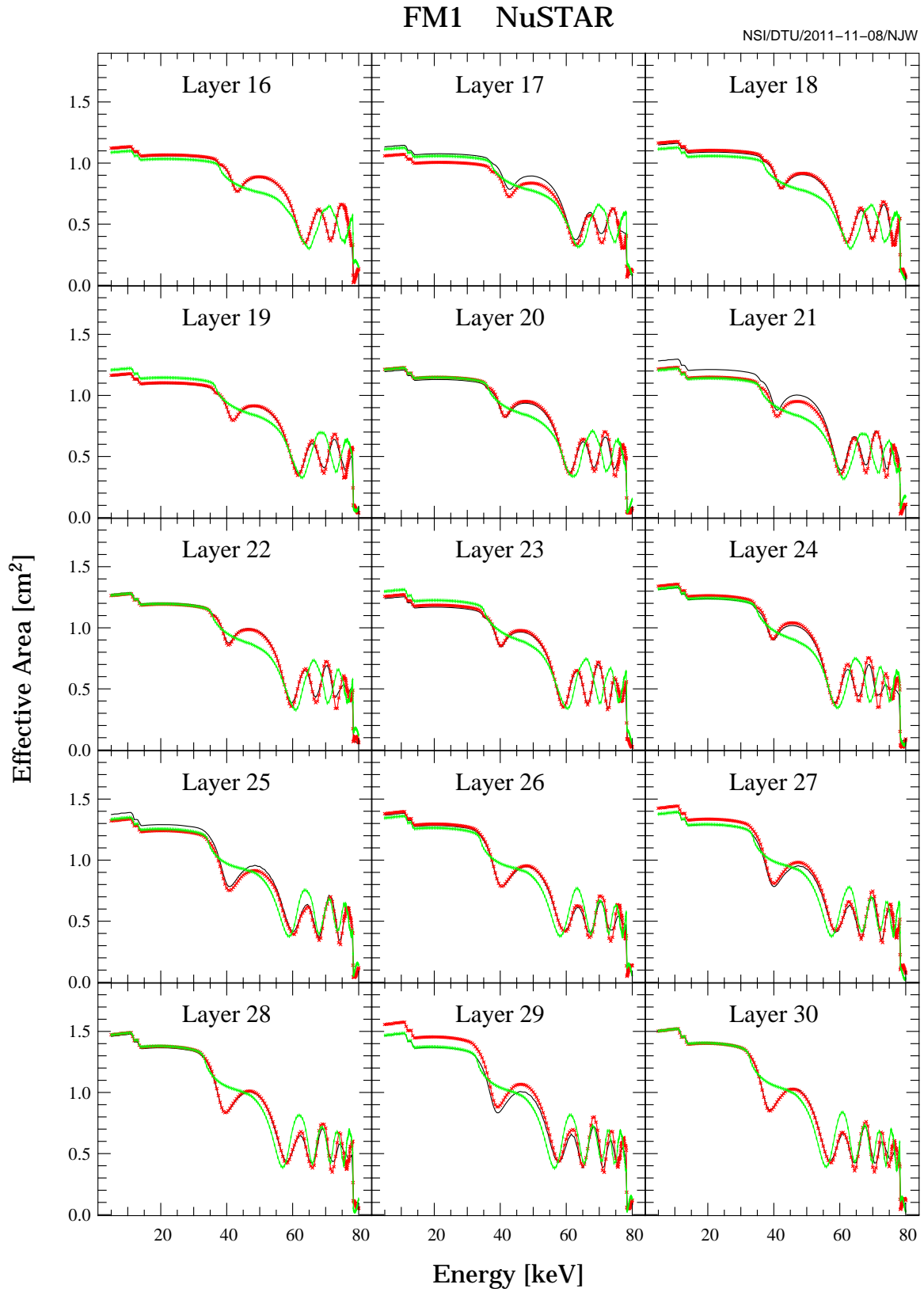
Figure 23: Comparing nominal and average recipe.

