Data Calculation of X-Ray and Auger Electron Arising from Nuclear Decay

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Abstract In nuclear decay process, internal conversion electron emission and electron capture leave vacancies in atomic shells. The vacancies in atomic shells give rise to rearrangements in the shells which are accompanied by the emission of X-ray and the ejection of Auger electrons. The energies of X-ray and Auger electron can be calculated on the basis of atomic-electron binding energies in different atomic shells. The intensities of X-ray and Auger electron can be also calculated from vacancy number, X-ray fluorescence yield and vacancy transfer coefficient of different atomic shells. The calculation methods of energies and absolute intensities of X-ray and Auger electron arising from nuclear decay are introduced briefly. The calculation codes and flow chart are presented. The application is also given by using some nuclear decays as an example.

Key words Auger electron, X-ray, data calculation, nuclear decay

1 Introduction

The X-ray and Auger electron data are relevant in nuclear decay data. In a gamma transition process, gamma transition energy will be transferred directly to an orbital electron in different atomic shells through electronic-magnetic interaction. The orbital electrons which have gotten transition energies overcome atomic-electron binding energy and will emit out from different atomic shells, and leave vacancies. In an electron capture (it is called simply EC decay, or ε decay) process, the atomic nuclei capture electrons in different capture probabilities from different atomic-electronic shells, the process of ($p + e^- \rightarrow n + \nu$) will be produced, and meanwhile the process leads also to the production of vacancies in the atomic shells of the atoms belonging to the disintegrating nuclei. The vacancies in atomic shells give rise to rearrangements in the shells which are accompanied by the emission of X-ray and the ejection of Auger electrons. The data calculation method of X-ray and Auger electron associated with nuclear decay, calculation codes and flow chart are introduced briefly in this paper. Some examples of nuclear decay are taken to show its application.

2 Data calculation of X-ray

2.1 Energy of X-ray

In general, we consider single line spectrum $XK_{\alpha 2}$, $XK_{\alpha 1}$ and complex spectrum XK_{β} and XL for K- and L-shell. The single line spectrum X-ray energies of different shells are calculated from atomic-electron binding energies of different atomic shells. These atomic-electron binding energies of different shells for different elements have been evaluated and published in Ref. [1]. The XK_{β} and XL of K-and L-shell for the general uses can be obtained by using average over single line spectrum energies. The single line spectrum $XK_{\alpha 2}$ and $XK_{\alpha 1}$ energies of K-shell and complex spectrum XK_{β} and XL energies of K-and L-shell are tabulated for different elements and contained in our calculation code RADLST.

2.2 Intensity of X-ray

2.2.1 Intensity of X-ray arising from internal conversion electron emission

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2.2.1.1 Internal conversion coefficient

Assume energy of i-th γ-ray for a radionuclide is $E_{\gamma i}$, its emission probability is $P_{\gamma i}$. The internal conversion coefficients of i-th γ-ray for K-, L-, M-, and N-Shell are α_{Ki}, α_{Li}, α_{Mi} and α_{Ni}, respectively. The total internal conversion coefficient is then α_i,

$$\alpha_i = \alpha_{Ki} + \alpha_{Li} + \alpha_{Mi} + \alpha_{Ni} = \sum_n \alpha_{ni}. \quad (1)$$

The internal conversion coefficients α_{Ki}, α_{Li}, α_{Mi}, α_{Ni} and α_i can be calculated by using calculation code HSICC[2]. It is based on the theoretical internal conversion coefficients (the data tables and curves are given as functions of atomic number Z, γ-ray energy E_γ, and its multipolarity E_1, E_2, E_3, E_4 and M_1, M_2, M_3, M_4, respectively). The conversion coefficients for specific γ-ray energy are determined by fitting with cubic spline function, and a set of fitting coefficients for a given Z, E_γ and multipolarity can be gotten, and then required set of internal conversion coefficients can be calculated by using fitting coefficients.

