PAPER

Catalog of x-ray spectra of Mo-, Rh-, and W-anode-based x-ray tubes from 10 to 50 kV

Steffen Ketelhut, Ludwig Büermann and Gerhard Hilgers
Physikalisch-Technische Bundesanstalt, Braunschweig, Germany
E-mail: steffen.ketelhut@ptb.de

Keywords: x-ray spectrometry, mammography, high-purity germanium detector

Abstract
This work presents a comprehensive catalog of x-ray spectra measured from x-ray tubes with tungsten, molybdenum, and rhodium anodes generated at tube potentials between 10 and 50 kV in steps of 1 kV. They can serve as an input for dose calculations, image quality calculations, investigations of detector features, and validations of computational spectral models, among other things. The measurements are performed by means of a high-purity germanium detector-based spectrometer 1 m from the x-ray sources without any added filtration. The x-ray tubes are characterized by thin beryllium exit windows (0.15−4 mm); thus, for energies above 15 keV, the spectra recorded can be considered approximately unfiltered. This allows potential users of the catalog to computationally add any filter to the spectra in order to create special radiation qualities of their choice. To validate this option, a small number of spectra are recorded with filter materials in place whose purity and thickness are known with high precision. These spectra are compared to the corresponding spectra from the catalog obtained by means of computationally added filters. The two types of spectra agree extremely well. Several typical mammographic radiation qualities are selected to compare the spectra obtained from the catalog presented here with corresponding spectra obtained from other catalogs published by Boone et al (1997 Med. Phys. 24 1863–74) and Hernandez et al (2017 Med. Phys. 44 2148–60). In contrast to the work presented here, those spectra rely partly or fully on calculations. A quantitative comparison is made by means of typical x-ray quality descriptors such as the mean energy and the first and second half-value layer. The results obtained from the Boone catalog match those of the current catalog sufficiently well for the Mo- and Rh-anode-based spectra. However, significant differences up to 10 times the estimated uncertainties are found for the quality descriptors evaluated from the spectra of Hernandez et al and the W-anode based spectra of Boone et al.

1. Introduction

In order to calculate mean glandular doses in mammography, the conversion factors $g$, $c$, and $s$ are calculated by means of Monte Carlo methods (Dance et al 2000). The $g$ factor is the conversion factor for the calculation of mean glandular dose from the air kerma measurement for a reference spectrum with a combination of molybdenum anode and filtration, and for an average glandularity of the breast. The $c$ factor corrects for different breast glandularities, and the $s$ factor corrects for different beam qualities. In order to calculate the factors with small uncertainty, realistic x-ray spectra are needed, similar to those in typical mammography facilities. For this purpose, it is advantageous to have an experimental catalog of spectra for a large variety of filters. Further applications for such a catalog include image quality calculations, investigations of detector features and development, and validations of catalogs of computational spectra.

Several spectra catalogs cover the mammography range from 15 to 50 kV. Birch and Marshall developed a semi-empirical spectral model which can be used to estimate spectra in the range of 30–150 kV generating potential (Birch and Marshall 1979). This model was used for the catalog of IPEM report 78 (Cranley et al 1997). Boone and Seibert used experimental spectra by Fewell, Shuping and Healy (Fewell et al 1981) in their TASMIP
model (Boone and Seibert 1997). The experimental spectra are interpolated with polynomials to generate the spectra in the range between 30 and 140 kV, which are not covered by the measurements. This spectral model was extended to cover the mammography spectra for tungsten, molybdenum and rhodium anodes in the TASMIP$M_{\text{T}}$, MASMI$P_{\text{M,T}}$, and RASMIP$M_{\text{T}}$ models (Boone et al 1997) based on spectra by Fewell and Shuping (Fewell and Shuping 1978). Hernandez et al took an alternative approach in the TASMICS model (Hernandez and John 2014). This approach is based purely on Monte Carlo-type calculations using MCNPX, with interpolations using cubic splines to cover the spectra not simulated in the range from 20 to 640 kV generating potential. An extension of the model specifically for mammography spectra is named TASMICS$M_{\text{T}}$, MASMIC$S_{\text{M,T}}$, RASMIC$S_{\text{M,T}}$ (Hernandez et al 2017). Another spectral model by Poludniowski, SpekCalc, is based on calculations and is validated against the model of Birch and Marshall (Poludniowski et al 2009). It is limited to the range of 30–300 kV generating potential and to tungsten anodes. An improved version of the SpekCalc spectral model has been developed and used in the SpekPy software (Bujila et al 2020). The second version of SpekPy allows tungsten, molybdenum, and rhodium anode spectra of generating potentials between 20 and 50 kV to be calculated.

While spectral models are available, there is a particular lack of experimental spectra in the mammography range. Spectrometry on medical equipment is challenging because of the limited space and high count rates involved. Most experimental work employ CdTe-detectors, but also other spectrometers (Boone et al 1998, Miyajima and Imagawa 2002, Miyajima 2003, Maeda et al 2005, Abbene et al 2010, 2012, Plagnard 2014, Santos et al 2017). However, no comprehensive experimental catalog of measured spectra covering the energy range of mammography in steps of 1 kV generating potential has been reported to date in literature to the knowledge of the authors.

This work presents a catalog of spectra measured at x-ray tubes containing tungsten, rhodium, and molybdenum anodes without any filter added between 10 and 50 kV generating potential in steps of 1 kV. These spectra can be computationally filtered to create any spectrum in the energy range typical for mammography.

2. Materials and methods

2.1. Experimental setup

The spectrometry was performed at the x-ray laboratories of the Physikalisch-Technische Bundesanstalt (PTB) Braunschweig which are otherwise used for calibration of secondary standard dosimeters. The high demands on the properties of the reference radiation fields for the use of high-precision dosimeter calibrations against primary air kerma standards cannot be achieved with medical x-ray systems as used in mammography. However, the measured spectra can be expected to be representative for those used in mammography (see section 4.2). A sketch of the experimental setup is given in figure 1. The x-ray tube and generator specifications are given in table 1. Before entering the spectrometer, the unfiltered x-ray beam passes the additional filter, a set of collimators, and a monitor chamber. All the filters of this work are purchased at Goodfellow GmbH, Hamburg, Germany. The monitor chamber is composed of three Suprorny$TM$ (PA) foils (Kalle GmbH, Wiesbaden, Germany) with a thickness of 25 μm which serve as entrance and exit windows and as a central electrode. The central electrode is coated with ≤2 μm of aluminum and ≤1 μm of carbon. The filtration of the x-ray beam by the monitor chamber is negligible.