FM1   NuSTAR
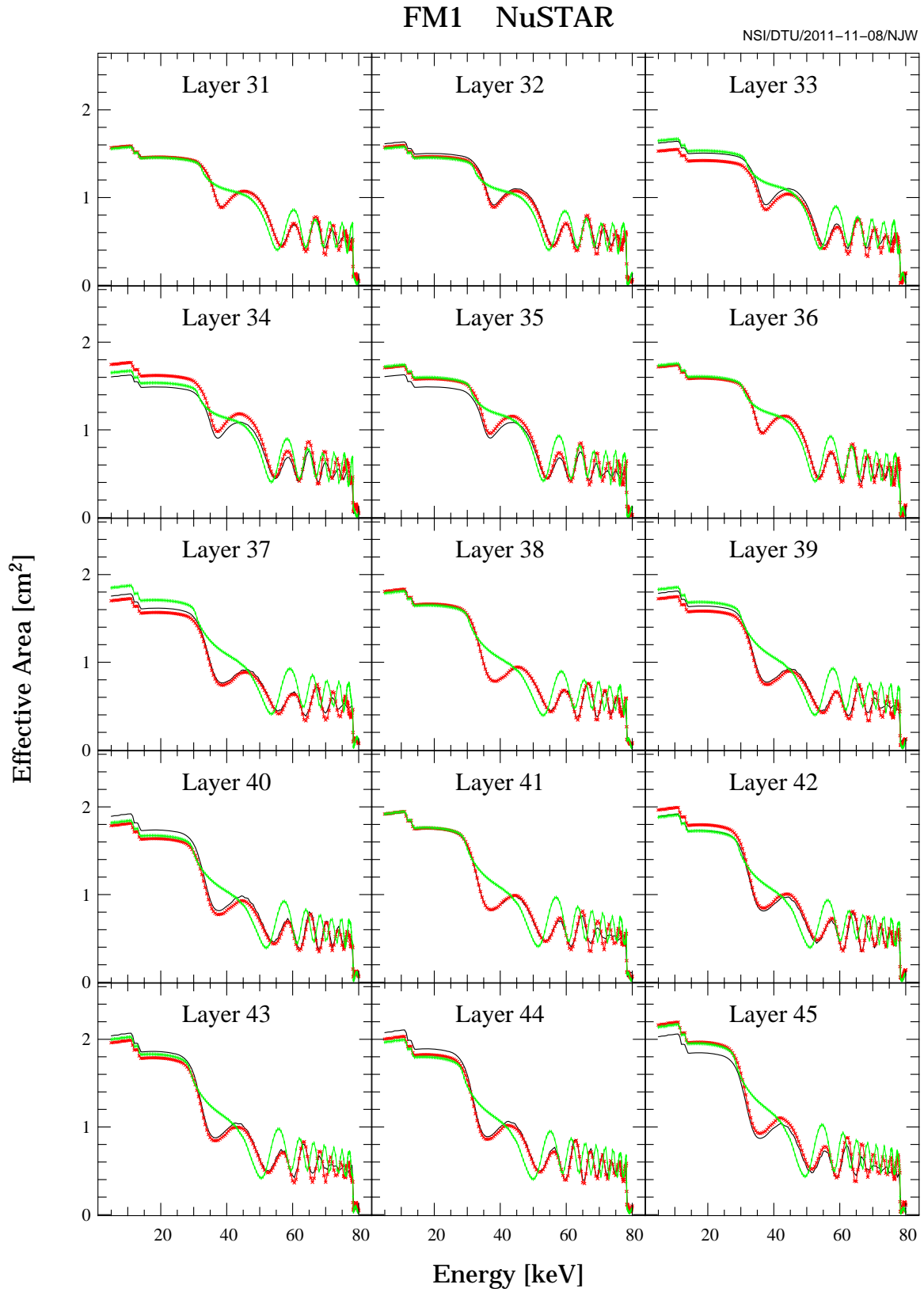
Figure 24: Comparing nominal and average recipe.

