Utilizing BP Neural Networks to Accurately Reconstruct the Tritium Depth Profile in Materials for BIXS

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Abstract

β-ray-induced X-ray spectroscopy (BIXS) is a promising method for tritium detection in solid materials because of its unique advantages, such as large detection depth, nondestructive testing capabilities, and low requirements for sample preparation. However, high-accuracy reconstruction of the tritium depth profile remains a significant challenge for this technique. In this study, a novel reconstruction method based on a backpropagation (BP) neural network algorithm that demonstrates high accuracy, broad applicability, and robust noise resistance is proposed. The average reconstruction error calculated using the BP network (8.0%) was much lower than that obtained using traditional numerical methods (26.5%). In addition, the BP method can accurately reconstruct BIX spectra of samples with an unknown range of tritium and exhibits wide applicability to spectra with various tritium distributions. Furthermore, the BP network demonstrates superior accuracy and stability compared to numerical methods when reconstructing the spectra, with a relative uncertainty ranging from 0 to 10%. This study highlights the advantages of BP networks in accurately reconstructing the tritium depth profile from BIXS and promotes their further application in tritium detection.

Full Text

Preamble

Accurate Reconstruction of Tritium Depth Profiles in Materials Using BP Neural Networks for BIXS

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β-ray-induced X-ray spectroscopy (BIXS) is a promising method for tritium detection in solid materials due to its unique advantages, including large detection depth, nondestructive testing capabilities, and minimal sample preparation requirements. However, high-accuracy reconstruction of the tritium depth profile remains a significant challenge for this technique. This study proposes a novel reconstruction method based on a backpropagation (BP) neural network algorithm that demonstrates high accuracy, broad applicability, and robust noise resistance. The average reconstruction error calculated using the BP network (8.0%) was substantially lower than that obtained using traditional numerical methods (26.5%). Additionally, the BP method can accurately reconstruct BIX spectra from samples with an unknown range of tritium and exhibits wide applicability to spectra with various tritium distributions. Furthermore, the BP network demonstrates superior accuracy and stability compared to numerical methods when reconstructing spectra with relative uncertainties ranging from 0 to 10%. This study highlights the advantages of BP networks in accurately reconstructing tritium depth profiles from BIXS data and promotes their further application in tritium detection.

Keywords: β-ray-induced X-ray spectroscopy, Tritium detection, BP network, Ridge regression, Reconstruction problem

Introduction

The development of nondestructive detection techniques for measuring tritium content and distributions in solid materials is essential for understanding tritium permeation processes in fields such as fusion research [1–8]. Among such methods, β-ray-induced X-ray spectroscopy (BIXS) offers distinct advantages, including large detection depth, low sample requirements, and convenient testing procedures [9–16]. The β-rays emitted from tritium excite X-ray emission from the base materials and testing gas, and the resulting X-ray spectrum contains information about the tritium depth profile in the materials. However, reconstruction of the tritium depth profile using BIXS presents a significant challenge due to its underdetermined, nonlinear, and ill-posed nature, which must be urgently addressed for further application of BIXS [17].

Numerous studies have reconstructed tritium depth profiles from BIXS using classical numerical methods. Matsuyama et al. employed a semi-empirical formula to calculate theoretical BIX spectra based on various assumed tritium distributions, then inferred the tritium depth profiles by comparing calculated and measured BIX spectra [18]. However, this reconstruction method struggles to handle BIX spectra with complex tritium distributions and fails to address the ill-posed nature of the inverse problem. An et al. utilized Monte Carlo methodology to simulate BIX spectra and introduced the Tikhonov regularization method, also known as ridge regression, to reconstruct the tritium depth profile [19]. The reconstruction error ranged from 2% to 40% with varying relative uncertainties and regularization codes, and the accuracy of the reconstruction results depended on the accuracy of testing. Furthermore, BIXS data obtained from samples with an unknown tritium distribution depth cannot be resolved using this method. Therefore, developing a reconstruction method with higher accuracy and broader applicability is necessary to improve the tritium detection capability of BIXS.