The pulse-height spectra are recorded by a high-purity germanium spectrometer 1 m from the source. The characteristics of the spectrometer are summarized in table 2. The detector is housed in a lead shield to inhibit stray radiation from entering the detector. In this work, the front part is equipped with a pinhole collimator made of TRIAMET$TM$ G17, an alloy comprising tungsten (90% of the weight) and nickel and iron (10% of the weight). The conical aperture has an entrance hole diameter of 0.136 mm, and an exit hole diameter of 4 mm. The transmission of stray radiation through the shield is tested using a sealing plug instead of a collimator, once with the radiation turned on and once with it turned off. A generating potential of 50 kV and the highest possible tube current are used. The spectra with and without stray radiation are identical within statistical uncertainty. Thus, the lead shield effectively shields the detector from scattered radiation in all of the radiation settings used.

2.2. Data processing

Data were acquired by means of the DSPEC 50$TM$ digital signal processing module manufactured by ORTEC, and the MAESTRO:32 MCA emulator software version 6.08. An optimal throughput and resolution were achieved using a rise time of 5.6 μs and a flat top width of 1.2 μs. A pile-up rejection circuit was not used. The range of count rates, integrated counts, and dead time of the data acquisition are given in table 3. A low-energy threshold of approximately 3 keV was set to suppress electrical noise. The raw spectra were collected into 4096 channels, such that one keV comprised approximately 10 channels. They were energy calibrated by means of the emission lines of a 133Ba source.
2.3. Detector spectral response correction

In an ideal detector, the full energy of all the photons are deposited in the detector. In a real detector, the following processes can cause a deposition of part of the energy: Compton scattering of the photons from the active detector material, escaping electrons and fluorescence photons from the active detector material, and the undesired detection of scattered photons from the surrounding non-active medium. With the help of the spectral response correction, the true spectrum is extracted from the measured one.

The measured spectrum is dependent on the incoming spectrum in the following way:

\[ M(E') = \int R(E, E') T(E) dE, \]  

where \( M(E') \) is the measured signal for energy \( E' \), \( T(E) \) is the impinging signal for energy \( E \), and \( R(E, E') \) is the response of the detector. For a discrete distribution, this can be expressed as:

**Figure 1.** Experimental setup of the x-ray tube, additional filter, collimators, monitor chamber and detector. The spectra for the tungsten anode and the rhodium and molybdenum anodes have been taken in different laboratories with dimensions as indicated. The parts are not true to scale.

**Table 1.** Main x-ray tube and generator specifications.

| Anode        | Tungsten | Molybdenum | Rhodium |
|--------------|----------|------------|---------|
| Tube manufacturer | Comet    | PANalytical | PANalytical |
| Tube type     | MXR 165  | PW 2185    | PW 2182 |
| Anode type    | Stationary | Stationary | Stationary |
| Anode angle   | 30°      | 26°        | 18°     |
| Be window thickness | 4 mm     | 1 mm       | 0.15 mm |
| Focal spot size | 5.5 mm × 5.5 mm | 9 mm × 16 mm | 9 mm × 16 mm |
| Generator manufacturer | Yxlon | Yxlon | Yxlon |
| Generator type | MGG46    | MGG43      | MGG43   |
| Frequency     | 40 kHz   | 40 kHz     | 40 kHz  |
| Ripple effect | ≤0.01%   | ≤0.01%     | ≤0.01%  |
| Tube potential inaccuracy | ≤0.01% | ≤0.01% | ≤0.01% |
\[ M_k = \sum_i R_{ki}^* T_i \cdot \Delta E, \] (2)

\[ = \sum_i R_{ki} \cdot T_i, \] (3)

\[ \hat{M} = \hat{R} \cdot \hat{T}, \] (4)

where \( M_k \) is the measured spectrum in channel \( k \), \( T_i \) is the incoming spectrum in channel \( i \) and \( R_{ki}^* \) is the response matrix. \( R_{ki} \) is related to the latter via \( R_{ki} \approx R_{ki}^* \cdot \Delta E \). \( \hat{M}, \hat{T} \), and \( \hat{R} \) are the corresponding vectors and the response matrix, respectively.

In order to derive the incoming x-ray spectrum \( \hat{T} \) from the measured spectrum \( \hat{M} \), (4) has been solved for \( \hat{T} \) using an iterative method based on Bayes’ theorem. Details of the method can be found in Sievers et al (2012), Kennett et al (1978), D’Agostini (1995). Using the notation of (4), Bayes’ theorem can be expressed as:

\[ P(T|M_k) = \frac{P(M_k|T)P(T)}{\sum_k P(M_k|T)P(T)}, \] (5)

for the probability \( P(T|M_k) \), that there is an event in channel \( i \) of the true spectrum, \( T_i \), given the observation of a count in channel \( k \) of the measured spectrum, \( M_k \). Using this equation and the relationship:

\[ P(T_i) = \sum_k P(T_i|M_k) P(M_k), \] (6)

one can derive the following equation:

\[ T_i^{(n+1)} \approx T_i^{(n)} \sum_k \frac{R_{ki} M_k}{\sum_j R_{kj} T_j^{(n)}}, \] (7)

In order to derive the undistorted spectrum \( T_i \) from the measured spectrum, (7) can be solved iteratively, with the measured spectrum as a starting point, \( T_i^{(0)} = M_i \). The resulting spectra are normalized to the same arbitrary area under the curve.

