INSTRUMENT CALIBRATION REPORT

ATOMIC SCATTERING CALIBRATION FILE AND XRISM XMA OPTICAL CONSTANTS

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**Goddard Space Flight Center
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Space Administration

Atomic Scattering Calibration File and XRISM XMA Optical Constants

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Preface

This document is an XRISM Project signature-controlled document. Changes to this document require prior approval of the applicable Product Design Lead (PDL) or designee. Proposed changes shall be submitted in the Technical Data Management System (TDMS) via a Signature Control Request (SCoRe) along with supportive material justifying the proposed change. Changes to this document will be made by complete revision.

All of the requirements in this document assume the use of the word "shall" unless otherwise stated.

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Change History Log

Revision	Effective Date	Description of Changes (Reference the SCoRe Approval Date)
-	08/24/2023	Released per RESOLVE-SCoRe-0474 Describes atomic scattering CalDB file – the entries are numerically identical in content to the Hitomi file. Provides background information on calculation of optical constants.

[Disclosure notice belongs here if applicable.]

NOTE to editors: The document name will be XRISM-CAL-RPT-XXXX, where XXXX is assigned by the TDMS system. The document will be cross-referenced in TDMS to the filename in the format XRISM-XXX-CALDB-FILEDESC-NN where XXX is the instrument or component (e.g., RESOLVE), FILEDESC refers to a specific calibration report (e.g., rmfparams) and NN the corresponding number assigned to that report by the SDC. For example the calibration report addressing the Resolve LSF calibration may be assigned XRISM-RESOLVE-CALDB-RMFPARAMS-01, that addressing the Resolve gain calibration XRISM-RESOLVE-GAINPIX-CALDB-02, etc. (where the numbers are to be provided by the SDC).

These documents are updated as needed, e.g., when the relevant CalDB files, or the relevant calibration data analysis, is revised. The document version will be assigned by the TDMS system. The tracking tool should be used to record changes.

This document must include the CalDB file name, an explanation of how the data were collected and the analysis conducted and, if using standard Ftools, the software version number. All revisions are consolidated into the same document to maintain a full record of all changes.

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Introduction

1.1   Purpose

This document describes the atomic scattering CalDB file, which provides the real (f_1) and imaginary (f_2) components of the scattering parameters as a function of energy. The document describes synchrotron measurements of mirror foil samples used to calculate f_1 and f_2 at Au absorption edges that, in combination with values from the literature (some of which is based on theory, not measurements), populate the CalDB file. The document also provides background information about how the mirror optical constants are calculated, as well as information about how the relevant CalDB files are organized and used by the XRISM software to calculate the reflectivity and transmissivity of the X-ray Mirror Assembly (XMA) mirror foils as a function of energy and incident angle.

1.2   Scientific Impact

Given the composition and density of a component of the XMA, the atomic scattering form factors as a function of energy (which are stored in a CalDB file) can be used to calculate the real and imaginary components of the optical constant as a function of energy for that component. From the complex optical constant function, we can calculate the reflectivity and transmissivity of the mirror foil coating layer as a function of X-ray energy and incident grazing angle.

The reflection and transmission probability functions calculated above are themselves stored in additional CalDB files and are used in downstream analysis software, along with a detailed geometrical model of the XMA, to calculate the XMA effective area, and point spread function (PSF), as functions of X-ray incident energy, off-axis angle, and azimuthal angle.

1.3   Background Information on Optical Constant Calculation

Although the atomic scattering factors can be calculated from theory (e.g., Pratt et al. 1994, and references therein), the theory breaks down around atomic absorption edges, and in certain energy ranges, depending on the detailed method and particular assumptions. Moreover, even the calculations away from absorption edges, published by different research groups, can be inconsistent with each other for some elements in some energy regimes due to variations in numerical methods and particular assumptions (see section 2.1). In practice, the XRISM software and CalDB adopt a hybrid approach whereby one theoretical set of tables is selected, but the atomic scattering factors are measured in ground experiments for critical elements, in energy regimes where the theory breaks down, and these measurements replace the relevant portions of theoretical tables.