FM1   NuSTAR
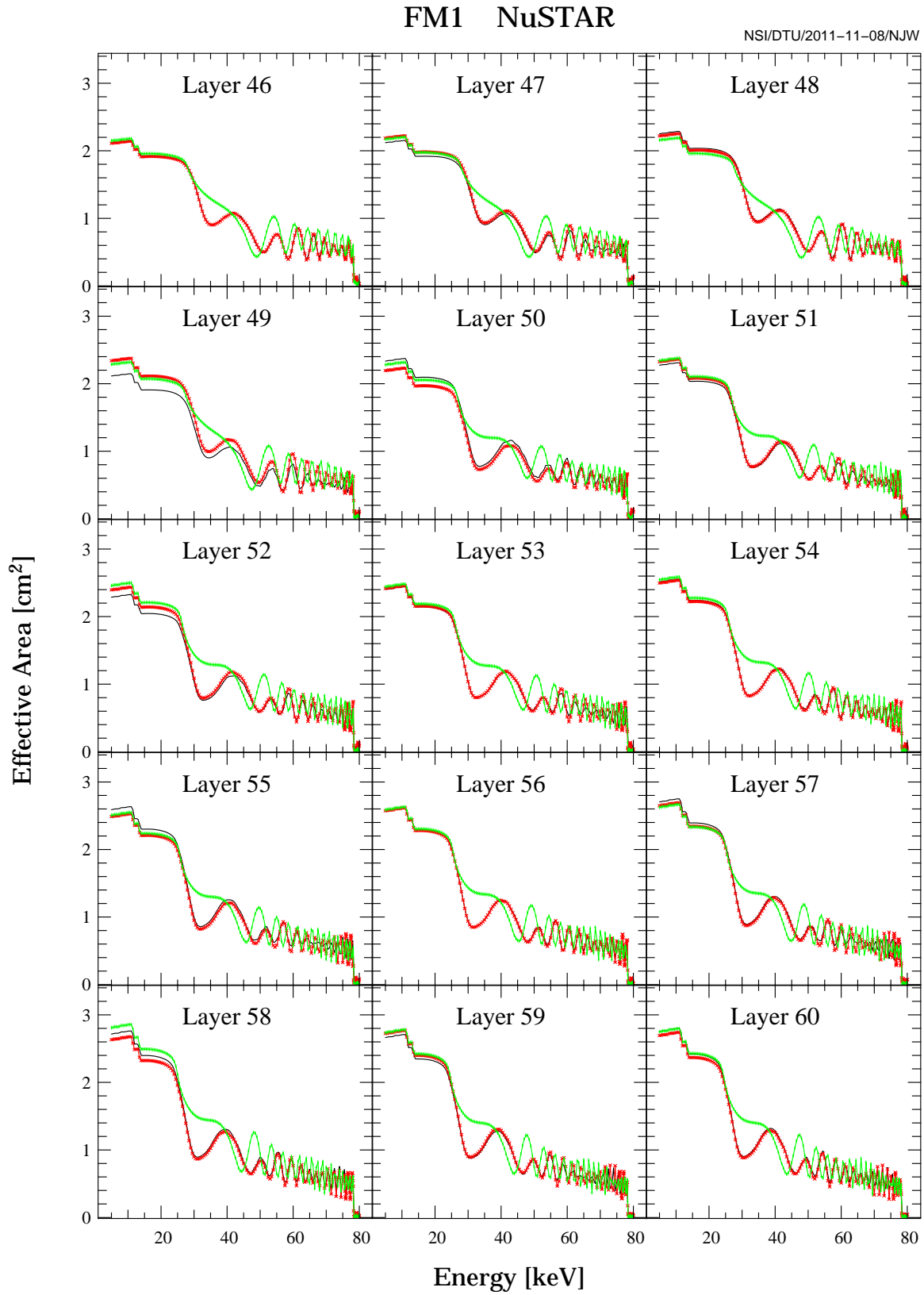
Figure 25: Comparing nominal and average recipe.