Classical numerical methods for BIXS reconstruction, such as ridge regression, inevitably face ill-posed equations. In contrast, an artificial neural network (ANN) algorithm may bypass this difficulty by directly modeling the complex and nonlinear relationships between the tritium depth profile and X-ray spectrum [20–23]. This capability can significantly improve the reliability and accuracy of reconstruction [24–26]. Numerous studies have highlighted the advantages of ANN algorithms in addressing inverse and unfolding problems in radiation detection [27–33]. Bagherzadeh-Atashchi et al. developed an ANN model to unfold the neutron energy spectrum and achieved a final error of less than 10% [34]. Jorge et al. utilized a multilayer perceptron (MLP) neural network to reconstruct linear accelerator spectra and achieved high concordance between 92% and 96% [35]. Given the analogous nature of various radiation detection reconstruction challenges, employing the ANN algorithm holds promise for achieving high-accuracy reconstruction of BIXS.

In this study, we propose a high-accuracy reconstruction approach for BIXS based on an ANN algorithm. Owing to their wide-ranging applicability, a back-propagation (BP) neural network was constructed and trained to reconstruct tritium depth profiles from BIX spectra. A Monte Carlo model was developed to simulate BIX spectra as a training database for the BP network. The number of neurons in the hidden layer of the network was optimized to minimize reconstruction errors. The reconstruction accuracies of the tritium depth profiles obtained from the BP network and traditional ridge regression were then compared using different distribution profiles. The BP network reconstruction algorithm achieved a lower average error of 8.0% compared to ridge regression, which had an average error of 26.5%. This was attributed to the high applicability of the BP network to different types of distributions and its ability to solve the BIX spectra of samples with an unknown range of tritium. The results of this study demonstrate the great potential of the ANN algorithm as a high-accuracy reconstruction method for BIXS.

II. Methods

A. Monte Carlo Simulations of BIXS

Training an ANN requires large amounts of BIXS data, including X-ray spectra and corresponding tritium depth profiles. However, this is difficult due to the challenges in controlling tritiated samples. Therefore, a Monte Carlo model was built using Geant4 code to simulate BIX spectra, which has been proven to be highly accurate in previous studies [4, 9, 36]. The left side of Fig. 1(a) shows a schematic of a BIXS device based on a silicon drift detector (SDD), which are known for their high sensitivity to soft X-rays. This type of detector is commonly employed in BIXS studies [12, 36].

The geometry of the SDD used in our model was based on an AXAS-D-H30 SDD manufactured by KETEK. The SDD had a diameter of 7 mm and thickness of 500 µm. The beryllium window on the SDD had a thickness of 8 µm. A tritiated sample was placed on a sample holder, and a collimation ring with an inner diameter of 10 mm was used to standardize the X-ray emission area. The entire system was placed in a sample chamber.

The corresponding model built in Geant4 is shown on the right-hand side of Fig. 1(a), encompassing all the primary components of a practical BIXS device to enhance the precision of the simulation. Tritium atoms were set in the sample region and generated using the G4GeneralParticleSource module. The tritium decay process was simulated using the G4RadioactiveDecayPhysics module, and the electron energy spectrum was set to the default Geant4 value. The energy range of β particles emitted from the tritium was 0–18.6 keV, with an average energy of 5.7 keV. The β particles were emitted isotropically in all directions within a 4π solid angle. The electromagnetic interactions between the electrons and materials were simulated using the PENELOPE model implemented in Geant4. Fluorescent X-rays and Auger transitions were considered in the simulations to enhance the accuracy of the calculated BIX spectra. The SDD shape was designated as the sensitive volume, and the BIX spectra were obtained by analyzing the energy distribution of the X-rays penetrating the SDD using the G4AnalysisManager module. The cutoff energy of the particles simulated in Geant4 was set at 100 eV, and the cutoff length was set at 10 nm to ensure high simulation accuracy.