For XRISM, the measurements of the atomic scattering factors (and therefore of the optical constants), are made just for Au (over critical energy ranges). Au forms the "front-side" reflective coating of the mirror foils. The remaining functions for all elements including Au, in

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the 0.010 to 30 keV range, are from the theoretical calculations of Henke, Gullikson, and Davis (1993; hereafter HENKE tables). The CalDB file described in this document (hereafter "atomic scattering file") contains this hybrid set of atomic scattering functions, as well as a compilation of other theoretical tables from principal studies in the literature (see section 2.1 for details). Although regular XRISM data analysis would not utilize these other sets of atomic scattering factors, they are included in the CalDB file for reference, and to facilitate theoretical studies investigating the effects of uncertainties in the optical constants for materials in the XMA. We note that the energy grid spacings of the atomic scattering factors in the theoretical tables are very coarse compared to the energy resolution of the XRISM Resolve instrument. For example, in the HENKE tables it is 30 eV or more in the 2-3 keV band, which includes the prominent Au M edges. However, the ground measurements are performed at a higher energy resolution that is more appropriate for the Resolve instrument, especially in the regimes where the optical constants are rapidly changing with energy.

In practice, the atomic scattering factors are not measured directly. It is the X-ray reflectivity of the material that is measured, and the atomic scattering factors (and therefore the optical constants) are inferred from the reflectivity measurements. The general scheme for calculating the relation between the atomic scattering factors and the reflectivity involves many steps, which are only presented here in outline form. Much of the details can be found in, e.g., Parratt 1954, Spiller 1994, de Boer et al. 1995, and references therein.
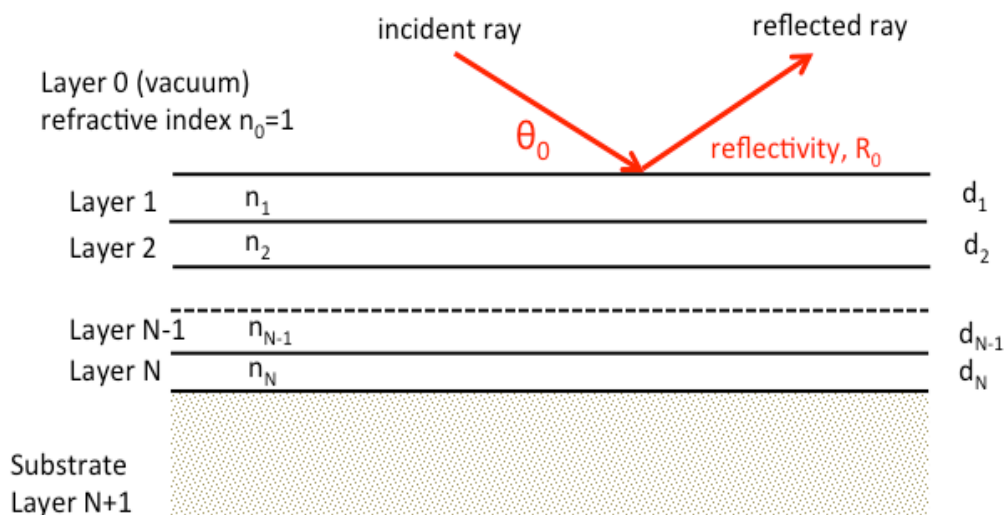

Figure 1:Illustration of a multilayer mirror coating stack. Thickness and (complex) refractive index for layer N are denoted by d_N and n_N respectively.

Here we summarize the steps linking the optical constants to reflectivity. Since the framework for the CalDB optical constants and reflectivity tables is based on the system designed for *Hitomi*, for completeness we outline the general relations for multilayer mirror foil coatings and specialize to the case of single-layer coatings at the end. Both of the XRISM XMA units have single layer Au

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coatings (thickness 2000 Å), as did SXT-1 and SXT-2 aboard *Hitomi*. (The hard X-ray telescopes aboard *Hitomi* had multilayer coatings.)

The complex refractive index of the coating layer l ($= 0 \dots N$, see Figure 1), at energy E is

(1) $n_l(E) = 1 - [\delta_l(E) + i\beta_l(E)]$,

where $\delta_l(E)$ and $\beta_l(E)$ are the real and imaginary components of the optical constants of the material in layer l respectively. If f_1 and f_2 are the real and imaginary components of the atomic scattering functions respectively (in the atomic scattering CalDB file), then

(2) $\delta_l(E) = \frac{r_e \lambda_{cm}^2 \rho_l N_A}{2\pi W_l} \sum_{k=1}^{k=K_l} M_{l,k} \, f_1(Z_{l,k}, E)$,

(3) $\beta_l(E) = \frac{r_e \lambda_{cm}^2 \rho_l N_A}{2\pi W_l} \sum_{k=1}^{k=K_l} M_{l,k} \, f_2(Z_{l,k}, E)$.