FM1   NuSTAR
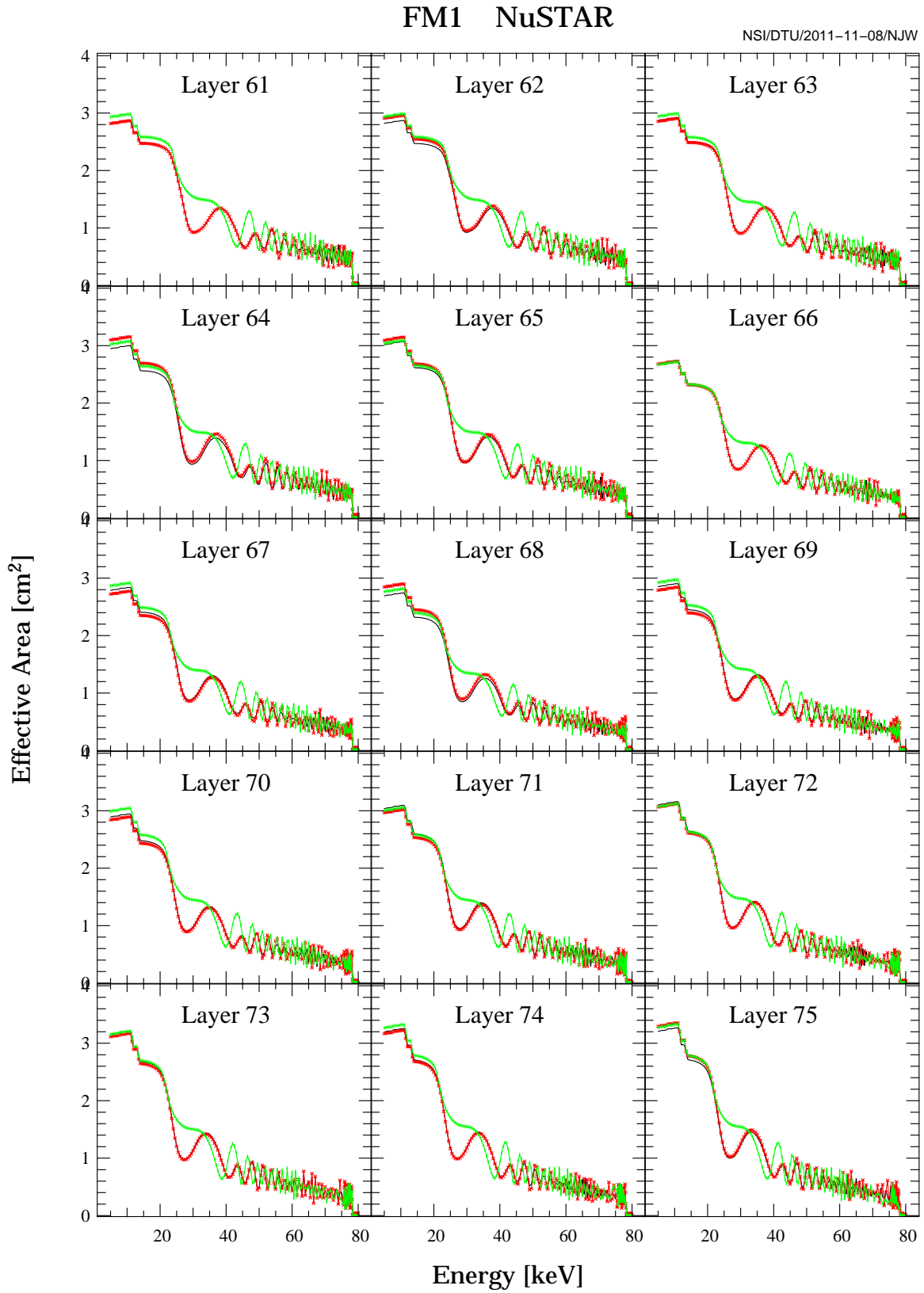
Figure 26: Comparing nominal and average recipe.

FM1   NuSTAR

NSI/DTU/2011−11−08/NJW
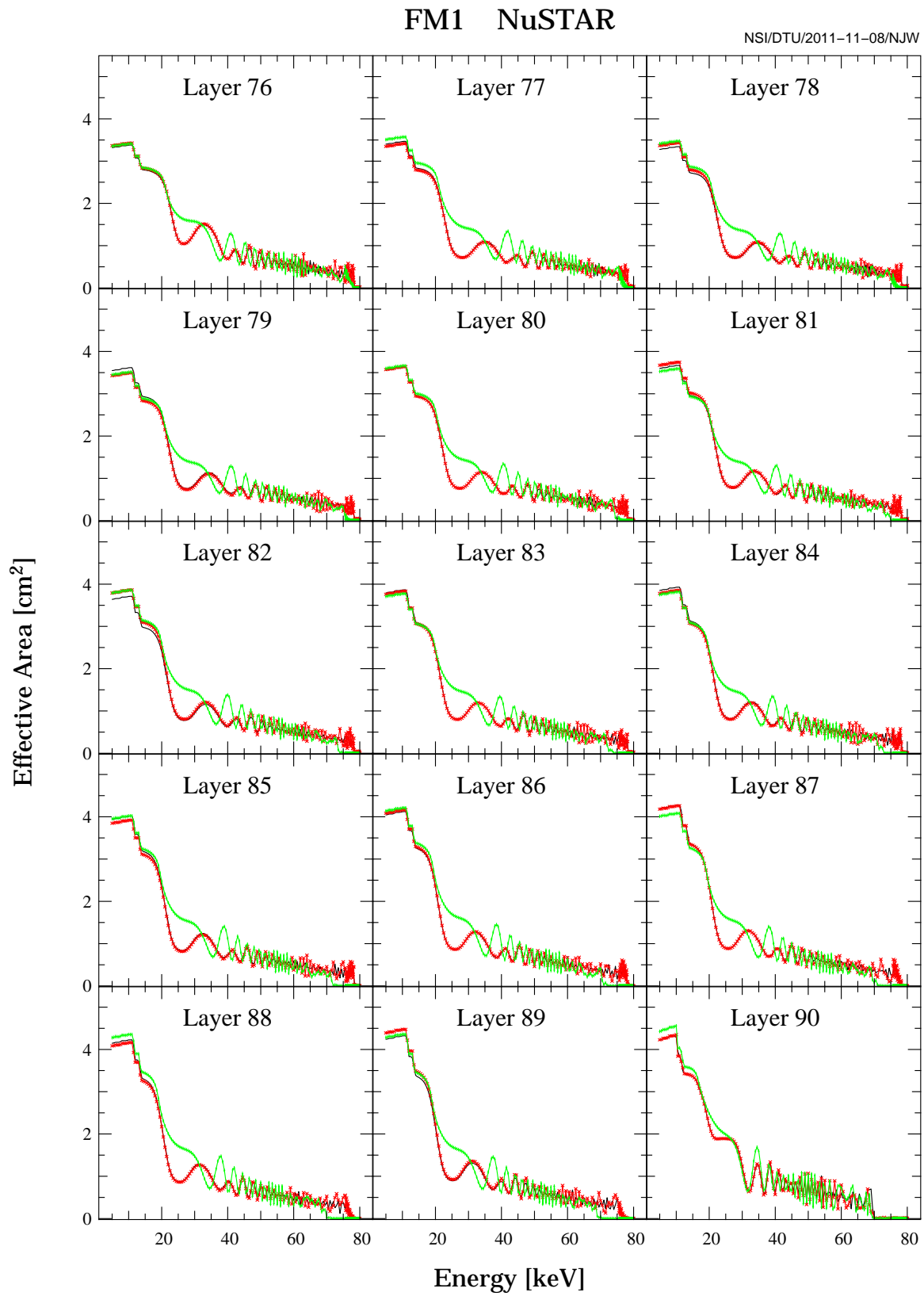
Figure 27: Comparing nominal and average recipe.