2.2.1.2 γ-ray absolute intensity

Assume relative intensity of the i-th γ-ray is $I_{\gamma i}$, the normalization factor for converting relative intensity to absolute intensity (emission probability per 100 radionuclide decays through the γ-ray transition) is N. The absolute intensity of i-th γ-ray can be obtained from formula (2),

$$P_{\gamma i} = NI_{\gamma i}, \quad (2)$$

where value N can be calculated from evaluated experimental decay data or decay scheme by data evaluator.

2.2.1.3 Internal conversion electron absolute intensity

It is assumed that absolute emission probability of i-th γ-ray for energy E_γ is P_γ, the internal conversion coefficient is α_n(n = K, L, M, N atomic shell), the internal conversion electron emission probability is P_{en}. It can be calculated by formula (3),

$$P_{en} = P_\gamma \cdot \alpha_n = NI_\gamma \cdot \alpha_n. \quad (3)$$

From formulas (1) and (3) we can get total internal conversion electron emission probability (absolute intensity) P_e of i-th γ-ray for energy E_γ,

$$P_e = \sum_{n=K} P_{en} = \sum_{n=K} P_\gamma \cdot \alpha_n = P_\gamma \sum_{n=K} \alpha_n = P_\gamma \cdot \alpha = NI_\gamma \sum_{n=K} \alpha_n, \quad (4)$$

where α is total internal conversion coefficient.

2.2.1.4 Vacancy number of internal conversion electron emission

It is known that the emission of internal conversion electron from different atomic shells leaves vacancy. In general, their absolute emission intensity (probability) is equal to the primary vacancy number directly arising from internal conversion electron emission. Assume absolute emission probability of i-th γ-ray is $P_{\gamma i}$. The primary vacancy number for the K-and L-shell is V_{Ki} and V_{Li}, respectively. And then, they can be calculated by formulas (5) and (6),

$$V_{Ki} = P_{\gamma i}\alpha_{Ki} = NI_{\gamma i}\alpha_{Ki}, \quad (5)$$

$$V_{Li} = P_{\gamma i}\alpha_{Li} = NI_{\gamma i}\alpha_{Li}. \quad (6)$$

The total vacancy number V_K and V_L of K- and L-shell for all radionuclide decay process are from summation of all V_{Ki} and V_{Li} for i-th γ-ray, respectively.

$$V_K = \sum_i P_{\gamma i}\alpha_{Ki} = N\sum_i I_{\gamma i}\alpha_{Ki}, \quad (7)$$

$$V_L = \sum_i P_{\gamma i}\alpha_{Li} = N\sum_i I_{\gamma i}\alpha_{Li}. \quad (8)$$

In formula (8), we did not consider the fact that the vacancy number increase in L-shell when a K-shell vacancy is filled by an electron from L-shell. The vacancy transfer coefficient n_{KL} describes the mean vacancy number increase in the L-shell produced by one vacancy in the K-shell. As noted above, the V_L is called as primary vacancy directly arising from internal conversion electron emission, V_L' is called as secondary vacancy associated with filling a K-shell vacancy by an electron from L-shell. The vacancy number increase V_L' can be calculated by formula (9),

$$V_L' = n_{KL} V_K. \quad (9)$$

In formula (9), n_{KL} can be obtained from Ref. [3]. From formulas (8) and (9), the total vacancy number in L-shell V(L) can be calculated by formula (10),

$$V(L) = V_L + V_L' = N\left(\sum_i I_{\gamma i}\alpha_{Li} + n_{KL}\sum_i I_{\gamma i}\alpha_{Ki}\right). \quad (10)$$

2.2.1.5 X-ray intensity

2.2.1.5.1　$XK_{\alpha 2}$, $XK_{\alpha 1}$ and XK_{β} ray intensity of K-shell

Assume XK ray intensity for K shell is I_{XK}. The K-shell fluorescence yield $\omega_K = I_{XK}/V(K)$ (X-ray emission probability per one vacancy in K-shell) has been evaluated and published in Ref. [3]. The XK ray intensity I_{XK} for K-shell can be calculated by using formula (11) as follows,

$$I_{XK} = V_K \omega_K = N\omega_K \sum_i I_{\gamma i}\alpha_{Ki}. \qquad (11)$$