The atmosphere in the BIXS system and the distance between the surface of the SDD and the sample were optimized using a model built in Geant4. Fig. 1(b) shows the calculated BIX spectra of a tritiated titanium sample under various atmospheres, including helium, nitrogen, neon, argon, and krypton gases. Each spectrum was simulated using 10^8 electrons in Geant4 and divided into 186 bins ranging from 0 keV to 18.6 keV. Most β particles emitted by the tritium stopped in the titanium sample, resulting in the generation of characteristic X-rays and bremsstrahlung. Therefore, all the X-ray spectra show two characteristic peaks at 4.5 keV and 4.9 keV, corresponding to the Kα and Kβ lines of titanium. The β-rays emitted from tritium at a superficial depth exit the sample and excite X-rays from the atmospheric gas. The BIX spectra obtained from atmospheres of helium, nitrogen, and neon exhibited only two characteristic titanium peaks because the characteristic X-ray energies of these gases are considerably low, typically below 1 keV. Consequently, the beryllium window absorbs these characteristic X-rays, causing the lack of corresponding peaks. The characteristic X-ray energy of krypton is very high at 12.6 keV; however, the efficiency of exciting krypton gas is hindered by the low energy of the β particles emitted by tritium. The characteristic X-ray energy of argon is moderate at 2.96 keV, leading to a distinct peak in the BIX spectrum, as shown in Fig. 1(b). The intensity of the characteristic peak of the atmospheric gas reflects information about tritium in the shallow regions of the sample, which is essential for reconstruction. Therefore, argon was selected as the testing environment, consistent with most previous studies [14, 36, 37]. Fig. 1(c) shows the energy deposition ratio of β particles emitted by tritium in argon at 1 atm. The energy of the β particles deposited in the argon gas decays exponentially, and a 5 mm-thick layer of argon gas can fully absorb the energy. Therefore, the distance between the surface of the SDD and the sample was set to 5 mm to convert all the β particle energy into characteristic X-rays. The Monte Carlo simulations described in the following section used the same settings.

B. Construction of Training Dataset

Fig. 2(a) shows the calculated BIX spectra of a tritiated titanium sample as a function of tritium depth. The parameters of the BIXS device were the same as those described above. The BIX spectra of Layers 1–20 were calculated when tritium was evenly distributed in each layer. The ith layer represents the distribution of tritium within the range from (i − 1) µm to i µm. Only the first ten layers are shown in Fig. 2(a). The total number and thickness of the layers could be adjusted based on the specific requirements of the BIXS test. All X-ray spectra show two characteristic peaks at 4.5 keV and 4.9 keV, corresponding to the Kα and Kβ lines of titanium, as shown in Fig. 1(b). Additionally, the total count of the X-ray spectra decreases as the depth of the layer increases because a portion of the X-rays generated inside the titanium was self-absorbed by the sample. Greater tritium depth results in a reduced proportion of detected X-rays. X-rays with lower energies exhibited a greater degree of self-absorption, leading to rapid changes in BIX spectrum shape on the low-energy side. The BIX spectrum of Layer 1 shows an additional characteristic peak at 3.0 keV, corresponding to the Kα line of argon. As mentioned above, β-rays emitted from tritium in shallower layers exit the sample and excite X-rays from the argon, whereas those emitted in deeper layers are absorbed by the sample, resulting in the absence of the characteristic argon peak.

The final BIX spectrum contains information about tritium at different depths with different weights and can be obtained using the following equation:

S(E) = (cid:88) f (i)Si(E)

where S(E) is the final X-ray spectrum obtained from the BIXS device, f(i) is the relative tritium content at the ith layer (i.e., the value of the probability distribution function f(x) when x = i), and Si(E) is the BIX spectrum with tritium distributed at the ith layer, as shown in Fig. 2(a). Four different tritium distribution functions were used to replicate practical depth profiles of tritium in samples, as shown in Fig. 2(b). The first two functions describe distributions caused by tritium diffusion, and the last two describe tritium implantation [38–41]. These four functions represent steady-state diffusion, unsteady-state diffusion, single-energy implantation, and dual-energy implantation of tritium. The specific probability distribution function for each type is described by Equations

2–5:

$f_1(x) = kx + b$
$f_2(x) = k[1 - erf(bx)] + c$
$f_3(x) = exp(- (x - u)^2) + c$
$f_4(x) = exp(- exp(- (x - u_1)^2 (x - u_2)^2) + c$

where k, b, σ, u, and c are coefficients that determine the detailed depth profiles, and erf is the Gaussian error function. These four distributions were selected with equal probability to generate the corresponding final BIX spectrum using Eq. (1). Additionally, the coefficients in each distribution were randomly selected within a reasonable range to ensure that each BIX spectrum corresponded to a unique depth profile shape. The detailed range of each coefficient is provided in Table 1 . The final randomly generated probability distribution function was normalized to ensure that the total probability equaled one. The generated database was used to train the BP network and test the reconstruction accuracy of both the network and ridge regression.