FM1   NuSTAR

NSI/DTU/2011−11−08/NJW
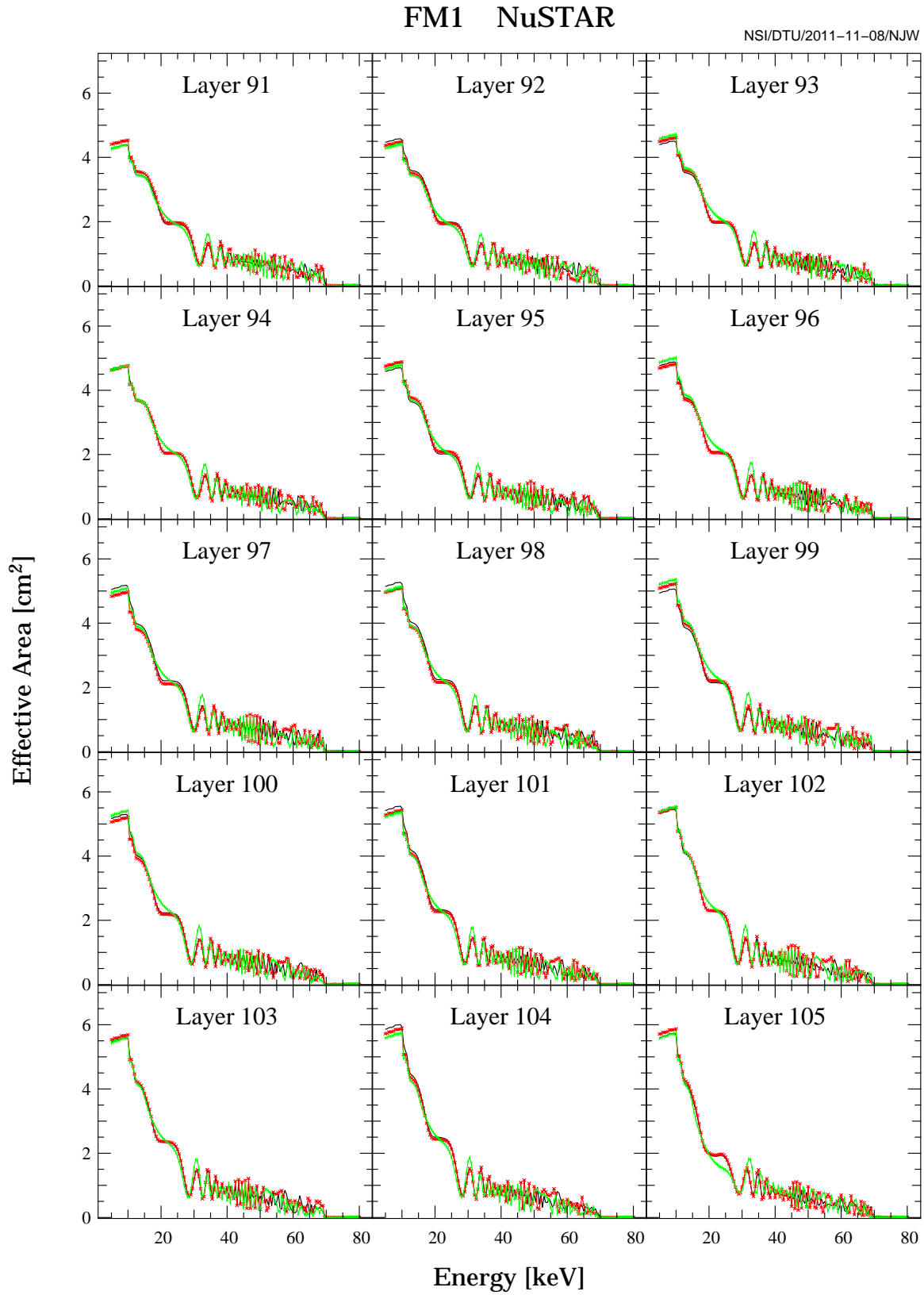
Figure 28: Comparing nominal and average recipe.