The XK ray intensity I_{XK} for K-shell can be divided into $I(K_{\alpha 2})$ and $I(K_{\alpha 1})$ for single line spectra $XK_{\alpha 1}$, and $I(K_{\beta})$ for complex spectrum XK_{β}. They are calculated by using formulas (12) and (13), respectively.

$$I_{XK} = I(K_{\alpha}) + I(K_{\beta}), \qquad (12)$$

$$I(K_{\alpha}) = I(K_{\alpha 1}) + I(K_{\alpha 2}). \qquad (13)$$

The following ratios are defined,

$$R_{\beta\alpha} = P(K_{\beta})/P(K_{\alpha}), \qquad (14)$$

$$R_{\alpha 2\alpha 1} = P(K_{\alpha 2})/P(K_{\alpha 1}), \qquad (15)$$

where $P(K_{\beta})$, $P(K_{\alpha})$, $P(K_{\alpha 2})$ and $P(K_{\alpha 1})$ are theoretical X-ray emission probabilities of XK_{β}, XK_{α}, $XK_{\alpha 2}$ and $XK_{\alpha 1}$, respectively. The values of ratios $R_{\beta\alpha}$ and $R_{\alpha 2\alpha 1}$ can be obtained from Ref. [3].

From formulas (14) and (15), the absolute emission intensities $I(K_{\alpha 2})$ and $I(K_{\alpha 1})$ of single spectra $XK_{\alpha 2}$ and $XK_{\alpha 1}$, and $I(K_{\beta})$ of complex spectrum XK_{β} can be calculated by following formulas respectively.

$$I(K_{\alpha}) = \frac{I_{XK}}{1 + R_{\beta\alpha}}, \qquad (16)$$

$$I(K_{\alpha 1}) = \frac{I(K_{\alpha})}{1 + R_{\alpha 2\alpha 1}} = \frac{N\omega_K \sum_i I_{\gamma i}\alpha_{Ki}}{(1 + R_{\alpha 2\alpha 1})(1 + R_{\beta\alpha})} \qquad (17)$$

$$I(K_{\alpha 2}) = I(K_{\alpha}) - I(K_{\alpha 1}) = \frac{I(K_{\alpha})R_{\alpha 2\alpha 1}}{1 + R_{\alpha 2\alpha 1}} = \frac{N\omega_K R_{\alpha 2\alpha 1}\sum_i I_{\gamma i}\alpha_{Ki}}{(1 + R_{\alpha 2\alpha 1})(1 + R_{\beta\alpha})}, \qquad (18)$$

$$I(K_{\beta}) = \frac{I_{XK}R_{\beta\alpha}}{1 + R_{\beta\alpha}} = \frac{N\omega_K R_{\beta\alpha}\sum_i I_{\gamma i}\alpha_{Ki}}{(1 + R_{\beta\alpha})} \qquad (19)$$

2.2.1.5.2　XL ray intensity of L-shell

Assume XL ray intensity for L shell is I_{XL}. The fluorescence yield of L-shell $\omega_L = I_{XL}/V(L)$ has been evaluated and published in Ref. [3]. The values ω_L for different elements are also obtained from Ref. [3]. As described above, X-ray absolute emission intensity of L-shell I_{XL} can be calculated by using formula (20),

$$I_{XL} = \omega_L V(L) = \omega_L(V_L + V_{L'}) = N\omega_L\left(\sum_i I_{\gamma i}\alpha_{Li} + n_{KL}\sum_i I_{\gamma i}\alpha_{Ki}\right). \qquad (20)$$

From formula (17) to (20), we can see that the relative intensities of each γ-ray, the normalization factor, internal conversion coefficients α_K and α_L, X-ray fluorescence yields ω_K and ω_L, and vacancy transfer coefficient n_{KL} must be known in order to calculate the X-ray intensities arising from internal conversion electron emission.