The matrix \( R_{ki} \) in (7) is calculated using the DOSRZnrc user package of the EGSnrc Monte Carlo simulation program (Kawrakow et al 2000). For the simulation, information on the detector geometry is obtained by means of the specifications provided by the manufacturer (see table 2) and an additional CT image. In order to determine the thickness of the absorbing inactive germanium layer at the crystal surface, the relative efficiency curve has been measured with calibrated point-shaped nuclide sources with energies around the germanium
K-absorption edge at 9.9 keV. The efficiency curve has been compared to simulations with a modified user package DOSRZnrc from the Monte-Carlo program EGSnrc. The modification consists of an extension giving access to the direct, non-normalized pulse height spectrum. In these simulations, the dead layer has been varied until the simulated efficiency curve resembled the experimental one, especially around the germanium K-absorption edge. An inactive germanium layer of 1.8 μm gives the best agreement between measurement and calculation. With these data, a geometrical model is built in the EGSnrc simulation. The detected pulse-height spectra for impinging monoenergetic beams are calculated for energies $E_i$ from 0.25 to 100 keV in steps of 0.25 keV. From the results, the matrix $R_i$ is constructed.

The detector response correction was checked with a $^{133}$Ba source using a response matrix calculated for energies from 1 to 400 keV in steps of 1 keV. The background between the full-energy peaks of the $^{133}$Ba lines is not completely removed in the unfolding process. However, both Compton edge and Compton plateau are substantially suppressed by the unfolding, leading to a significant reduction of the background in the area of the spectrum affected by Compton scattering, i.e. around and below the Compton edge. Moreover, the relative intensities of the peaks were compared to literature values (Bé et al 2016), and were found to agree within a few percent.

2.4. Calculation of filtered photon spectra and x-ray quality descriptors

Filtered photon spectra and x-ray quality descriptors like mean energy and half-value layers (HVLs) were calculated with a FORTRAN inhouse code named ‘specman’. In this section we describe the underlying formulas and procedures used in this code. Filters positioned in the x-ray beam close to the x-ray focus (see figure 1) attenuate the beam intensity and modify the shape of the photon energy spectrum. Due to the special geometric arrangement it is unlikely that filter-scattered photons contribute to the spectrum at the point of measurement. Thus, the filtered spectrum can be calculated by the linear attenuation law. The distribution of the photon fluence with respect to energy is given by $\Phi_E = d\Phi/dE$, where $d\Phi$ is the fluence of photons of energy $E$.

$\Phi_E$ the attenuated distribution, $\Phi_{E, att}$ is calculated as $\Phi_{E, att} = \Phi_E e^{-\mu_{mat}(E) t_{mat}}$, where $\mu_{mat}(E)$ and $t_{mat}$ are the linear attenuation coefficient at the energy $E$ and the thickness of the material. Attenuation coefficients of the materials were calculated with the NIST XCOM program (Berger and Hubbell 1987). This program allows to generate mass attenuation coefficients of pure and mixed materials for an energy grid defined by the user. The relative uncertainties of the mass attenuation coefficients in the energy region from 5 to 50 keV and filter materials relevant for this work is estimated at about 2% or less (see figure 3 in Yves et al 2019).

The XCOM material data input files used by specman were generated for energies between 0.25 and 400 keV in steps of 0.25 keV (1600 energies in total). For the purpose of interpolation with respect to photon energy, the total attenuation coefficients are approximated by log–log cubic-spline fits as functions of energy.

Fluence-weighted mean energies $\bar{E}_\Phi$ were calculated according to

$$\bar{E}_\Phi = \frac{\int_0^{E_{max}} \Phi_E E dE}{\int_0^{E_{max}} \Phi_E dE}. \quad (8)$$

The air kerma $K_{air}$ of a spectrum was calculated according to

$$K_{air} = \int_0^{E_{max}} \Phi_E E \left(\frac{\mu_{air}}{\rho}\right)_E dE, \quad (9)$$

where $\left(\frac{\mu_{air}}{\rho}\right)_E$ is the mass energy transfer coefficient of air at the energy $E$ which were taken from the calculations of Seltzer (1993). The attenuated air kerma was calculated as

$$K_{air, att} = \int_0^{E_{max}} \Phi_E e^{-\mu_{mat} t_{mat}} E \left(\frac{\mu_{air}}{\rho}\right)_E dE. \quad (10)$$

The first HVL of a spectrum with respect to aluminum, HVL$_{Al,spec}$, was calculated by an iterative process. First, the HVL$_{Al}$ of a monoenergetic photon beam of the mean energy $\bar{E}_\Phi$ was calculated according to

$\text{HVL}_\text{Al} (\bar{E}_\Phi) = t_{1/2 Al} (\bar{E}_\Phi) = \ln(2) / \mu_{Al} (\bar{E}_\Phi).$ This value is expected to be already close to HVL$_{Al,spec}$. Next, the inequality $|K_{air}/K_{air,att}(t_{Al}) - 2| \leq 0.001$ was solved iteratively by varying the aluminum thickness $t_{Al}$ starting with $t_{Al} = t_{1/2 Al} (\bar{E}_\Phi)$ and then by increasing or decreasing $t_{Al}$ in steps of 0.0001 · $t_{Al}$ until the inequality is fulfilled. The same iterative procedure was used to calculate the second HVL.

It is noted that the same code was applied to all evaluations of spectra discussed in this paper. Thus, if differences in mean energies or HVL values occur between nominally the same spectra but published by different authors it is not caused by differences in the interaction coefficients or interpolation procedures.
Table 4. Area density, density and thickness from the measurements of the filter thickness of four typical filters. The density values are taken from Greenwood and Earnshaw (1997).

| Material   | \(d_{\text{nominal}}\) \(\mu m\) | Area density \(\text{mg cm}^{-2}\) | Density \(\text{g cm}^{-3}\) | \(d_{\text{max}}\) \(\mu m\) |
|------------|----------------------------------|---------------------------------|----------------------------|----------------------------|
| Molybdenum | 30                               | 30.56(10)                       | 10.28(2)                   | 29.73(11)                 |
|            |                                  | 31.12(10)                       |                            | 30.27(11)                 |
|            |                                  | 30.54(10)                       |                            | 29.71(11)                 |
| Molybdenum | 60                               | 59.64(19)                       | 10.28(2)                   | 58.02(22)                 |
|            |                                  | 59.76(19)                       |                            | 58.13(22)                 |
|            |                                  | 60.90(19)                       |                            | 59.24(22)                 |
| Rhodium    | 25                               | 30.44(10)                       | 12.38(2)                   | 24.39(9)                  |
|            |                                  | 31.45(10)                       |                            | 25.40(9)                  |
|            |                                  | 30.73(10)                       |                            | 24.82(9)                  |
| Silver     | 50                               | 51.40(16)                       | 10.49(2)                   | 49.00(18)                 |
|            |                                  | 51.81(16)                       |                            | 49.39(18)                 |
|            |                                  | 51.64(16)                       |                            | 49.23(18)                 |