FM1   NuSTAR

NSI/DTU/2011−11−08/NJW
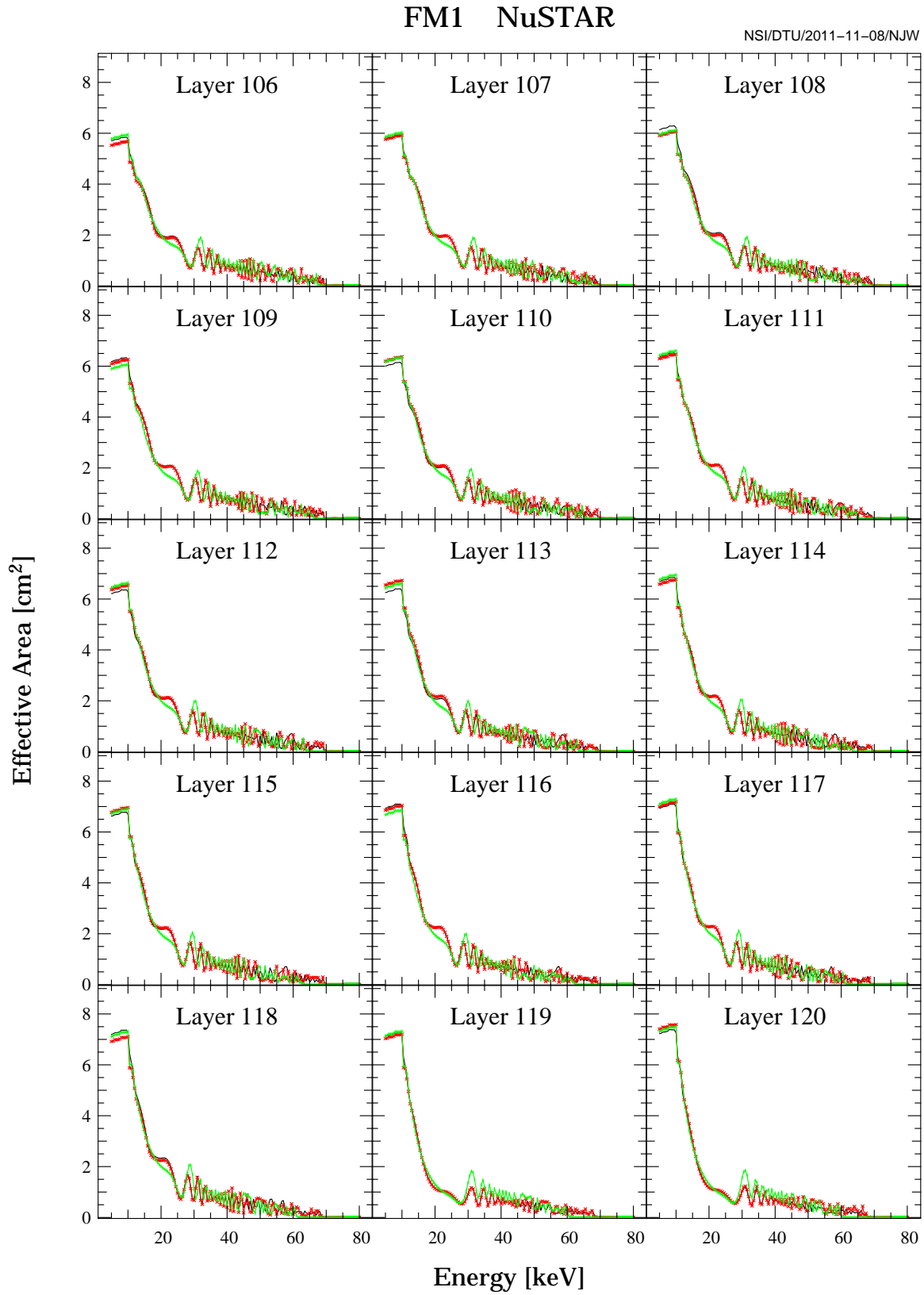
Figure 29: Comparing nominal and average recipe.
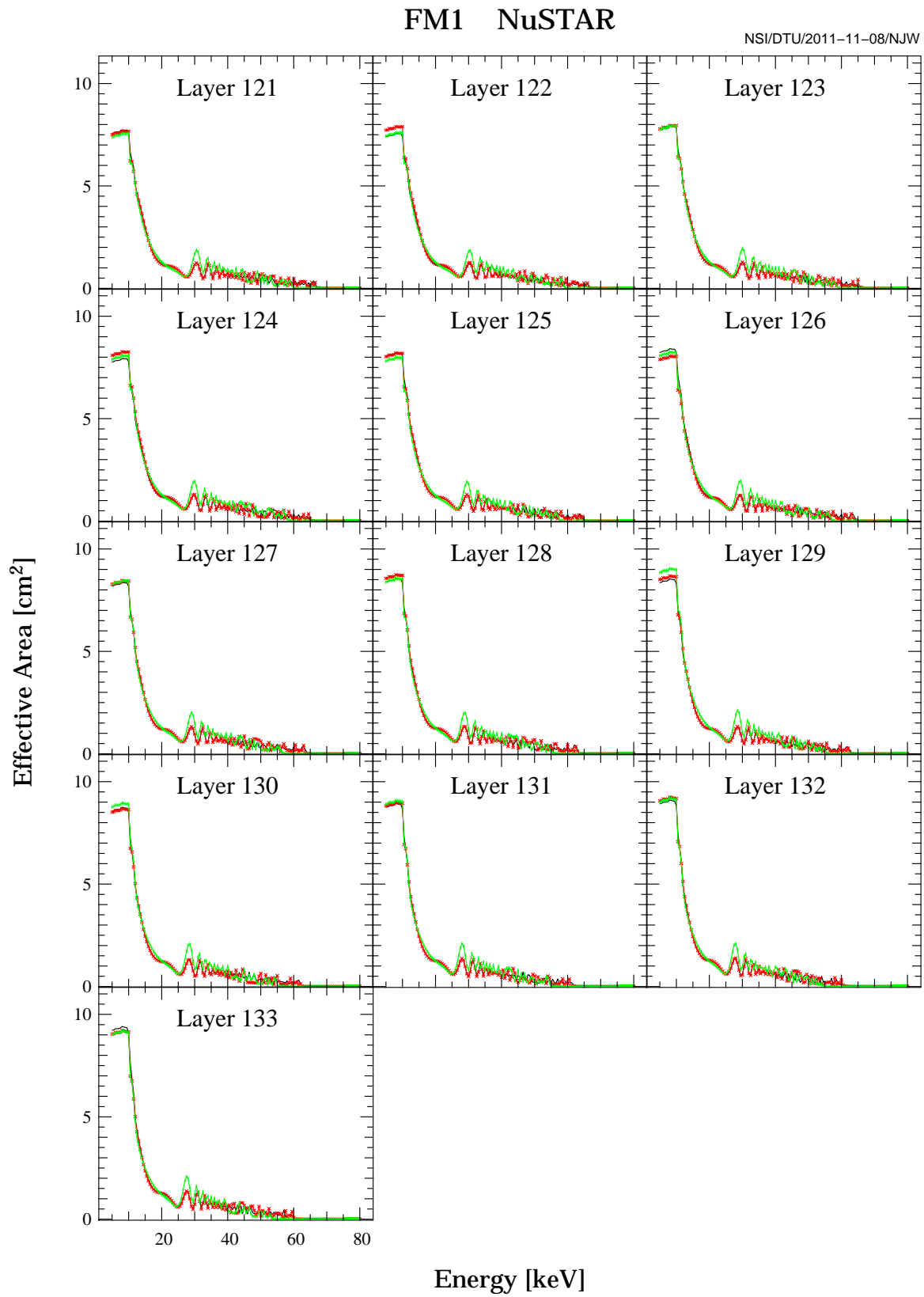
FM1   NuSTAR

NSI/DTU/2011−11−08/NJW

Figure 30: Comparing nominal and average recipe.

17 Appendix: Calculating the z-array needed for FRESNEL

Design recipe:

$$d_i = \frac{a}{(b+i)^c} \tag{1}$$

where i is the bilayer number, 1 at the top (facing vacuum) and N at the bottom (facing the mirror substrate), N being the total number of bilayers.