C. Structure of the BP Network

Fig. 3 [Figure 3: see original paper] shows the structure of the BP network used in this study for BIXS reconstruction. It consisted of three layers: input, hidden, and output. The input layer contained 186 neurons, each corresponding to one of the 186 bins in the BIX spectrum. The output layer contained 20 neurons representing the values of the probability distribution function within the range 0–20 µm. The three layers in the network were fully connected, meaning that each neuron in the previous layer was connected to all neurons in the next layer. The network was trained using an error backpropagation algorithm. The training process of a BP network optimizes the connection coefficients to minimize error, which helps the network accurately establish nonlinear relationships between tritium depth profiles and BIX spectra.

The BP network was written in Python 3 using the PyTorch library. A sigmoid function was used as the activation function, introducing nonlinearity into the BP network and enabling it to effectively model a wide range of curves. Sigmoid functions are commonly used nonlinear functions that transform input values into a range between zero and one, making them well-suited for models where outputs represent probabilities. Since the network in this study was required to output the tritium depth profile, which reflects the probabilities of relative tritium contents at different depths, a sigmoid function was used as the activation function. The mean square error (MSE) was used as the loss function to calculate the average of the squares of errors between predicted values and actual labels. MSE is commonly employed in regression problems where it is essential to model and analyze relationships between variables. Since the tritium depth profile was reconstructed based on the relative intensity of each bin in the BIX spectrum, MSE was utilized to enhance the performance of the BP network. Additionally, because the reconstruction of tritium depth profiles from BIXS requires consideration of data along with their corresponding relative uncertainties, the adaptive moment estimation algorithm (Adam) was used as the optimization algorithm, chosen for its suitability in handling datasets with significant volume and noise.

TABLE 1. Ranges of the coefficients used in the four distribution functions

Function 1	Function 2	Function 3	Function 4
Coefficient Range	Coefficient Range	Coefficient Range	Coefficient Range
k: $(-0.08, 0)$	k: (0, 1)	σ: (1, 10)	u_1: (0.4, 0.6)
b: (0.05, 0.4)	b: (0.05, 0.7)	u: (1, 5)	u_2: (1, 5)
c: (0, 0.01)	c: (0, 0.01)	c: (0, 0.01)	c: (0, 0.01)

III. Results and Discussions

A. Training of the BP Network

Fig. 4(a) shows the trend of training and testing MSE obtained by the BP network with 5000 hidden neurons as training epochs progressed. Ten thousand pairs of different probability distribution functions and BIXS spectra were generated to train the BP network, with the training and testing datasets set at a 7:3 ratio. The BP network was trained using a single GPU with an FP32 performance of 30 TFLOPS for 10 hours. The results illustrate a rapid initial decrease in MSE, followed by leveling off in both training and testing datasets. The MSE obtained using the BP network barely decreased after 200 epochs. The strong convergence of the BP network demonstrates its effectiveness in learning BIXS data and establishing a correlation between BIX spectra and tritium depth profiles. Moreover, the MSE obtained for both datasets exhibits minimal divergence as the number of epochs increases, indicating no overfitting during the training process.

The performance of the trained BP network was subsequently evaluated based on the average error in reconstructing the tritium depth profile (δ) as defined by the following equation presented by Long and An [19]:

δ = (cid:80)M (cid:80)M × 100 i=1 |arec,i − aori,i| i=1 aori,i

where arec,i and aori,i are the reconstructed and original probability distribution values at the ith layer, respectively. The value of δ obtained by the BP network with 5000 hidden neurons was 11.4%. This can be further improved by increasing the number of hidden neurons, which is the primary parameter affecting the fitting capability of the BP network. Fig. 4(b) shows the average reconstruction errors of the trained BP network in the training and test datasets plotted against the number of hidden neurons. As the number of hidden neurons increased from 5000 to 40000, the value of δ decreased from 11.4% to 8.0% at a decreasing rate of change. This result demonstrates the effectiveness of increasing hidden neurons in reducing reconstruction errors. However, a substantial increase in hidden neurons does not lead to a significant reduction in reconstruction error, as shown in Fig. 4(b). The values of δ obtained in the training and test datasets were very close for each BP network, implying no overfitting with the addition of hidden neurons and indicating the outstanding quality of the BP network. Consequently, a BP network with 40000 hidden neurons was used for subsequent reconstruction tests and compared to traditional numerical methods.