2.5. Measurements
In the following, measurements of unfiltered spectra are presented which are generated by tungsten, molybdenum, and rhodium anode x-ray tubes. The spectra presented range from 10 to 50 kV generating potential in steps of 1 kV. The spectra have a resolution of 0.25 keV and a minimum energy of 3 keV. Additionally, measured filtered spectra of reference qualities are presented in order to compare them to the unfiltered spectra, which are computationally filtered. In this way, the indirect method of generating the spectra is tested. The main concerns are the high count rate in the measurement of the unfiltered spectra and deviations due to the use of the ideal computationally added filtration as compared to the physical filters.

In order to distinguish the measured filtered spectra and the measured unfiltered spectra, the former are called physically filtered spectra and the latter computationally filtered spectra.

2.6. Filter thickness
The nominal filter thicknesses have been taken for the calculation of computationally-filtered spectra. In order to estimate the typical deviation of the thicknesses from their nominal values, four filter thicknesses have been determined experimentally.

Molybdenum filters with a nominal thickness of 30 and 60 \(\mu m\), a rhodium filter with a nominal thickness of 25 \(\mu m\) and a silver filter with a nominal thickness of 50 \(\mu m\) were measured precisely. All filter materials have a purity of \(\geq 99.95\%\). Three filters of each type were weighed by means of an analytical balance of type Kern model ABT 124-4M (Kern & Sohn GmbH, Balingen, Germany) with an uncertainty of \(\pm 0.1\%\). Their area was determined by scanning the filters and counting the pixels using ImageJ, an image editing program. Using these values, the area density of the filters was determined (see table 4). With the known density, the filter thickness could be determined with an uncertainty of better than 0.3 \(\mu m\).

2.7. Notation
The following notation is adopted for the radiation qualities: the elemental abbreviation of the anode material, i.e. W, Rh or Mo, is followed by the thickness of the filter in \(\mu m\), the elemental abbreviation of the filter material, and the generating potential of the beam in kV. For example, for a beam from a tungsten anode filtered by 60 \(\mu m\) of molybdenum at a generating potential of 28 kV, the radiation quality code is W60Mo28.

3. Results
3.1. Filtered spectra
Examples of computationally filtered x-ray spectra are shown in figure 2 for the molybdenum, rhodium, and tungsten anodes with generating potentials of 25 and 35 kV. The characteristic peaks for the \(K_{\alpha}\) and \(K_{\beta}\) lines of molybdenum at around 17 and 19 keV and those of rhodium at around 20 and 23 keV are clearly visible. The fine structure of the \(K_{\alpha}\) and \(K_{\beta}\) lines with peak separations in the range of 0.1–0.3 keV lies within the resolution of the measurement system and cannot be resolved.

Tube currents were chosen such that the dead time did not exceed approximately 5\%. In this case, the pile up in the spectra is small, in general only \(< 0.1\%\). An exception were the unfiltered tungsten spectra with high generating potential, for which the tube current could not be reduced sufficiently, and the dead time rose to
approximately 10%. The effect of pile up on the spectral shape was tested by recording tungsten spectra of 30 kV and varying tube current, and was found to be negligible.

3.2. Comparison of computationally filtered spectra and physically filtered spectra

Physically filtered spectra and computationally filtered spectra are shown in figure 3 for Mo25Rh28, Mo30Mo28, Rh1000Al28, Rh25Rh28, W500Al28, and W50Ag28. The spectra are chosen to include typical reference spectra, and to comprise a large variety of anode materials and filtrations. All spectra are recorded at a generating potential of 28 kV. Qualitatively, the spectra agree well. The ratio of the fluence in the physically and computationally filtered spectra is very close to one for the largest part of the spectra. Some deviations can be seen at low energies and close to 28 keV, where the number of counts is low, and the absolute difference of the fluence therefore small, and close to the absorption edges, where the fluence in the computationally-filtered spectra drops down more steeply.

In order to quantitatively compare the spectra, their mean energies and first and second HVLs for aluminum have been calculated and are presented in table 5. All spectra agree very well in terms of their mean energy with respect to fluence within 0.1 keV. The agreement of the HVLs between the physically and computationally filtered spectra is at or below 1.0% for the molybdenum and rhodium spectra, confirming the qualitatively good agreement in figures 3(a)–(d). The W50Ag28 spectra also agree well, with the difference of the first HVLs being 1.2% and that of the second HVLs being 0.4%. The only spectra with larger deviations are for W500Al28, with a difference of 4.5% for the first HVLs and 2.3% for the second HVLs.

3.3. Comparison to the ASMIP and ASMICS spectral models

The computationally filtered spectra of this work are compared to the corresponding computationally filtered spectra from the MASMIP, RASMIP, and TAMSIP models from Boone et al (1998) and the spectra of the
MASMICS, RASMICS, and TASMICS models from Hernandez et al (2017). In tables 6–8, the mean energy, the first and second HVLs for aluminum of the Mo30Mo series, the Rh25Rh series, and the W60Mo series are given for generating potentials between 20 and 40 kV.

For all three parameters, a general trend is apparent: the computationally filtered spectra show the best agreement with the physically filtered spectra, followed by the spectra obtained by Boone et al and then by Hernandez et al. The average differences for the mean energies are 0.3%, 1.8%, and 4.0% for the spectra of this

Figure 3. Example spectra for computationally filtered and physically filtered spectra with different anode-filter combinations at a generating potential of 28 kV. \( \Phi_{E,\text{norm}} \) denotes the photon fluence with respect to energy, normalized to the total fluence. Below each spectrum, the ratio of the physically filtered to computationally filtered spectrum is given. The ratio is restricted to bins with a count number of at least 0.2% of the maximum count number in a bin.
work, those obtained by Boone et al. and by Hernandez et al., respectively. For the first HVLs, these numbers are 1.5%, 5.7%, and 11.2%, respectively, and for the second HVLs, 1.0%, 4.7%, and 10.5%, respectively.

