UDK 543.428.2:544.171.7
Original scientific article/Izvirni znanstveni članek

ISSN 1580-2949
MTAEC9, 49(3)435(2015)

USING SIMULATED SPECTRA TO TEST THE EFFICIENCY OF SPECTRAL PROCESSING SOFTWARE IN REDUCING THE NOISE IN AUGER ELECTRON SPECTRA

UPORABA SIMULIRANEGA SPEKTRA ZA PREIZKUS UČINKOVITOSTI PROGRAMSKE OPREME PREDELAVE SPEKTRA PRI ZMANJŠANJU ŠUMA SPEKTRA AUGERJEVIH ELEKTRONOV

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Prejem rokopisa – received: 2015-01-04; sprejem za objavo – accepted for publication: 2015-01-21

doi:10.17222/mit.2015.013

When attempting to automate Auger spectra analyses it becomes necessary to have a deeper knowledge of the constituent elements of the spectra. In order to obtain a reliable analysis, the unavoidable spectral noise must be reduced, thus giving a clearer view to the spectral peaks and the spectral background. Therefore, the necessary step is to analyze the spectral noise and to find a way to evaluate the noise-reduction algorithms. A method in which simulated Auger electron spectra are used for testing the efficiency of noise-reduction routines has been proposed. The performance of noise-reduction procedures on measured spectra cannot be evaluated since the intrinsic noiseless spectra is never available for reference; therefore, the spectra were simulated and the noise-reduction routines were used on the simulated spectra. After the processing, the simulated noiseless spectrum is subtracted from the complete spectrum, leaving the remaining noise for further analysis and a comparison with the exactly known simulated noise. For each spectrum data point the noise ratios are calculated by dividing the remaining noise levels by the initial noise. When plotting the noise ratios for each respective processing route, it was found that most of the noise ratios lie in the interval –1 to +1, indicating an improvement in regard to the initial noise. Such a plot of the noise ratios offers a convenient way for assessing the efficiency of the noise-reduction routine at a glance.

Keywords: Auger electron spectroscopy, spectra simulator, spectral noise, noise reduction

Avtomatizacija postopka analize Augerjevih spektrov zahteva dobro poznanje posameznih sestavnih elementov spektra. Zanesljivost avtomatske analize je v prvi vrsti odvisna od tega, v kolikšni meri nam uspe zmanjšati spektru primešan šum, ki sicer zamegli tako spektralne vrhove kot tudi spektralno ozadje. Zato moramo najprej analizirati lastnosti šuma, primešanega spektrom, in poiskati načine za ovrednotenje delovanja orodij, ki šum zmanjšujejo. V članku predlagamo uporabo simulatorja Augerjevih spektrov, ker sicer pri izmerjenih spektrih nikoli ne poznamo oblike primešanega šuma in torej nimamo osnove za dobro ovrednotenje delovanja uporabljenih orodij. Po uporabi orodja za zmanjševanje šuma, ki deluje na simuliranem spektru, odstranimo natančno poznano spektralno ozadje in spektralne vrhove. Tako dobimo preostali šum, ki ga primerjamo z znanim začetnim šumom. V vsaki točki spektra so izračunana razmerja med začetnim in končnim šumom. Razmerja so nato prikazana v grafu in v veliki večini spektralnih točk ležijo v intervalu –1, 1. Tako dobimo vizualno predstavitev delovanja orodij za zmanjševanje šuma, ki omogoča hitro oceno učinkovitosti preizkušanega orodja.

Ključne besede: Augerjeva elektronska spektroskopija, simulator spektra, spektralni šum, zmanjševanje šuma

1 INTRODUCTION

Auger electron spectroscopy is a technique often used for the elemental characterization of the surface of conductive samples.[1–8] Apart from a high surface sensitivity,[9] due to the fact that the primary electron beam can be focused down to approximately 10 nm in diameter,[10] analyses with very good spatial resolution can also be performed. This fact makes it possible to analyze features on a nanometer scale on the surface through this technique.

To interpret the measured spectra the measured data have to be manipulated by software for signal processing. This manipulation inevitably leaves its mark on the results obtained.[11]

Smoothing is one of the methods that are used for the purpose of reducing the noise in Auger electron spectra.[12] Very little can be said about the efficiency of such procedures in reducing the noise when applying them in measured spectra, because noise in both the input and the output spectra is at unknown levels. The aim of this work is to show a simple way in which the performance of the noise-reduction techniques can be assessed using simulated spectra. Using simulated spectra to assess the efficiency of noise-reduction routines is very appropriate. This comes about due to the fact that the values for the different components of the simulated AE spectra (including the noise) are known before processing, and thus any change due to the processing route may be found and then compared to the initial preprocessed values.