2.2.2　Intensity of X-ray arising from electron capture decay

2.2.2.1　Electron capture probability

When electron capture decay energy Q_ε is more than 1.02 MeV, not only ε decay but also β^+ decay will be produced. Assume relative electron capture probability to j-th level of daughter-nuclei from parent-nuclei is $P_{\varepsilon j}$, and β^+ decay relative probability to j-th level is $P_{\beta^+ j}$, respectively. The formula (21) can be obtained,

$$P_{\varepsilon j} + P_{\beta^+ j} = 1. \qquad (21)$$

Assume the relative electron capture probabilities of j-th level from K, L, M, and N atomic shells are $P_{\varepsilon Kj}$, $P_{\varepsilon Lj}$, $P_{\varepsilon Mj}$ and $P_{\varepsilon Nj}$, respectively. Formula (22) can be written as following,

$$P_{\varepsilon j} = P_{\varepsilon Kj} + P_{\varepsilon Lj} + P_{\varepsilon Mj} + P_{\varepsilon Nj} = \sum_n P_{\varepsilon nj}, \qquad (22)$$

where n = K, L, M, N atomic shell.

The relative electron capture probabilities of j-th level, $P_{\varepsilon nj}$, can be calculated by using LOGFT code[12]. The electron radial wave function data have been evaluated and included in code LOGFT as its input data file. In general, ε decay data file must be transferred into ENSDF formatted data file because ENSDF (Evaluated Nuclear Structure Data File) format is adopted in input data file of code LOGFT. We run LOGFT code and obtain relative electron capture probabilities of j-th level $P_{\varepsilon Kj}$, $P_{\varepsilon Lj}$, $P_{\varepsilon Mj}$ and $P_{\varepsilon Nj}$.

If ε decay energy Q_ε is not more than 1.02 MeV, β^+ decay will be not produced. Therefore,

$$P_{\beta^+ j} = 0 \text{ and } P_{\varepsilon j} = 1.$$

2.2.2.2 Electron capture absolute intensity

Assume relative intensity of $(\varepsilon + \beta^+)$ decay for the j-th level is $I(\varepsilon + \beta^+)_j$, the normalization factor for converting relative total intensity to absolute total intensity (emission probability per 100 radionuclide decays through the $(\varepsilon + \beta^+)$ decay) is $N(\varepsilon + \beta^+)$. The absolute total intensity $P(\varepsilon + \beta^+)_j$ of j-th level can be obtained from formula (23),

$$P(\varepsilon + \beta^+)_j = N(\varepsilon + \beta^+) I(\varepsilon + \beta^+)_j, \quad (23)$$

where value $N(\varepsilon + \beta^+)$ can be calculated from evaluated experimental decay data or decay scheme by data evaluator.

2.2.2.3 Vacancy number of electron capture decay

The vacancy number for the K- and L-shell is V_{Kj} and V_{Lj}, respectively. From formula (23), they can be calculated by formulas (24) and (25),

$$V_{Kj} = P(\varepsilon + \beta^+)_j P_{\varepsilon Kj} = N(\varepsilon + \beta^+) I(\varepsilon + \beta^+)_j P_{\varepsilon Kj}, \quad (24)$$

$$V_{Lj} = P(\varepsilon + \beta^+)_j P_{\varepsilon Lj} = N(\varepsilon + \beta^+) I(\varepsilon + \beta^+)_j P_{\varepsilon Lj}. \quad (25)$$

The total vacancy number V_K and V_L of K- and L-shell for all ε decay process is from summation of all V_{Kj} and V_{Lj} for j-th level, respectively.

$$V_K = \sum_j P(\varepsilon + \beta^+)_j P_{\varepsilon Kj} = N(\varepsilon + \beta^+) \sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon Kj}, \quad (26)$$

$$V_L = \sum_j P(\varepsilon + \beta^+)_j P_{\varepsilon Lj} = N(\varepsilon + \beta^+) \sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon Lj}. \quad (27)$$

In formula (27), we did not consider that vacancy number increase in L-shell when a K-shell vacancy is filled by an electron from L-shell. The vacancy transfer coefficient n_{KL} describes the mean vacancy number increase in the L-shell produced by one vacancy in the K-shell. The vacancy number increase associated with filling a K-shell vacancy by an electron from L-shell V'_L can be calculated by formula (28),

$$V'_L = n_{KL} V_K. \quad (28)$$

In formula (28), n_{KL} can be obtained from Ref. [3]. From formulas (27) and (28), the total vacancy number in L-shell $V(L)$ can be calculated by formula (29),

$$V(L) = V_L + V_{L'} = V_L + n_{KL} V_K = N(\varepsilon + \beta^+)\left[\sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon Lj} + n_{KL} \sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon Kj}\right]. \quad (29)$$