Here, r_e is the classical electron radius (in cm), λ_{cm} is the wavelength of incident radiation (in cm), ρ_l is the density of the material (in g cm^{-3}) in layer l, N_A is Avogadro's number, W_l is the total atomic weight of the material in layer l, $M_{l,k}$ is the number of atoms of element k in a molecule in layer l, $Z_{l,k}$ is the atomic number of element k in layer l, where $k=1,2,3..K_l$.

To derive the reflectivity of the mirror system based on the index of refraction calculated in equation (1), one must calculate two quantities that are proportional to the momentum transfer, one for *S*-polarization ($f_{S,l}$), and one for *P*-polarization ($f_{P,l}$).

(4) $f_{S,l} = \frac{1}{\mu_l} \frac{2\pi}{\lambda_{cm}} g_l$,

(5) $f_{P,l} = \frac{\mu_l c^2}{n_l^2} \frac{2\pi}{\lambda_{cm}} g_l$.

Here, μ_l is the relative magnetic permeability of the material in layer l, and

(6) $g_l = (n_l^2 - \cos^2\theta_0)^{\frac{1}{2}}$,

where θ_0 is the grazing angle of incidence between the X-ray and the reflective surface.

Next, we calculate the reduction factor for electric field amplitudes due to roughness (thermal lattice vibrations). The XRISM CalDB reflectivity/transmissivity files use the formalism of Névot & Croce (1980):

(7) $Q_l(\theta_0, E) = \exp\left[-2\left(\frac{2\pi}{\lambda}\right)^2 \sigma_{l+1}^2 (n_l^2 + \sin^2\theta_0 - 1)^{\frac{1}{2}} (n_{l+1}^2 + \sin^2\theta_0 - 1)^{\frac{1}{2}}\right]$.

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Here, σ_{l+1} is the roughness parameter between layer l and $l+1$. In the next step we calculate the complex Fresnel coefficients for S- and P-polarization between layers l and $l+1$, modified by the roughness attenuation factor:

$$(8) \quad F_{S,l,l+1} = \left[\frac{f_{S,l} - f_{S,l+1}}{f_{S,l} + f_{S,l+1}}\right] Q_l(\theta_0, E)$$

and

$$(9) \quad F_{P,l,l+1} = \left[\frac{f_{P,l} - f_{P,l+1}}{f_{P,l} + f_{P,l+1}}\right] Q_l(\theta_0, E).$$

A recursion relation can then be constructed between the reflected amplitude ratio, r, at the bottom of layer l and the top of layer $l + 1$, for $l > 0$:

$$(10) \quad r_{S,l} = \left[\frac{F_{S,l,l+1} + r_{S,l+1}}{1 + F_{S,l,l+1}\, r_{S,l+1}}\right] \exp\left[id_l(\frac{4\pi}{\lambda})(n_l^2 - \cos^2\theta_0)^{\frac{1}{2}}\right]$$

and

$$(11) \quad r_{P,l} = \left[\frac{F_{P,l,l+1} + r_{P,l+1}}{1 + F_{P,l,l+1}\, r_{P,l+1}}\right] \exp\left[id_l(\frac{4\pi}{\lambda})(n_l^2 - \cos^2\theta_0)^{\frac{1}{2}}\right]$$

For $l = 0$ (the ambient layer), by definition of the formalization of the problem (see e.g., Parratt 1954), the exponential factor is replaced by unity (i.e., d_l is effectively 0 in the above equations), for both S- and P-polarizations. Finally, we invoke the boundary condition that the reflected amplitudes at the boundary between the final layer and the (semi-infinite) substrate are 0. Then we can use the recursion relations to arrive at the reflection amplitude ratios at the coating surface, $r_{S,0}$ and $r_{P,0}$. The reflectivity is equal to the square of the reflected amplitude ratio, and the net reflectivity, $R_0(E, \theta_0)$, for unpolarized radiation is obtained by taking the average of the squares of the reflected amplitude ratios for S- and P-polarizations:

$$(12) \quad R_0(E, \theta_0) = \frac{1}{2}\left(|r_{S,0}|^2 + |r_{P,0}|^2\right).$$

Calculation of the transmissivity of a multilayer stack follows along similar lines but we do not give explicit expressions here.