The greatest differences exist for the tungsten-anode spectra, followed by the molybdenum and rhodium-anode spectra. Additionally, for the W60Mo spectra, there is a trend of growing differences in terms of HVLs towards higher generating potentials. No clear trends are apparent in the Mo30Mo series or the Rh25Rh series.

| Quality code | Phys/Comp | Phys | 1st HVL | 2nd HVL |
|--------------|------------|------|---------|---------|
| Mo25Rh28     | Phys       | 1.5% | 0.375   | 0.478   |
|              | Comp       | 1.5% | 0.373   | 0.475   |
| Mo30Mo28     | Phys       | 5.7% | 0.314   | 0.408   |
|              | Comp       | 5.7% | 0.315   | 0.406   |
| Rh1000Al28   | Phys       | 11.2%| 0.564   | 0.694   |
|              | Comp       | 11.2%| 0.569   | 0.701   |
| Rh25Rh28     | Phys       | 1.0% | 0.354   | 0.485   |
|              | Comp       | 1.0% | 0.357   | 0.484   |
| W50Ag28      | Phys       | 4.7% | 0.558   | 0.697   |
|              | Comp       | 4.7% | 0.565   | 0.700   |
| W50Al28      | Phys       | 10.5%| 0.395   | 0.563   |
|              | Comp       | 10.5%| 0.413   | 0.576   |

Table 5. Comparison of the energy and half-value layers of some physically and computationally filtered reference spectra.

Table 6. Mean energies of the Mo30Mo, Rh25Rh, and W60Mo spectra of this work (physically and computationally filtered), of Boone et al. (1998) and of Hernandez et al. (2017). The uncertainty of the mean energy for the spectra of this work is 0.6% for \(k = 1\) (see section 4.1).

| Quality code | Phys. filtered | Comp. filtered | Boone et al | Hernandez et al |
|--------------|----------------|----------------|-------------|-----------------|
|               | \(E_{\text{mean}}\) keV | \(E_{\text{mean}}\) keV | \(E_{\text{mean}}\) keV | \(E_{\text{mean}}\) keV |
| Mo30Mo20     | 14.6           | 14.6           | 16.9        | 19.9            |
| Mo30Mo30     | 17.1           | 17.0           | 18.8        | 21.5            |
| Mo30Mo40     | 18.9           | 18.9           | 18.8        | 21.9            |
| Rh25Rh20     | 14.9           | 14.9           | 16.9        | 19.9            |
| Rh25Rh30     | 18.4           | 18.5           | 18.5        | 20.3            |
| Rh25Rh40     | 20.5           | 20.5           | 20.5        | 22.7            |
| W60Mo20      | 15.9           | 15.9           | 15.6        | 17.4            |
| W60Mo30      | 17.8           | 17.6           | 17.1        | 18.9            |
| W60Mo40      | 22.6           | 22.8           | 21.7        | 23.0            |

Table 7. First HVLs of the Mo30Mo, Rh25Rh, and W60Mo spectra of this work (physically and computationally filtered), of Boone et al. (1998) and of Hernandez et al. (2017). The uncertainty of the first HVLs for the spectra of this work is 2.2% for \(k = 1\) (see section 4.1).

| Quality code | Phys. filtered | Comp. filtered | Boone et al | Hernandez et al |
|--------------|----------------|----------------|-------------|-----------------|
|               | 1st HVL mm | 1st HVL mm | 1st HVL mm | 1st HVL mm |
| Mo30Mo20     | 0.222 | 0.220 | 0.207 | 0.192 |
| Mo30Mo30     | 0.339 | 0.333 | 0.327 | 0.302 |
| Mo30Mo40     | 0.401 | 0.396 | 0.394 | 0.366 |
| Rh25Rh20     | 0.240 | 0.241 | 0.232 | 0.215 |
| Rh25Rh30     | 0.376 | 0.383 | 0.381 | 0.343 |
| Rh25Rh40     | 0.472 | 0.487 | 0.487 | 0.448 |
| W60Mo20      | 0.315 | 0.319 | 0.290 | 0.280 |
| W60Mo30      | 0.397 | 0.392 | 0.351 | 0.346 |
| W60Mo40      | 0.479 | 0.472 | 0.411 | 0.394 |
4. Discussion

4.1. Uncertainty

The filter thickness determination is the main source of uncertainty for the determination of the mean energy and the first and second HVLs.

Five typical anode-filter combinations were chosen for the filters given in section 2.6. For those anode-filter combinations, the differences in \( E_{\text{mean}} \) and 1st HVL and 2nd HVL were calculated in the range between 20 and 40 kV. In each case, the maximum was taken as a conservative estimate of the uncertainty. The average of these uncertainties is taken as an estimate for the overall uncertainties, as shown in table 9.

Other sources of uncertainty were negligible. The source-to-detector distance (SDD) can be reproduced with a precision of 0.5 mm, and the absolute distance is known to be better than 2.0 mm. Even for a change in SDD of 3 mm, the change in mean energy and first and second HVLs for aluminum is less than 0.1 keV and 0.002 mm, respectively. Using SpekPy, the variations of the anode angle and Be window thickness were evaluated for the radiation qualities given in table 5. Variations were below 0.1%. As shown in table 1, the tube potential accuracy is better than 0.01%, and the ripple effect smaller than 0.01%. The uncertainty caused by the spectral correction method is not significant. The overall uncertainties for the mean energy, the first HVLs, and the second HVLs are therefore estimated to be \( u_{E_{\text{mean}}} = 0.6\% \), \( u_{1\text{st HVL}} = 2.2\% \), and \( u_{2\text{nd HVL}} = 1.4\% \), respectively.