B. Comparison of Reconstruction Accuracy

Fig. 5(a) shows box charts for reconstruction errors calculated using the BP network and ridge regression. The charts present the mean value, median value, and 25%–75% and 5%–95% ranges of the 3000 errors calculated using the testing dataset. The ridge regression method was implemented using the RidgeCV model from the SciPy library. Ridge regression is an improved least-squares method where the tritium depth profile was calculated using the following equation:

x = (ST 20S20 + αI T 20)−1ST 20S(E)

where x is the tritium depth distribution vector, S_{20} is a matrix containing the BIX spectra from Layers 1 to 20, α is the ridge coefficient, and I_{20} is a unit matrix. The optimal ridge coefficient for each BIX spectrum was automatically selected using a cross-validation method in the RidgeCV model. The average error of tritium depth profiles reconstructed by the BP network was 8.0%, significantly smaller than that calculated by ridge regression (26.5%). Additionally, the standard deviation of δ calculated by the BP network was smaller than that of ridge regression, indicating greater reconstruction reliability.

Fig. 5(b) illustrates detailed reconstruction errors of BIX spectra using four different distribution functions calculated by both methods. The BP network outperformed ridge regression across all distributions. The average reconstruction errors for BIX spectra with steady-state diffusion, unsteady-state diffusion, single-energy implantation, and dual-energy implantation distributions calculated using the BP network were 5.5%, 3.5%, 6.3%, and 17.6%, respectively. The corresponding errors calculated using ridge regression were 19.2%, 25.5%, 26.7%, and 36.1%. The dual-energy implantation distribution was the most difficult to reconstruct, as both methods exhibited their largest errors when solving this distribution.

One reason for the smaller reconstruction error in the BP network is its ability to address BIX spectra from samples with an unknown range of tritium. Figs. 5(c) and 5(d) show reconstruction results obtained using both methods compared to original set values. Both distributions were steady-state distributions. The sample shown in Fig. 5(c) had a 20-µm tritium distribution range, meaning all values of the probability distribution function were positive. The reconstruction error for this sample calculated using ridge regression (4.6%) was very close to that calculated using the BP network (4.2%). The ridge regression method demonstrated the ability to effectively solve BIX spectra from samples with a known tritium depth range. However, the sample shown in Fig. 5(d) had an unknown distribution range, implying some probability values were zero. The reconstruction error for this sample calculated by ridge regression (27.4%) was much larger than that of the BP network (1.6%). Consequently, the average reconstruction error and standard deviation obtained using ridge regression were much higher than those obtained using the BP network, as shown in Fig. 5(b). The presence of zeros in the probability distribution functions complicates resolution of an ill-posed system of equations using ridge regression. Simultaneously, the strategy of randomly selecting distribution function coefficients generated a substantial training dataset for the BP network, which aids the network in capturing nonlinear relationships between X-ray spectra and tritium depth profiles with various ranges.

Another advantage of the BP network in BIXS reconstruction is its broad applicability to various types of tritium distributions, particularly its ability to address complex tritium depth profiles. The dual-energy implantation distribution was the most complicated distribution used in this study, and the average reconstruction errors for this distribution using the BP network and ridge regression were the highest among all four distributions, as shown in Fig. 5(b). Fig. 5(e) shows a reconstruction example with the dual-energy implantation distribution obtained from the BP network and ridge regression, compared to the set value. The reconstruction error for this sample calculated by the BP network (6.0%) was remarkably lower than that of ridge regression (31.4%), indicating the ability of the BP network to reconstruct BIX spectra with complex tritium depth profiles.

The broad applicability of the BP network was also reflected in its ability to accurately reconstruct mixed BIX spectra, indicating that at least two types of tritium depth profiles were present in the sample. Fig. 6 shows an example of reconstruction results for BIX spectra mixed with two different types of tritium distribution functions using a BP network. Fig. 6(a) shows the two original tritium depth profiles, one belonging to the single-energy implantation distribution (Distribution 1) and the other to the steady-state distribution (Distribution 2). The reconstruction errors for these two distributions using the BP network were 7.6% and 4.0%, respectively. A mixed BIX spectrum was generated by combining these two tritium distribution functions in different ratios, as described by the following equation:

fm(x) = (cid:88) akfk(x)