For mirror foils with single-layer coatings, as is the case for both XMA units on XRISM, according to the model theoretical framework described above, there is only one dielectric boundary, and that is between the vacuum and coating surface. At the "bottom" of the coating

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layer, the reflected amplitude is zero, or, $r_{S,1}=0$ and $r_{P,1} = 0$. The recursion relations then lead to expressions for $r_{S,0}$ and $r_{P,0}$.

(13)

$$r_{S,0} = \left[\frac{\sin\theta_0 - (n_1^2 - \cos^2\theta_0)^{1/2}}{\sin\theta_0 + (n_1^2 - \cos^2\theta_0)^{1/2}}\right] \times \exp\left[-2\left(\frac{2\pi}{\lambda}\right)^2 \sigma_1^2 \, (n_1^2 + \sin^2\theta_0 - 1)^{1/2} \sin\theta_0\right]$$

$$r_{P,0} = \left[\frac{n_1^2\sin\theta_0 - (n_1^2 - \cos^2\theta_0)^{1/2}}{n_1^2 \sin\theta_0 + (n_1^2 - \cos^2\theta_0)^{1/2}}\right] \times \exp\left[-2\left(\frac{2\pi}{\lambda}\right)^2 \sigma_1^2 \, (n_1^2 + \sin^2\theta_0 - 1)^{1/2} \sin\theta_0\right]$$

$$R_S(E, \theta_0) = \left[\mathrm{Re}(r_{S,0})\right]^2 + \left[\mathrm{Im}(r_{S,0})\right]^2,$$

with a similar expression for $R_P(E, \theta_0)$, so that

$$R_0(E, \theta_0) = \frac{1}{2}\left\{\left[\mathrm{Re}(r_{S,0})\right]^2 + \left[\mathrm{Im}(r_{S,0})\right]^2 + \left[\mathrm{Re}(r_{P,0})\right]^2 + \left[\mathrm{Im}(r_{P,0})\right]^2\right\}$$

In the above, the ambient medium is the vacuum, for which $n_0 = 1$, and $\mu_0 = 1$.

The above calculations can be performed by the HEASoft tool xrtreftable. This tool takes the atomic scattering CalDB file (the subject of this report), and the telescope description file (TDF) as inputs, and produces a FITS output file containing the reflectivity and transmissivity of the thin-film coatings on the "front-sides" of similar groups of mirror foils, as a function of energy and incident grazing angle. However, the tool only calculates the transmissivity of thin-film coatings and does not calculate the transmission probabilities for the substrate and other "thick" materials making up a mirror foil (including the epoxy layer between the front-side coating and the main foil body). This must be done separately by calculating the mass-absorption coefficients, $\mu_{\mathrm{abs},m}$, for material m from the imaginary components of the atomic scattering factors, f_2, for all of the relevant materials:

(14)

$$\mu_{\mathrm{abs},\,m} = \frac{2r_e\,\lambda_{\mathrm{cm}}\,N_A}{W_m} \sum_{k=1}^{k=K_m} M_{m,k}\,f_2\left(Z_{m,k}, E\right)\ \mathrm{cm}^2\ \mathrm{g}^{-1}$$

If d_m is the thickness of the component for material m that has a density of ρ and a mass-absorption coefficient of $\mu_{\mathrm{abs},m}$, then the transmission probability is

(15) $T_m(E) = \left[1 - R_0(E, \theta_0)\right]\,\exp\left[-(\mu_{\mathrm{abs},\,m}\ \rho_m\,d_m)/\sin\theta_0\right],$

where $R_0(E, \theta_0)$ is the net front-side reflectivity for the mirror foil calculated earlier.

1.4 How to Update the Atomic Scattering CalDB File with New XRISM Data

In principle, it is possible that after the launch of XRISM, continued calibration efforts may improve the characterizations of the Au optical constants around the M and/or L edges. In that case the atomic scattering CalDB file would need to be updated accordingly. In order to preserve back-compatibility with *Hitomi,* no modifications should be made to the data in the HENKEMODSXT extension of the file. Instead, a new extension should be created called HENKEMODXMA. The data in this extension would begin as a copy of the data in HENKEMODSXT, and then the data would be modified according to improved calibration. The only downstream software that uses the atomic scattering CalDB file is the tool xrtreftable, and one would simply specify HENKEMODXMA for the input parameter "atmsctng," instead of HENKEMODSXT.