2.2.2.4 X-ray intensity

2.2.2.4.1 $XK_{\alpha 2}$, $XK_{\alpha 1}$ and XK_β ray intensity of K-shell

In electron capture process of radionuclide decay, not only Auger electron is ejected but also X-ray is emitted. The K-shell fluorescence yield ω_K (X-ray emission probability per one vacancy in K-shell) has been evaluated and published, and the values ω_K can be got[3]. The K-shell X-ray intensity I_{XK} is calculated by formula (30),

$$I_{XK} = V_K \omega_K = \omega_K N(\varepsilon + \beta^+) \sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon Kj}, \quad (30)$$

$$I_{XK} = I(K_\alpha) + I(K_\beta), \quad (31)$$

$$I(K_\alpha) = I(K_{\alpha 1}) + I(K_{\alpha 2}). \quad (32)$$

From formwlas (12), (13), (14) and (15), the absolute emission intensities $I(K_{\alpha 2})$ and $I(K_{\alpha 1})$ of single line spectrum $XK_{\alpha 2}$ and $XK_{\alpha 1}$, and $I(K_\beta)$ of complex spectrum XK_β can be calculated by following formulas, respectively.

$$I(K_\alpha) = \frac{I_{XK}}{1 + R_{\beta\alpha}}, \quad (33)$$

$$I(K_{\alpha 1}) = \frac{I(K_\alpha)}{1 + R_{\alpha 2\alpha 1}} = \frac{N(\varepsilon + \beta^+)\omega_K \sum_j I(\varepsilon + \beta^+) P_{\varepsilon Kj}}{(1 + R_{\alpha 2\alpha 1})(1 + R_{\beta\alpha})}, \quad (34)$$

$$K_{\alpha 2}) = I(K_\alpha) - I(K_{\alpha 1}) = \frac{I(K_\alpha) R_{\alpha 2\alpha 1}}{1 + R_{\alpha 2\alpha 1}} = \frac{N(\varepsilon + \beta^+)\omega_K R_{\alpha 2\alpha 1} \sum_j I(\varepsilon + \beta^+) P_{\varepsilon Kj}}{(1 + R_{\alpha 2\alpha 1})(1 + R_{\beta\alpha})}, \quad (35)$$

$$I(K_\beta) = \frac{I_{XK} R_{\beta\alpha}}{1 + R_{\beta\alpha}} = \frac{N(\varepsilon + \beta^+)\omega_K R_{\beta\alpha} \sum_j I(\varepsilon + \beta^+) P_{\varepsilon Kj}}{(1 + R_{\beta\alpha})}. \quad (36)$$

2.2.2.4.2　XL ray intensity of L-shell

The fluorescence yield of L-shell ω_L has been evaluated and published, and the values ω_L can be obtained[3]. As indicated above, X-ray absolute emission intensity of L-shell I_{XL} can be calculated by using following formula,

$$I_{XL} = \omega_L V(L) = N(\varepsilon + \beta^+)\omega_L\Big(\sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon L_j} + n_{KL}\sum I(\varepsilon + \beta^+)_j P_{\varepsilon K_j}\Big). \quad (37)$$

From formulas (34) to (37), we can see that the relative intensities of electron capture, their normalization factor, electron capture probabilities. X-ray fluorescence yields ω_K and ω_L and vacancy transfer coefficient n_{KL} must be known in order to calculate the X-ray intensities arising from electron capture decay.

3 Data calculation of Auger electron

3.1 Energy of Auger electron

In general, we consider complex spectrum e_{AuL} and e_{AuK} for L- and K-shell. The single line spectrum Auger electron energies of KLL, KLX and KXY, and LXL, LXX and LXY (The first letter describes shell that has the initial vacancy, the second defines the shell from which an electron fills this vacancy, and the third specifies the shell from which the Auger electron is ejected; it means that the Auger electron ejection process is two closely connected and not independent processes) are calculated from atomic-electron binding energies of different shells and sub-shells. The atomic-electron binding energies of different shells for different elements have been evaluated and published in Ref. [1]. By average over above single line spectrum energies, one obtains these Auger electron energies of complex spectrum e_{AuL} and e_{AuK} for L-and K-shell for general uses. The Auger electron energies of complex spectrum e_{AuL} and e_{AuK} of L-shell and K-shell are given in tabulated form for different elements and contained in our calculation code RADLST.