where fm(x) is the mixed tritium depth profile, fk(x) is the kth independent tritium depth profile, ak is the ratio of the kth tritium depth profile, and n is the total number of tritium depth profiles (n = 2). The mixed tritium depth profile was further normalized, and the mixed BIX spectrum was calculated using Eq. (1). Fig. 6(b) shows reconstruction errors obtained from mixed BIX spectra using the BP network plotted against the ratio of Distribution 2. The reconstruction error consistently remained below 10% across a ratio range of 0–100%, highlighting the high reconstruction accuracy of the BP network on mixed BIX spectra. A peak reconstruction error was observed around the 50% ratio position, where the mixed BIX spectrum exhibited the most significant deviation from the two original BIX spectra. The insets in Fig. 6(b) show the mixed tritium depth profiles with 25%, 50%, and 75% ratios of Distribution 2 along with corresponding reconstruction results and detailed errors. As the ratio of Distribution 2 increased, the peak of the mixed tritium depth profile became indistinct, and the tail of the curve became linear. When the ratios of the two distribution functions were equal, the mixed tritium depth profile exhibited characteristics of both functions. The reconstructed tritium depth profiles (scatter plots) were very close to the true values, with reconstruction errors of 6.0%, 8.3%, and 6.4% at the specified ratios when using the BP network. Despite the absence of information regarding these mixed spectra in the training dataset, the BP network demonstrated high accuracy in reconstructing these spectra. This result convincingly demonstrates the broad capability of the BP network to reconstruct BIX spectra with various tritium depth distributions.

C. Comparison of Noise Resistance

Noise resistance is another crucial figure of merit for reconstruction methods, reflecting the accuracy and stability of results when BIX spectra contain additional relative uncertainties. Gaussian noise of varying intensity was added to the dataset to emulate measurement uncertainty. A dataset containing BIX spectra with 0–10% relative uncertainty was used to train the BP network. Fig. 7(a) shows the trend of training and testing MSE obtained by the BP network with 40000 hidden neurons as a function of epoch. The trend in MSE obtained with a dataset containing 0–10% Gaussian noise closely resembles the pattern depicted in Fig. 4(a). The MSE of the BP network continued to exhibit significant convergence with increasing epochs, demonstrating the effectiveness of the BP network in modeling the correlation between tritium depth profiles and BIX spectra despite varying levels of noise interference. The addition of relative uncertainties increased variability of convergence, thereby inducing fluctuations in the MSE curve of the testing dataset. Additionally, the consistency of MSE in the training and testing datasets did not exhibit the same level of perfection as shown in Fig. 4(a); however, the specific disparity was less than 10%, indicating an ideal fit of the BP network to the dataset with 0–10% relative uncertainty.

Fig. 7(b) presents reconstruction errors of the tritium depth profile calculated using the BP network and ridge regression as functions of the relative uncertainty of BIX spectra. Each point was obtained by calculating the average and standard deviation of 10000 reconstruction errors. When the relative noise of BIX spectra increased from 0% to 10%, the average reconstruction errors calculated by the BP network increased from 8.0% to 23.2%, which is a much lower range than that of ridge regression, which increased from 26.5% to 56.0%. Additionally, the standard deviation of errors calculated by the BP network barely increased with increasing noise, whereas those of ridge regression significantly increased from 14.5% to 37.7%. The detailed averages and standard deviations of errors obtained using both methods are listed in Table 2 . This result demonstrates the high noise resistance of the BP network method, which is extremely important for practical BIXS applications.

TABLE 2. Averages and standard deviations of errors calculated by the BP network and ridge regression as a function of the relative uncertainty of BIX spectra

Relative uncertainty (%)	BP network	Ridge regression
	Average errors	Standard deviation
0	8.0%	4.2%
2	11.3%	4.5%
4	14.7%	4.8%
6	18.1%	5.2%
8	20.7%	5.5%
10	23.2%	5.9%

Fig. 8 [Figure 8: see original paper] shows a detailed example of how additional noise in the BIX spectrum affects reconstruction results obtained by the BP network and ridge regression. Fig. 8(a) shows the initially calculated BIX spectrum of a tritiated titanium sample with a single-energy implantation distribution of tritium compared to BIX spectra incorporating 5% and 10% Gaussian noise. The BIX spectra are presented in semi-logarithmic coordinates, and it is apparent that the addition of relative uncertainty did not change the shape of the BIX spectra. The major effect of relative uncertainty was an alteration in the intensity ratio between the characteristic peak and bremsstrahlung. Since the intensity of the characteristic peak was significantly higher than that of the bremsstrahlung, the relative uncertainty resulted in more pronounced absolute intensity fluctuations in the characteristic peak. As mentioned in Figs. 1 and 2, the characteristic peak of argon indicates relative tritium content in the superficial layer beneath the sample surface, and fluctuation of this peak caused by additional Gaussian noise is likely to result in larger reconstruction errors.