2 First Delivery-20201115

The atomic scattering file described in this document was first released as a CalDB file for the *Hitomi* mission. The initial file for XRISM, "xa_gen_atmsca_20190101v001.fits", is numerically identical in content to "ah_gen_atmsca_20140101v001.fits" for the *Hitomi* mission that was released with the final *Hitomi* CalDB. For XRISM, only the extension named "HENKEMODSXT" is used, and the data in this extension correspond to the theoretical calculations of Henke, Gullikson, and Davis (1993), with sections of the data for Au replaced by the measurements described elsewhere in this document.

File name	Validity date	Issue date	File(s) as delivered	Delivery Version
xa_gen_atmsca_20190101v001.fits	2015-02-28	2020-11-15	f1f2_HenkeModSXT.fits	1.0

Table 1: Attributes of the atomic scattering CalDB file.

2.1 Data Description

The atomic scattering CalDB FITS file contains 12 extensions. Each extension contains tables of different compilations of the atomic scattering factors as a function of energy for most, but not all, of the elements in the periodic table. (Different elements are missing in different tables.) Each FITS extension has five columns, as described below.

Column name	Description	Note
Z	Atomic number of element	
rowindex	Energy bin number for a given element	Starts at 1 for each Z
energy	Photon energy	
f1real	Real part of the atomic scattering factor	
f2img	Imaginary part of the atomic scattering factor	

Table 2: Column descriptions for the FITS tables in the atomic scattering CalDB file. The data for all atomic elements have a common energy grid, and the data are listed sequentially in a single FITS table, by energy, and then by atomic number, without a break. The "rowindex" column is used to assign a particular row to an energy bin: this column avoids the table-reading code having to calculate the energy bin assignment for every row.

Following are descriptions and references for the compilations of atomic scattering tables in each extension of the CalDB file. The extension names are given in parentheses.

- Extension 1: (henke97): Henke, B. L., Gullikson, E. M., & Davis, J. C., (1993), Atomic Data and Nuclear Data Tables Vol. 54 (no.2), 181-342, but with data for Au modified to fit ASCA data better around the Au edges (Tamura et al. 2006, SPIE Vol. 6266).

- Extension 2: (BrennanCowan) Brennan, S., and Cowan, P. L. (1992), Rev. Sci. Instrum. 63, 850.

- Extension 3: (Chantler) Chantler, C. T., Journal of Physical and Chemical Reference Data (1995), 24, 71.

- Extension 4: (CromerLiberman) Cromer, D. T. (1983) J. Appl. Cryst. 16, 437-437.

- Extension 5: (EPDL97) "EPDL97 The Evaluated Data Library, 97 Version," Cullen, D. E., et al. (1997) UCRL-50400, Vol 6, Rev 5.

- Extension 6: (Henke2013) Henke data downloaded in November 2013 from http://henke.lbl.gov/optical_constants/asf.html, containing updates for several elements compared to the data in Henke et al. (1993). The Au data in this extension are *not* modified in any way.

- Extension 7: (Kissel) Kissel, L., Radiation physics and chemistry 59 (2000) 185-200.

- Extension 8: (Sasaki) Sasaki, S. (1989) Numerical Tables of Anomalous Scattering Factors Calculated by the Cromer and Liberman Method, KEK Report, 88-14, 1-136.

- Extension 9: (Windt) Atomic scattering factors calculated by D. Windt (see http://www.rxollc.com/idl/).

- Extension 10: (Shadow) A concatenation of three sources of atomic scattering factors. 0.1-2 keV: Henke et al. (1982) Atom. Data Nucl. Data Tables, 27., 1; 2-10 keV: Auerbach et al., Software for Reflectivity calculations of X-ray mirrors, LLNL Report UCRL91230 (1984); 10-100 keV: Sasaki, S. (1989), KEK Report, 88-14, 1-136.

- Extension 11: (HenkeSskChantler): A concatenation of 3 sources of atomic scattering factors. In the energy range 0.03-4.275 keV the data are the same as in the Henke2013 extension; In the energy range 4.275-123 keV the data are the same as in the Sasaki

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extension for all except the three elements, H, He, and Be. For these three elements the data are identical to the corresponding data in the extension Chantler.

- Extension 12: (HENKEMODSXT): Henke 2013 data (as in extension 6), modified over certain energy ranges for Au, by replacement with ground measurements, as described in section 2.2.