4.2. Are the measured spectra representative for those used in mammography?

The anode angles of the three x-ray tubes used in this work are 18°, 26° and 30°. The effective anode angle (the actual anode angle plus the physical tube tilt) in mammography x-ray systems is usually 22° or 24° (depending on the type). These values of effective anode angles are comparable with those of the x-ray tubes used in this work. The influence of different anode angles on the shape of the spectrum is visible if the filtration is minimal (i.e. only the inherent Be window of the tube and no additional filtration). However, these differences nearly vanish if one adds filtrations as used in mammography. This behavior is demonstrated in table 10 where W-anode spectra are compared which were measured at two different x-ray tubes with anode angles of 20° and 30° with an added filtration of 60 \( \mu \text{m} \) of molybdenum and generated with tube potentials between 20 and 40 kV. The differences in the mean energies and first and second HVLs are not more than a few percent. There is a large difference between the focal spot sizes of the tubes used in this work (see table 1) and those of typical mammography x-ray systems.

### Table 8. Second HVL of the Mo30Mo, Rh25Rh, and W60Mo spectra of this work (physically and computationally filtered), of Boone et al (1998) and of Hernandez et al (2017). The uncertainty of the second HVLs for the spectra of this work is 1.4% for \( k = 1 \) (see section 4.1).

| Quality code | 2nd HVL (phys. filtered) mm | 2nd HVL (comp. filtered) mm | Boone et al 2nd HVL mm | Hernandez et al 2nd HVL mm |
|--------------|-----------------------------|-----------------------------|------------------------|--------------------------|
| Mo30Mo20     | 0.274                       | 0.272                       | 0.255                  | 0.240                    |
| Mo30Mo30     | 0.435                       | 0.428                       | 0.421                  | 0.397                    |
| Mo30Mo40     | 0.506                       | 0.500                       | 0.497                  | 0.469                    |
| Rh25Rh20     | 0.293                       | 0.293                       | 0.282                  | 0.264                    |
| Rh25Rh30     | 0.524                       | 0.525                       | 0.521                  | 0.475                    |
| Rh25Rh40     | 0.667                       | 0.671                       | 0.665                  | 0.627                    |
| W60Mo20      | 0.365                       | 0.368                       | 0.346                  | 0.330                    |
| W60Mo30      | 0.477                       | 0.467                       | 0.432                  | 0.420                    |
| W60Mo40      | 0.646                       | 0.638                       | 0.563                  | 0.512                    |

### Table 9. Maximum uncertainty of the mean energy and the first and the second HVLs of selected radiation qualities in percent due to uncertainty \( \Delta d \) in the thickness of the filters.

| Quality code | \( \Delta d \) (\( \mu \text{m} \)) | \( (\Delta E_{\text{mean}})_{\text{max}} \) \( \% \) | \( (\Delta 1\text{st HVL})_{\text{max}} \) \( \% \) | \( (\Delta 2\text{nd HVL})_{\text{max}} \) \( \% \) |
|--------------|-------------------------------|-----------------|-----------------|-----------------|
| Mo30Mo20—Mo30Mo40 | 1.0                           | 0.7             | 1.8             | 1.1             |
| Mo25Rh20—Mo25Rh40 | 1.0                           | 0.7             | 2.1             | 1.4             |
| Rh25Rh20—Rh25Rh40 | 1.0                           | 0.6             | 2.2             | 1.7             |
| W60Mo20—W60Mo40  | 3.0                           | 0.6             | 2.3             | 1.4             |
| W50Ag20—W50Ag40  | 2.0                           | 0.5             | 2.3             | 1.5             |
| Mean           | 0.0                           | 0.6             | 2.2             | 1.4             |
mammography systems (0.1 or 0.3 mm). Only a fraction of the photons emitted from the large focus will pass the aperture with the very small diameter of 0.136 mm. Thus, the measured spectra belong to photons emitted from a small area within the large focal spot. Due to the Heel effect the target self-absorption reduces the intensity in the cathode to anode direction and therefore the spectral shape will change as well if one moves the pinhole along this direction in a way that photons emitted from another position within the focal spot reach the germanium detector. However, these changes in the spectral shape are only visible in the minimally filtered spectra and are nearly not visible in measured spectra with added filtrations as used in mammography. On the other hand, in classical mammography one makes use of the special intensity variation caused by the Heel effect by using the so-called half-field geometry. Thus, these small differences in the spectral shape are also present in real mammography. In conclusion, despite the large differences in x-ray tube design used in this work and in real mammography units it is justified to regard the measured spectra at the special x-ray tubes used in this work as being representative for those in real mammography if one adds the usual filtrations.

### 4.3. Deviations between computationally filtered spectra and physically filtered spectra

The computationally filtered and the physically filtered spectra agree very well within the uncertainty in terms of the mean energy and the HVLs (see tables 5–8). Nevertheless, some differences remain, especially for W500Al28, which shows a difference in the first and second HVLs of 4.5% and 2.3%, respectively, between computationally filtered and the physically filtered spectra. These deviations may be caused by differences in the x-ray generation, in the filtration of the spectrum, or in the measurement setup.

The generation of the x-ray beam can be ruled out as a source of deviation. The x-ray generation is identical in both data sets, as the unfiltered and filtered spectra were measured at the same x-ray tube, with the same anode angle and Be window thickness, and in the same laboratory.

The larger HVLs indicate that the beam has been hardened more for the computationally filtered spectra, which suggests that the thickness of the physical filter is smaller than of the nominal filter. In contrast to this, the aluminum filter thickness was measured for the filter in the measurement to be 503(2) μm. Also, the larger filter thickness increases the first HVLs by 0.5(3)% and the second HVLs by 0.2(2)%, which causes deviations which are much smaller than the described deviations above.

A collimator with a very small entrance hole (0.136 mm) was used due to the high fluence rate especially in the recording of the unfiltered spectra. Here, possible issues include misalignment of the small collimator, pile-up counts in the spectrum and transmission through the edges of the collimator. The alignment was carried out with great care, and no signs of misalignment were present (for example, in the form of tungsten x-rays from increased scattering events in the collimator). Thus, misalignment is not the cause of the differences. A contribution from pile up is unlikely, as explained in section 3.1. Transmission through the edges is only possible if the collimator is misaligned, which is not the case, as explained above.