3.2 Intensity of Auger electron

The X-ray intensity calculations both for internal conversion electron emission and for electron capture decay processes have been presented above, respectively. The electron vacancy number calculation for X-ray and Auger electron for K and L shell is the same. The difference of their intensity calculation is their different emission probabilities from electron vacancy for K and L atomic shell. As known above, the X-ray emission probabilities from electron vacancy for K and L shell are ω_K and ω_L. The Auger electron emission probabilities from electron vacancy for K and L shell are $(1 - \omega_K)$ and $(1 - \omega_L)$, respectively. Therefore, the intensity calculation for Auger electron is simpler if the electron vacancy number for K and L shell is known. It is presented as follows.

3.2.1　Intensity of Auger electron arising from internal conversion electron emission

The electron vacancy number $V(K)$ for K shell is known from formula (7), the Auger electron intensity I_{AuK} for K shell can be calculated by using formula (38),

$$I_{AuK} = (1 - \omega_K)V(K) = N(1 - \omega_K)\sum_i I_{\gamma i}\alpha_{Ki}. \quad (38)$$

The electron vacancy number $V(L)$ for L shell is known from formula (10), the Auger electron intensity I_{AuL} for L shell can be calculated by using formula (39),

$$I_{AuL} = (1 - \omega_L)V(L) = N(1 - \omega_L)\cdot\Big(\sum_i I_{\gamma i}\alpha_{Li} + n_{KL}\sum_i I_{\gamma i}\alpha_{Ki}\Big). \quad (39)$$

3.2.2　Intensity of Auger electron arising from electron capture decay

The electron vacancy number $V(K)$ for K shell is known from formula (26), the Auger electron intensity I_{AuK} for K shell can be calculated by using formula (40),

$$I_{AuK} = (1 - \omega_K)V(K) = (1 - \omega_K)N(\varepsilon + \beta^+)\cdot\sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon K_j}. \quad (40)$$

The electron vacancy number $V(L)$ for L shell is known from formula (29), the Auger electron intensity I_{AuL} for L shell can be calculated by using formula (41),

$$I_{AuL} = (1 - \omega_L)V(L) = (1 - \omega_L)N(\varepsilon + \beta^+)\cdot\Big[\sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon L_j} + n_{KL}\sum_j I(\varepsilon + \beta^+)_j P_{\varepsilon K_j}\Big].$$

4 Calculation codes and flow chart

The data calculation codes for X-ray and Auger electron arising from internal conversion electron emission and electron capture decay and their functions are listed in Table 1. We get it from ENSDF physics analysis codes[2], which are maintained and updated by the National Nuclear Data Center (NNDC) at Brookhaven National laboratory, USA, for the International Network of Nuclear Structure and Decay Data Evaluation. We run it normally at VAX and ALPHA computer, and PC computer. They are very useful for the nuclear structure and decay data evaluation. In Table 1, HSICC, LOGFT and RADLST codes contain other data files for their data calculation requirement.

Table 1. Codes[2] and functions of data calculation for atomic radiation arising from nuclear decay.

Code name	Main function
FMTCHK	ENSDF formatted data check
HSICC	Internal conversion coefficient calculation of α_n (n = K, L, M, N atomic shell) and α
LOGFT	Electron capture probability calculation of $P_{\varepsilon n}$ (n = K, L, M, N atomic shell)
RADLST	Energy and intensity calculation for atomic radiations
ENSDAT	Calculation data output shown in tables and drawings

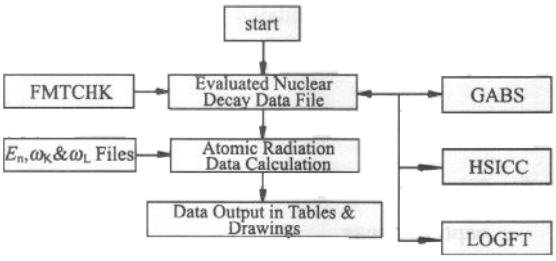

Fig.1. Flow chart of data calculation of X-ray and Auger electron.
(E_n, ω_K & ω_l files) means atomic-electron binding energies and X-ray fluorescence yields ω_K and ω_L, and vacancy transfer coefficients n_{KL} data files.