2.2   Data Analysis

Photon paths that include "double reflections," which lead to a focused image on the focal plane, occur on the XMA mirror foil "front-side" surfaces that are coated with a layer of Au with thickness 2000 Å. Fine structure in the Au optical constants occurs in the ~2.1-3.7 keV and ~11.5-15 keV bands due to M and L edges respectively. In order to fully take advantage of the energy resolution of Resolve (~5-7 eV FWHM), the optical constants in these energy ranges should be measured with an energy resolution of ~1 eV. Using a witness sample, the reflectivity curves around the M and L edges were obtained at the radiation facilities KEK and Spring-8, respectively. The f_1 atomic scattering factor, as well as the roughness, σ, were calculated by fitting the reflectivity curve with local software at ISAS/JAXA. The results are given below. Due to the limitations of the KEK data, the f_2 atomic scattering factor was not measured for the energy band covering the Au M edges. Therefore, although the HENKEMODSXT extension in the CalDB atomic scattering file has the HENKE table f_2 values replaced by measurements in the regime of the Au L edges, it retains values of f_2 from the HENKE table, unmodified in the regime of the Au M edges. (Note that in the regimes that the HENKE data are retained, the table values are mapped onto a finer energy grid than that native to the HENKE data.)

In principle, f_2 can be derived from f_1, since the two are not independent, but are mathematically related via the Kramers-Kronig dispersion relation (e.g., Peiponen and Vartiainen 1991). However, it turns out that while going from f_2 to f_1 is straightforward, the reverse is highly non-trivial to calculate accurately because the denominator in the integral goes to infinity in the energy regime of the atomic fine structure, where the greatest accuracy is required (e.g., see https://pypi.org/project/kkcalc/). This means that f_1 and f_2 are not strictly self-consistent in the regime of the Au M edges in the CalDB file, and this ultimately contributes to the error budget in the effective area calibration of the XMA in the energy range around the Au M edges.
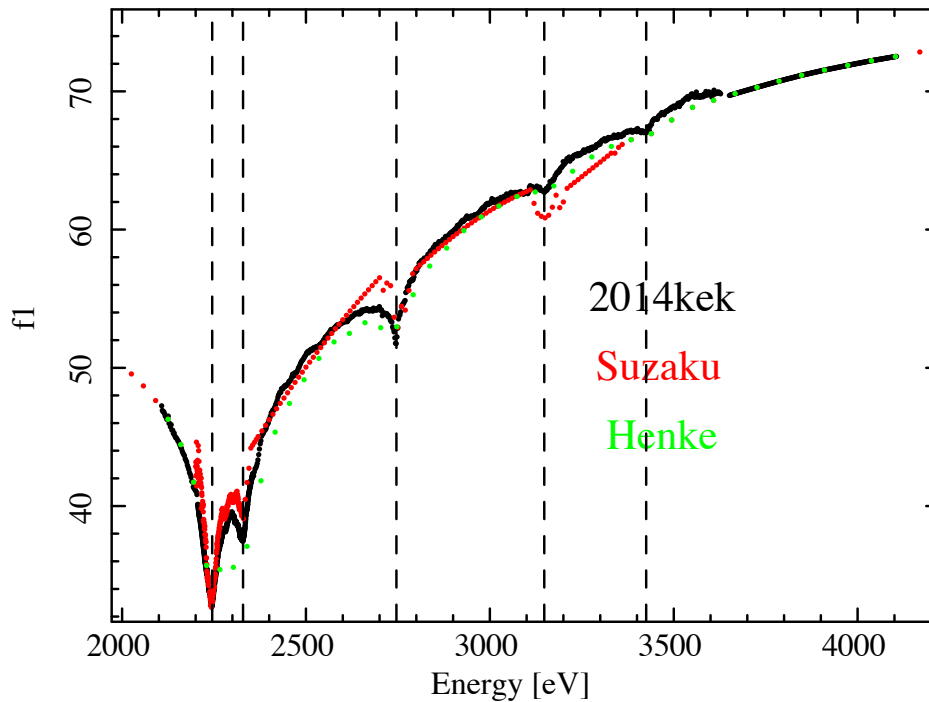
Figure 2: Atomic scattering factor f_1 around the Au M edges. The black data were adopted and included in the atomic scattering CalDB file, replacing the HENKE table values in the energy range shown (see Kurashima et al. 2016, proceedings of SPIE, 9905, doi:10.1117/12.2231173). For f_2, the HENKE table values are used at all energies except around the Au L edges in the range ~11.5-15 keV.