### 4.4. Deviations from the ASMIP and ASMICS spectral models

The spectra models by Boone et al and by Hernandez et al rely partly or fully on calculations. Therefore, the catalog with experimental spectra of this work can be taken as a validation of these models. As can be seen from tables 6–8, the spectra of computationally filtered spectra are generally closer to the experimental spectra than those obtained by Boone et al and by Hernandez et al. This is expected due to the high correlation, as the x-ray generation for both measurements was identical and as a similar measurement setup was used.

In order to compare to the spectral models, the x-ray generation has to be taken into account. In table 11, the specifications for the generation of the tungsten-anode spectra are listed. There are differences in the thicknesses of the Be exit window, in the distances between the source and the detector, and in the effective anode angles.

The differences in the HVLs and the mean energies caused by the different filtering of the Be exit window and the air volume between source and detector were investigated using two standard radiation quality series, W50Ag and W60Mo. The spectra were generated as computationally filtered spectra. The differences from the

### Table 10. Mean energy and first and second HVLs for filtered spectra measured for anode angles of 20° and 30° for radiation qualities from W60Mo20 to W60Mo40, i.e. 60 μm molybdenum filtered tungsten spectra.

| kV | Anode angle of 20° | Anode angle of 30° | Difference to 30° spectrum |
|---|---|---|---|
| | $E_{mean}$ keV | 1st HVL mm | 2nd HVL mm | $E_{mean}$ keV | 1st HVL mm | 2nd HVL mm | 1st HVL % | 2nd HVL % |
| 20 | 15.8 | 0.302 | 0.358 | 15.9 | 0.312 | 0.366 | −0.6 | −3.2 | −2.2 |
| 25 | 16.6 | 0.344 | 0.414 | 16.7 | 0.353 | 0.418 | −0.3 | −2.5 | −1.0 |
| 30 | 17.4 | 0.364 | 0.447 | 17.4 | 0.372 | 0.449 | 0.0 | −2.2 | −0.4 |
| 40 | 22.1 | 0.427 | 0.585 | 21.8 | 0.430 | 0.574 | 1.4 | −0.7 | 1.9 |
spectra of any possible anode-
0.5%
or in the development of mammography facilities among other things.
computationally
fi
Additional Be and air
range of generating potentials used in mammography. The spectra can be mathematically
measured un
Braunschweig for molybdenum, rhodium, and tungsten anodes. The catalog provided in this work includes
Spectra without additional
fi
spectra obtained by Boone et al and by Hernandez et al, which had less filtering, were calculated by means of an
additional Be and air filtering of the same amount. The mean energy, and first and second HVLs increase by
0.5%–1.8%, 3.5%–5.8% and 2.3%–5.3% in the case of Hernandez et al, and by 0.0%–1.3%, 2.3%–3.8% and
1.5%–3.5%, respectively, in the case of Boone et al.

The differences caused by the change in anode angle were investigated by experiments evaluating spectra
from two x-ray sources with two different anode angles of 20° and 30°. The results are presented in table 10. The
relative differences in mean energy and first and second HVLs are ≤3.2% for W60Mo radiation qualities with
20–40 kV generating potential. For molybdenum and rhodium anodes, smaller deviations are expected, as the
anode angles of this work are 18° and 26°, and therefore closer to the 22.4° in the work by Hernandez et al. Also,
differences caused by different anode angles are smaller for these anode materials due to the smaller atomic
number.

A list of the differences in the HVLs and the mean energy between the physically filtered spectra and the
spectral models is given in table 12 for the W60Mo series. The purely experimental spectra of this work show the
best agreement compared to the semi-empirical spectra obtained by Boone et al, and the largest deviations are
found for the spectra obtained by Hernandez et al. For some of the spectra, the deviations are larger than the
stated uncertainty of approximately 2%, even after taking into account the different anode angle and inherent
filter thickness. Whether this is relevant when using the spectra for calculations, depends on the kind of
application.

5. Conclusion

Spectra without additional filtration have been measured at the x-ray facility of the department 6.2 of the PTB
Braunschweig for molybdenum, rhodium, and tungsten anodes. The catalog provided in this work includes
measured unfiltered x-ray spectra with generating potentials between 10 and 50 kV in steps of 1 kV, covering the
range of generating potentials used in mammography. The spectra can be mathematically filtered to provide
spectra of any possible anode-filter combination available in mammography, thus providing a full catalog of
radiation qualities which can be used to estimate of mean glandular dose in mammography, in detector testing
or in the development of mammography facilities among other things.

Additionally, filtered spectra have been recorded. These spectra are used for a consistency check of
computationally filtered spectra. The overall agreement was very good, and sufficient for most applications.

The spectra of this catalog were compared to spectral models by Boone et al (1997) and Hernandez et al
(2017). The spectra of this work were closer to the spectra by Boone et al in terms of the mean energy and the first
and second HVLs for aluminum. The model by Boone et al is calculated with a semi-empirical approach based on
measured spectra. The model by Hernandez et al, on the other hand, was generated solely by means of
calculations performed using MCNP.

Table 11. Specifications for the generation of the tungsten-anode spectra for the TASMIP and
TASMICS catalogs and the data from this work.

| Spectral model | Hernandez et al | Boone et al | this work |
| ---------------|----------------|-------------|-----------|
| Effective anode angle | 22.4° | N/A | 30.0° |
| Inherent filtration | 0.77 mm Be | 0.5 mm Be | 4 mm Be |
| Source-to-detector distance | 668 mm | 1000 mm | 1000 mm |
| Focal spot size | 0.3 mm | 0.3 mm | 5.5 mm × 5.5 mm |

Table 12. Difference in the mean energy and first and second HVLs of computationally filtered spectra of this work (1), of
the spectra from Boone et al (2), and of the spectra from Hernandez et al (3) from physically filtered spectra for W60Mo.
The values are given as % difference to the physically-filtered spectra.

| Quality code | \( \Delta E_{\text{mean}} \) | \( \Delta 1\text{st HVL} \) | \( \Delta 2\text{nd HVL} \) |
|-------------|----------------|----------------|----------------|
| W60Mo20     | (1) | (2) | (3) | (4) | (5) | (6) | (7) |
| W60Mo30     | −1.1 | −3.9 | −5.1 | −1.3 | −11.6 | −12.8 | −2.1 | −9.4 | −11.9 |
| W60Mo40     | 0.9 | −4.0 | −10.2 | −1.5 | −14.2 | −17.7 | −1.2 | −12.8 | −20.7 |
Data resources

The unfiltered spectra are available at Ketelhut and Büermann (2021). They are provided as ASCII files in a two-column format in which the first column gives the energy at the top of the bin, and the second column the flux, normalized to the total fluence of the spectrum and the bin width.