Additional parameters for the multilayer description are the gamma values (ratio of LZ material thickness to the total bilayer thickness) and the interface roughness parameter (often called sigma).

NB's procedure for fitting the witness sample reflection measurements utilizes the above expression including individual changes of the upper six layers as well as a change of the gamma value for layer no. 2 and 3 (layer 1 has a special 'top-gamma' value).

The NJW IDL code:

```
function mk_recipe, params, dump=dump, debug=debug
;
; Standard (nominal) design recipe with alterations:
;
;    Use d = a/(b+i)^c  prescription
;                Then 'params' must at least be
;              [n, dmin, dmax, c, topgam, gamma]
;
;    but it might be expanded with:
;        [gtot2, gtot3, dtot1, dtot2, dtot3, dtot4, dtot5, dtot6]
;
;-------------------------

  nelem = n_elements(params)
  if nelem lt 6 then begin
     print,'Syntax: z = mk_recipe( params[, /dump][, /debug]'
     print,''
     print,'The number of elements in params must at least be 6'
     print,' [n, dmin, dmax, c, topgam, gamma]'
     print,' but it might be expanded with:'
     print,' [gtot2, gtot3, dtot1, dtot2, dtot3, dtot4, dtot5, dtot6]'
     print,' (failing to set all dtot will make the rest equal 1.00)'
     return,0;
  endif

  dbg = 0
  if keyword_set(debug) then dbg = 1

  ; If nelem == 6 then basic formula is used without modifications

  if nelem gt 6 then begin
     p = replicate(1.,14);
     p(0:nelem-1) = params
     if nelem eq 7 then p(7) = p(6);  ensure that gtot3 has a reasonable value
  endif else begin
     p = params;  Basic formula
  endelse
```

```
   if dbg then begin
      print,'*mk_recipe* p:',p
   endif

   n = long(p(0)+0.01); Counteract rounding errors
   dmin = p(1)
   dmax = p(2)
   c    = p(3)
   topgam = p(4)
   gamma = p(5)

; ---  produce the nominal layer thicknesses

   z_arr = dblarr( 2*n )

   k = (dmin/dmax)^(1./c)
   b = (1. - n*k)/(k - 1.)
   a = dmin * (b + n)^c

   if keyword_set(dump) then begin
      filename = get_next_filename( 'recipe_????.scm' )
      openw, lun, filename, /get_lun
      printf,lun,date(3),format='("// ",a)'
      printf,lun,n,format='("// N = ",i3)'
      printf,lun,dmin,format='("// dmin = ",f10.4)'
      printf,lun,dmax,format='("// dmax = ",f10.4)'
      printf,lun,c,format='("// c = ",f10.4)'
      printf,lun,topgam,format='("// topgam = ",f10.4)'
      printf,lun,gamma,format='("// gamma = ",f10.4)'
      if nelem gt 6 then begin
         printf,lun,p(6),format='("// gtot2 = ",f10.4)'
         printf,lun,p(7),format='("// gtot3 = ",f10.4)'
         printf,lun,p(8),format='("// dtot1 = ",f10.4)'
         printf,lun,p(9),format='("// dtot2 = ",f10.4)'
         printf,lun,p(10),format='("// dtot3 = ",f10.4)'
         printf,lun,p(11),format='("// dtot4 = ",f10.4)'
         printf,lun,p(12),format='("// dtot5 = ",f10.4)'
         printf,lun,p(13),format='("// dtot6 = ",f10.4)'
      endif
      printf,lun,'// Layer thicknesses - one line is one bilayer'
      printf,lun,'//   #  Light      Heavy  Bilayer thickness'
   endif

   for i = 1, n do begin;  NB! counting from 1
      d = a / (b + i)^c
      if i eq 1 then begin
         d_use = d
         if nelem gt 6 then d_use = d_use * p(8)
         heavy_thick = d_use * topgam
         light_thick = d_use * (1. - topgam)
      endif else begin
         g_use = gamma
         d_use = d
         if nelem gt 6 and i le 3 then g_use = p(i+4)
         if nelem gt 6 and i le 6 then d_use = d_use * p(i+7)
         heavy_thick = d_use * g_use
         light_thick = d_use * (1. - g_use)
      endelse
```

```
    z_arr(2*(i-1)) = light_thick
    z_arr(2*(i-1)+1) = heavy_thick

    if keyword_set(dump) then printf, lun, i, light_thick, heavy_thick, d_use, $
                format='(i5,f10.4,f10.4,f10.4)'

endfor


if keyword_set(dump) then close, lun
if keyword_set(dump) then free_lun, lun

return, z_arr

end
```