The 2-4 keV f_1 data (labeled 2014KEK) are shown in Figure 2, and the 11.0-15.5 keV f_1 data (labeled SPring-8), along with the Henke f_2 function over the same energy range, are shown in Figure 3. The energy ranges and corresponding sources of data in the atomic scattering table for Au in the CalDB file are summarized in Table 3, along with the energy pitch in each energy band.

Energy band (keV)	f_1	f_1 Energy pitch (eV)	f_2	f_2 Energy pitch (eV)
0.01-2.220	Henke 2013	0.16 – 35.5	Henke 2013	0.16-35.5
2.220-2.355	KEK PF	0.25	Henke 2013	36.1 – 37.9
2.355-3.628	KEK PF	0.20	Henke 2013	38.5-58.4
3.628-11.30	Henke 2013	59.3-182.3	Henke 2013	59.3-182.3
11.30-14.00	Spring 8	0.4-0.7	Spring 8	0.4-0.7
14.00-14.90	Spring 8	0.4-0.7	Henke 2013	0.20-247.3
14.90-30.00	Henke 2013	251.3-477.5	Henke 2013	251.3-477.5

Table 3: Energy ranges and corresponding sources of data in the atomic scattering table for Au in the CalDB file, along with the energy pitch in each energy band.
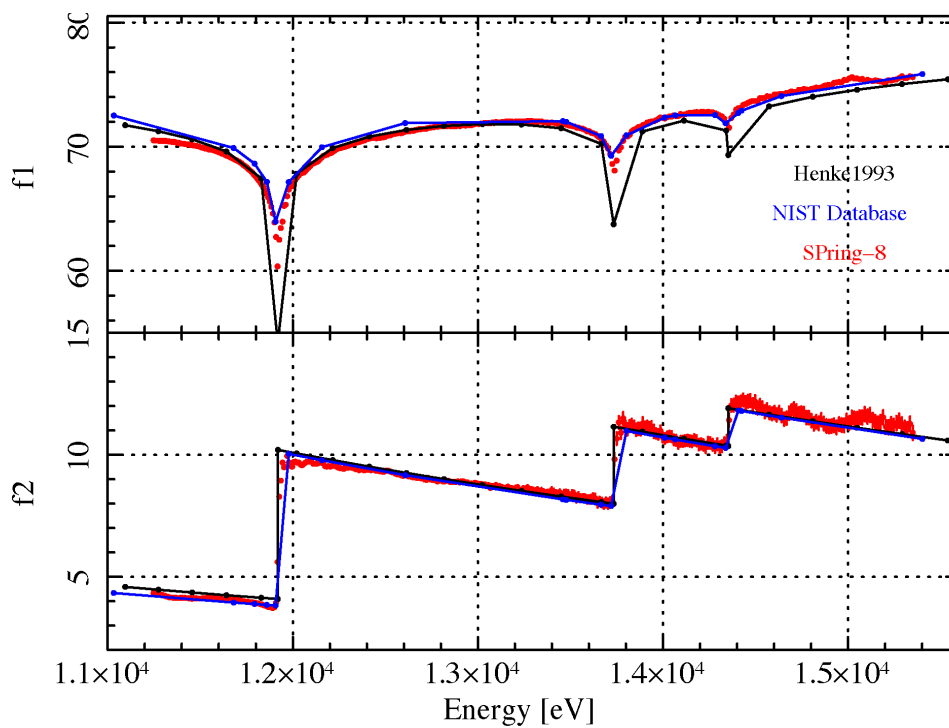
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Figure 3: The atomic scattering factors f_1 and f_2 around the Au L edges (see Kikuchi et al. 2016, Optics Express, 24, 25548). The red data are adopted and included in the atomic scattering CalDB file, replacing the HENKE table values in the energy range shown in Table 3.