The main flow chart of data calculation of X-ray and Auger electron arising from nuclear decay is shown in Fig.1. (1) Preparation, at first the ENSDF format data file for data calculation of X-ray and Auger electron of radionuclide decay must be setup because ENSDF format of input data of calculation code is adopted. In general, atomic electron binding energy data file and X-ray fluorescence yield data file, LOGFT (electron radial wave function) data file, and internal conversion electron data file have been contained in data calculation codes. The ENSDF format check must be done before data calculation so that data calculation can be reliable. (2) Run HSICC code, internal conversion electron coefficients α_n and α are calculated and put into the ENSDF format decay data file. (3) Run LOGFT code, electron capture probabilities $P_{\varepsilon n}$ are calculated and put into the ENSDF format decay data file prepared. (4) γ-ray intensity normalization factor N is calculated and put into the ENSDF format decay data file prepared, and then γ-ray absolute intensity is calculated. (5) Electron capture intensity normalization factor $N(\varepsilon+\beta^+)$ is calculated and put into the ENSDF format decay data file prepared, and then electron capture absolute intensity $P(\varepsilon+\beta^+)_j$ can be calculated. (6) Run RADLST code, the energies and intensities of atomic radiation (X-ray, Auger electron and internal conversion electron) and other decay radiation data are calculated. (7) Calculation data output is shown in tables and drawings.

5 Application

5.1 Example 1, data calculation of X-ray and Auger electron arising from internal conversion electron emission

^{129}I β^- decay scheme[4] is relatively simple. It is taken as an example and the calculation results are given. In Table 2, the internal conversion coefficients α_K, α_L, α_M, and α are listed and calculated by HSICC code, and normalization factor $N = 1$ is given to calculate γ-ray absolute intensities. In Table 3, the calculation parameters of X-ray and Auger electron data for K- and L-shell are given. In Table 4, the radiation data of ^{129}I β^- decay are given. In Fig.2, the scheme of ^{129}I β^- decay is shown.

Table 2. γ-ray intensity and internal conversion coefficients for ^{129}I β^- decay.

E_γ/keV	I_γ	α_K	α_L	α_M	α
39.578	7.51# 23	10.4943	1.428 11	0.2882 23	12.31 1

uncertainties ("Errors"): The uncertainty in any number is given one space after the number itself. For an example, 7.51 23 means 7.51 ± 0.23. (the same in following tables)

Table 3. Calculation parameters[3] for atomic radiation data for ^{129}I β^- decay.

element	ω_K	ω_L	n_{KL}	R_{β_0}	R_{a2a1}
$_{54}$Xe	0.888 * 5	0.097 5	0.902 4	0.2327 24	0.5398 25

Table 4. Radiation data of ^{129}I β^- decay.

Radiation type	energy/keV	Absolute intensity(%)
β_1^- max	154 3	
avg	40.9 12	100
e_{AuL}	3.430	74 5
e_{AuK}	24.60	8.8 4
XL	4.11	7.9 25
$XK_{\alpha 2}$	29.458 1	19.9 9
$XK_{\alpha 1}$	29.779 1	36.9 17
XK_β	33.6	13.2 6
γ_1	39.578 4	7.51 23
e_{CeIK}	5.017 4	79 4
e_{CeIL} *	34.125 4	10.7 5
e_{CeIM}	38.436 5	2.16 10

* e_{CeIL} means internal conversion electron of γ_1 ray from L-shell.