Figs. 8(b–d) show true and calculated tritium depth profiles using the BP network and ridge regression, reconstructed from the original BIX spectrum, BIX spectrum with 5% Gaussian noise, and BIX spectrum with 10% Gaussian noise, respectively. The reconstruction errors from the original BIX spectrum using the BP network and ridge regression were 4.1% and 8.5%, respectively, as shown in Fig. 8(b). The reconstructed tritium depth profile calculated using the BP network fits well with the true profile; the type of tritium distribution function could be clearly identified, and the peak position of the tritium depth distribution was consistent with set values. In contrast, the reconstruction error of the tritium depth profile calculated using ridge regression was slightly larger.

The relative tritium distribution contents in the superficial layer of the samples calculated using ridge regression were close to the set value, while those in the deeper region had slightly larger deviations. In this example, the difference in reconstruction errors calculated using the two methods was not significant when no additional Gaussian noise was present.

When the BIX spectrum contained 5% Gaussian noise, reconstruction errors for the tritium depth profile calculated using both the BP network and ridge regression increased, as shown in Fig. 8(c). The reconstruction error calculated using the BP network increased to 10.3%, which remains within an acceptable range, and the type of tritium distribution function could still be identified from the reconstructed profile. Meanwhile, the reconstruction error calculated using ridge regression increased significantly to 32.3%, and the tritium distribution function could not be clearly discerned between single-energy implantation and unsteady-state diffusion. The disparity in reconstruction error became more pronounced as the relative uncertainty of the BIX spectrum increased to 10%, as shown in Fig. 8(d). The BP network demonstrated robust resistance to noise, as evidenced by a reconstruction error of 17.1%. The reconstructed tritium depth profile remained reliable, and the tritium distribution function could be identified. In contrast, the reconstruction error calculated using ridge regression increased to 59.2%, and the calculated tritium depth profile exhibited a high degree of chaos, including negative values. The example shown in Fig. 8 clearly demonstrates the feasibility of training a BP network with robust noise resistance using a BIXS dataset with preset relative uncertainties. This also highlights the advantage of the BP network in accurately and stably reconstructing BIX spectra with specific levels of relative uncertainty.

The findings of this study were based on simulated BIXS data. A crucial factor in validating the accuracy of the BP network method in practical measurements is guaranteeing the accuracy of the simulated BIX spectra. We intend to measure BIX spectra using standard tritiated samples and calibrate the simulated data. Finally, the calibration coefficients will be used to generate a high-accuracy BIXS database. Different networks are required for various types of base materials and layer spacings. Selecting an appropriate number of hidden layers within the convergence region guarantees high reconstruction accuracy. The upper limits of the BP network method in BIXS applications lie in its noise resistance, as additional uncertainty in practical BIXS measurements is inevitable. The uncertainty caused by uneven planar distribution and X-rays emitted from activation products in the sample should be considered in future studies.

IV. Conclusion

In conclusion, this study demonstrated a highly accurate and reliable reconstruction method for BIXS using a BP network algorithm. A Monte Carlo model was built to simulate BIX spectra, and four different tritium distribution functions with random coefficients were incorporated to generate a training database for the BP network. The number of neurons in the hidden layer of the BP network was optimized to minimize reconstruction errors. The BP network method demonstrated higher accuracy, broader applicability, and greater noise resistance than the traditional ridge regression method. The average reconstruction error calculated by the BP network was 8.0%, much lower than that calculated by ridge regression (26.5%). The BP network method accurately reconstructed BIX spectra from samples with an unknown range of tritium and outperformed ridge regression across all distribution types. Moreover, the BP network retained higher accuracy and stability than ridge regression with increasing relative uncertainty of BIX spectra. Our study explored a novel approach for BIXS reconstruction and demonstrated the potential of BIXS for detecting tritium depth profiles in solid materials.

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Note: Figure translations are in progress. See original paper for figures.