Acknowledgments

The authors would like to thank Hartmut Drehsler and Reinulf Böttcher for their help in recording the spectra.

ORCID iDs

Steffen Ketelhut https://orcid.org/0000-0003-2099-3452

References

Bé M-M et al 2016 Table of Radionuclides (Vol. 8 - A = 41 to 198) Bureau International des Poids et Mesures (http://www.hnhb.fr/nuclear-data/nuclear-data-table/)

Abbene L, Gerardi G, Principato F, Del Sordo S, Ienzi R and Raso G 2010 High-rate x-ray spectroscopy in mammography with a CdTe detector: a digital pulse processing approach Med. Phys. 37 6147–56

Abbene L, Gerardi G, Principato F, Del Sordo S and Raso G 2012 Direct measurement of mammographic x-ray spectra with a digital ccd detection system Sensors 12 8390–404

Berger M J and Hubbell J H 1987 XCOM: Photon cross sections on a personal computer Technical Report NBSIR 87-3597 National Bureau of Standards Washington (DC), United States

Birch R and Marshall M 1979 Computation of bremsstrahlung x-ray spectra and comparison with spectra measured with a Ge(Li) detector Phys. Med. Biol. 24 505–17

Boone J M, Fewell T R and Jennings R J 1997 Molybdenum, rhodium, and tungsten anode spectral models using interpolating polynomials with application to mammography Med. Phys. 24 1863–74

Boone J M and Seibert J A 1997 An accurate method for computer-generating tungsten anode x-ray spectra from 30 to 140 kV Med. Phys. 24 1661–70

Boone J M, Yu T and Seibert A 1998 Mammography spectrum measurement using an x-ray diffraction device Phys. Med. Biol. 43 2569–82

Bujila R, Omar A and Poludniowski G 2020 A validation of SpekPy: a software toolkit for modelling x-ray tube spectra Phys. Med. Biol. 24 505–17

Cranley K, Gilmore B J, Fogarty G W A and Deponds L 1997 Catalogue of diagnostic x-ray spectra and other data Phys. Med. Biol. 24 505–17

Dance D R, Skinner C L, Young K C, Beddett J R and Kotre C J 2000 Additional factors for the estimation of mean glandular breast dose using the UK mammography dosimetry protocol Phys. Med. Biol. 45 3225–40

D’Agostini G 1995 A multidimensional unfolding method based on Bayes’ theorem Nucl. Instrum. Methods Phys. Res. A 362 487–98

Fewell T R and Shuping R E 1978 Handbook of mammographic x-ray spectra HEW Publication (FDA) 79-8071 (Washington, D.C.: U.S. Government Printing Office)

Fewell T R, Shuping R E and Healy K E 1981 Handbook of computed tomography x-ray spectra HHS Publication (FDA) 81-8162 (Washington, D.C.: U.S. Government Printing Office)

Greenwood N N and Earnshaw A 1997 Chemistry of the Elements 2nd edn (Oxford: Butterworth-Heinemann)

Hernandez A M and Boone J M 2014 Tungsten anode spectral model using interpolating cubic splines: unfiltered x-ray spectra from 20 to 640 kV Med. Phys. 41 042101

Hernandez A M, Seibert J A, Norastieh A and Boone J M 2017 Generation and analysis of clinically relevant breast imaging x-ray spectra Med. Phys. 44 2148–60

Kawrakow I, Rogers D W O, Mainegra-Hing E, Tessier F, Townson R W and Walters B R B 2000 EGSnrc Toolkit for Monte Carlo Simulation of Ionizing Radiation Transport (https://doi.org/10.4224/40001303)

Kennett T J, Prestwich W V and Robertson A 1978 Bayesian deconvolution: I. Convergent properties Nucl. Instrum. Methods 151 285–92

Ketelhut S and Büermann L 2021 Catalogue of Unfiltered X-ray Spectra from Tungsten-, Molybdenum-, and Rhodium-Anode-Based X-ray Tubes with Generating Voltages from 10 to 50 kV in Steps of 1 kV (Braunschweig: Physikalisch-Technische Bundesanstalt) (https://doi.org/10.7795/720.20201118)

Maeda K, Matsumoto M and Taniguchi A 2003 Compton-scattering measurement of diagnostic x-ray spectrum using high-resolution Schottky CdTe detector Med. Phys. 32 1342–27

Miyajima S 2002 Thin CdTe detector in diagnostic x-ray spectroscopy Med. Phys. 30 771–7

Miyajima S and Imagawa K 2002 CdZnTe detector in mammographic x-ray spectroscopy Phys. Med. Biol. 47 3959–72

Plagnard J, Omar A and Poludniowski G 2014 Comparison of measured and calculated spectra emitted by the x-ray tube used at the Gustave Roussy radiobiological service X-ray Spectrom. 43 298–304

Poludniowski G, Landry G, DeDilis F, Evans P M and Verhaegen F 2009 SpekCalc: a program to calculate photon spectra from tungsten anode x-ray tubes Phys. Med. Biol. 54 N433–8

Santos J C, Tomal A, Furquim T A, Fausto A M F, Nogueira M S and Costa P R 2017 Direct measurement of clinical mammographic x-ray spectra using a CdTe spectrometer Med. Phys. 44 3504–11

Seltzer S M 1993 Calculation of photon mass energy-transfer and mass energy-absorption coefficients Radiat. Res. 136 147–70

Sievers P, Weber T, Michel T, Klammert J, Büermann L and Anton G 2012 Bayesian deconvolution as a method for the spectroscopy of x-rays with highly pixelated photon counting detectors J. Instrum. 7 P03003

Yves M, Christophe D and Marie-Christine L 2019 Advances in the measurements of the mass attenuation coefficients X-ray Spectrom. 48 330–5

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