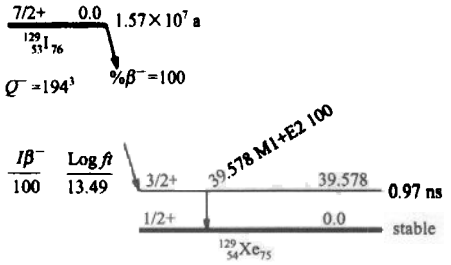

Fig.2. ^{129}I β^- decay scheme.

5.2 Example 2, data calculation of X-ray and Auger electron arising from electron capture decay

^{55}Fe ε decay scheme[5] is very simple. It is taken as an example and the calculation results are given. In Table 5, the electron capture intensity and probabilities are listed and calculated by LOGFT code, and normalization factor $N(\varepsilon + \beta^+) = 1$ is given to calculate electron capture absolute intensities. In Table 6, the calculation parameters of X-ray and Auger electron data for K- and L-shell are given. In Table 7, the radiation data of ^{55}Fe ε decay are given. In Fig. 3, the scheme of ^{55}Fe ε decay is shown.

Table 5. Electron capture intensity and probability for ^{55}Fe ε decay.

E_L/keV	$I(\varepsilon + \beta^+)$	P_{ε_K}	P_{ε_L}	P_{ε_M}	P_ε
0.0	100	0.8854	0.0975	0.01709	1.0

Table 6. Calculation parameters[3] for atomic radiation data for ^{55}Fe ε decay.

element	ω_K	ω_L	n_{KL}	R_{β_0}	R_{a2a1}
$_{25}$Mn	0.321 5	0.0047 7	1.478 4	0.1359 14	0.5099 25

Table 7. Radiation data of ^{55}Fe ε decay.

Radiation type	Energy/keV	Radiation intensity(%)
EC_1		100.
e_{AuL}	0.610	140 4
e_{AuK}	5.19	60.1 3
XL	0.640	0.42 1
$XK_{\alpha 2}$	5.888 1	8.24 11
$XK_{\alpha 1}$	5.899 1	16.29 12
XK_β	6.49	3.29 7

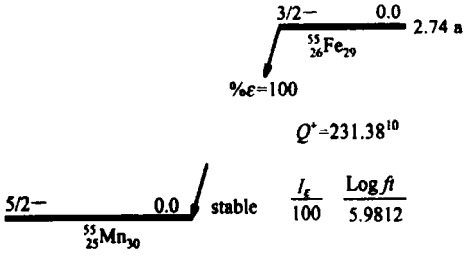

Fig.3. ^{55}Fe ε decay scheme.

6 Discussion

How to calculate the total intensity of X-ray and Auger electron arising from internal conversion electron emission and electron capture decay is interesting. As described above, the independent X-ray intensity calculations arising from internal conversion electron emission and electron capture decay have been introduced, respectively. Therefore, the total intensity calculation of X-ray and Auger electron arising from internal conversion electron emission and electron capture decay is simpler. It is equal to sum of both X-ray intensities and both Auger electron intensities, respectively.

7 Summary

In this paper, the physics formulas of data calculation of X-ray and Auger electron arising from internal conversion electron emission and electron capture decay are derived, calculation codes and flow chart are also present-

ed. Some examples for data calculation of atomic radiation are given. The X-ray and Auger electron data are very important for nuclear medical science, nuclear technology application and so on. For an example, radiotherapy is a major medical treatment for cancer. The accurate nuclear data are required for nuclear data application. It may be helpful for interesting readers to get some data from this paper.

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核衰变产生的X射线和俄歇电子数据计算

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摘要 核衰变过程中,内转换电子发射和电子俘获能在原子电子壳层内留下空穴.其他原子电子壳层的电子将填补这些空穴,其原子电子位置将重排,并发射X射线和俄歇电子.X射线和俄歇电子的能量由原子电子结合能计算得到,X射线和俄歇电子的强度分别由内转换电子发射和电子俘获在原子电子壳层内留下的空穴数,X射线荧光产额,和空穴转移系数计算得到.本文简要介绍核衰变产生的X射线和俄歇电子数据的计算方法、计算程序与工作流程,并以核衰变为例说明其具体应用和简要讨论与总结.

关键词 X射线 俄歇电子 数据计算 核衰变

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