2.3 Results

The final tables of f_1 and f_2 cover the energy range 0.030 to 30.0 keV. These tables are placed in the HENKEMODSXT extension of the atomic scattering file "xa_gen_atmsca_20190101v001.fits", and f_1 and f_2 as a function of energy are shown in Figure 4. The XRISM software and CalDB use the data in the HENKEMODSXT extension of the atomic scattering file to calculate the optical constants, reflectivity, and transmissivity.
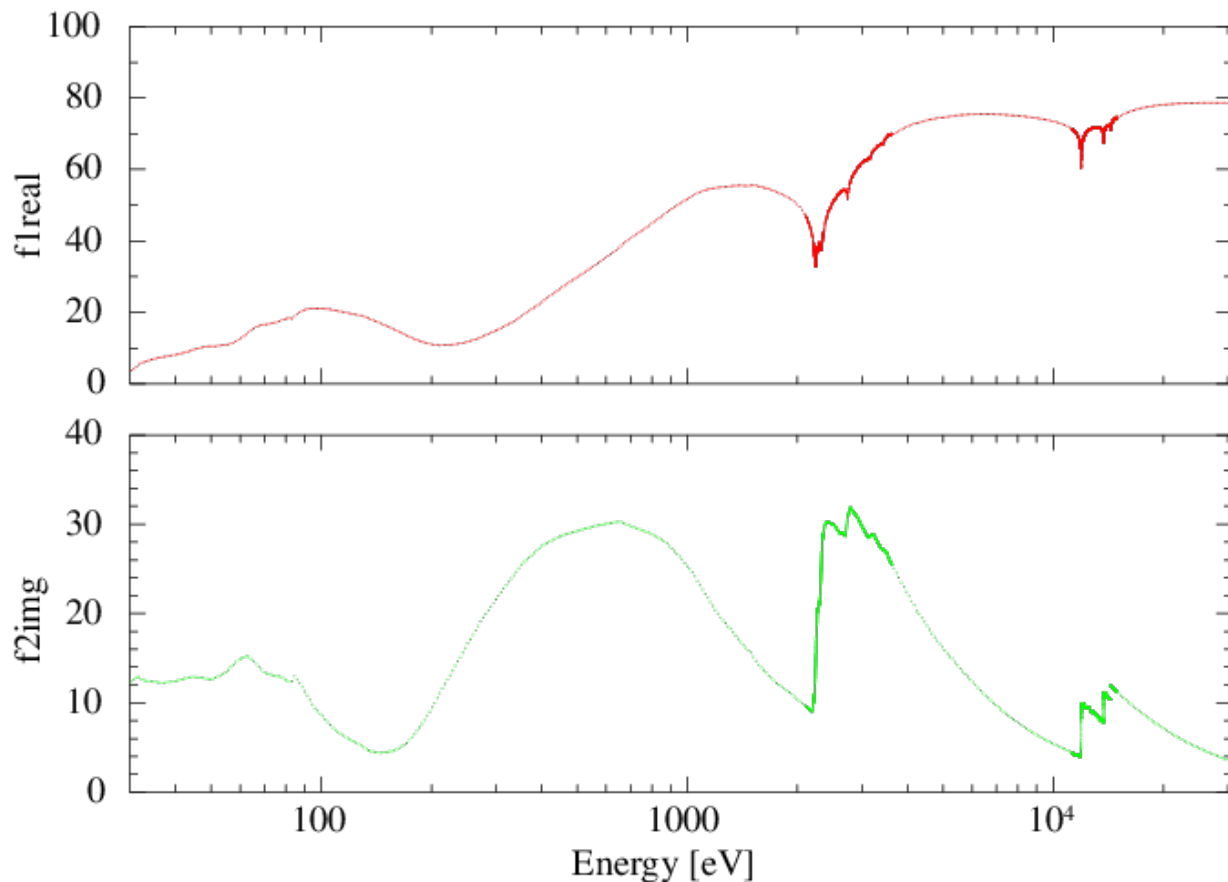
Figure 4: The atomic scattering factors f_1 and f_2 in the 30-30,000 keV band that are in the HENKEMODSXT extension of the atomic scattering file "xa_gen_atmsca_20190101v001.fits", constructed from a combination of measurements and HENKE table values, as described in this document. The red and green data are f_1 and f_2, respectively. The values around the Au M and L edges are tabulated at a fine energy resolution of ~1 eV (see Table 3), in order to properly sample Resolve's spectral resolution.

2.4   Comparison with Previous Releases

The atomic scattering file that is described in this document and that will be used in the CalDB at the time of the launch of XRISM ("xa_gen_atmsca_20190101v001.fits"), has content that is numerically identical to that in the corresponding file that was included in the final release of the *Hitomi* CalDB ("ah_gen_atmsca_20140101v001.fits").

2.5   Final Remarks

It is expected that this version of the atomic scattering file will not change before the launch of XRISM.

3   References

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