2 EXPERIMENT

The construction of the simulator for gathering the simulated spectra used for this assessment is described in detail in[11]. For the construction of this simulator a number of measured AE spectra obtained from spring-steel samples were closely inspected. The neural network was used to model the primary background by selecting a number of representative points for the background and including them in the training data set for the neural network. After carefully observing the behavior of the background in the measured spectra an equation was derived, which then would be used for generating various primary backgrounds that would resemble those observed in the measured spectra. After removing the primary background defined in this way the peak base and the peaks remained. The peak base was also modeled in the same way using the neural network, and the removal of the defined peak base left only the characteristic peaks. The peak base and the peaks of various elements were saved in the database. Combining the generated primary backgrounds, on the one hand, and the peak base and characteristic peaks from the database, on the other, produced the simulated spectrum. The generated noise that was then added to such a spectrum was also made to resemble the noise observed in measured spectra. It is important to note that while the components of the simulated spectra such as the background and noise are made to resemble those of the measured spectra, their exact values are simulated and therefore known and stored in the computer (**Figure 1**).

Through the modeling of the background, which was performed using the neural network, we have found that the AE spectra consist of three main components: the primary background, the peak base, and the peaks (**Figure 2**).

From the set of standard AE spectra that were obtained using COMPRO10, a freely available online spectral database, the peak base and the peaks of elements such as Al, C, Co, Cu, Fe, Au, Ni, O, Si, Ag, Ti, and V were extracted (as shown in **Figure 3** for the case of iron) and were stored separately.

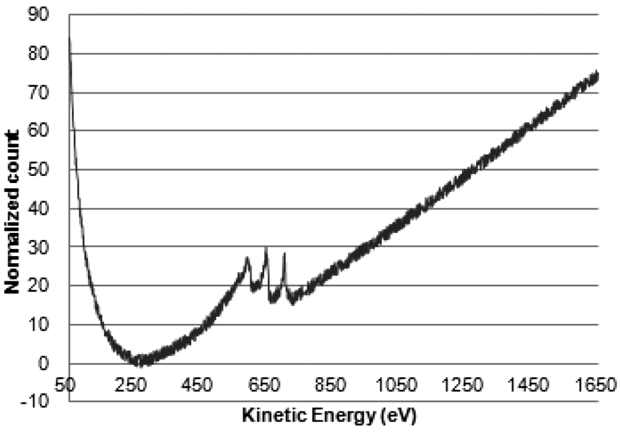

Figure 1: Simulated Auger electron spectrum
Slika 1: Simuliran spekter Augerjeve elektronske spektroskopije

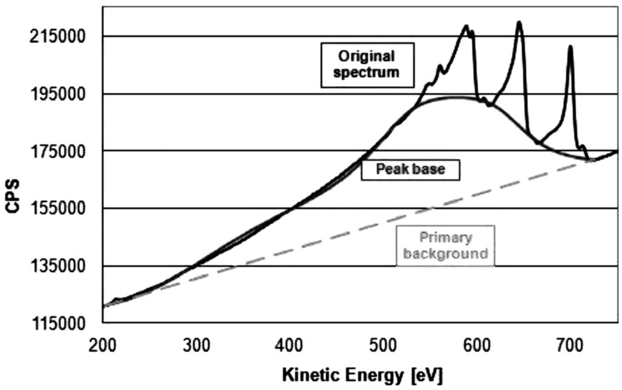

Figure 2: The AE spectra constituent elements: the primary background, the peaks base, and the peaks
Slika 2: Sestavni elementi AE-spektra: primarno ozadje, podlaga spektralnih vrhov in spektralni vrhovi

The AE spectra simulator combines the extracted peak base and the peaks from various standard elements, and it combines them with the randomly defined primary background (**Figure 4**) to form the complete simulated spectrum without the noise.

At the end of the simulation process the random noise is added and also stored separately for further use. We have ensured that the properties of the simulated noise resemble the properties of the noise in the measured AE spectra.

Other AE spectra simulators can be used for this purpose as well. One such simulator is SESSA (Simulation of Electron Spectra for Surface Analysis). SESSA is

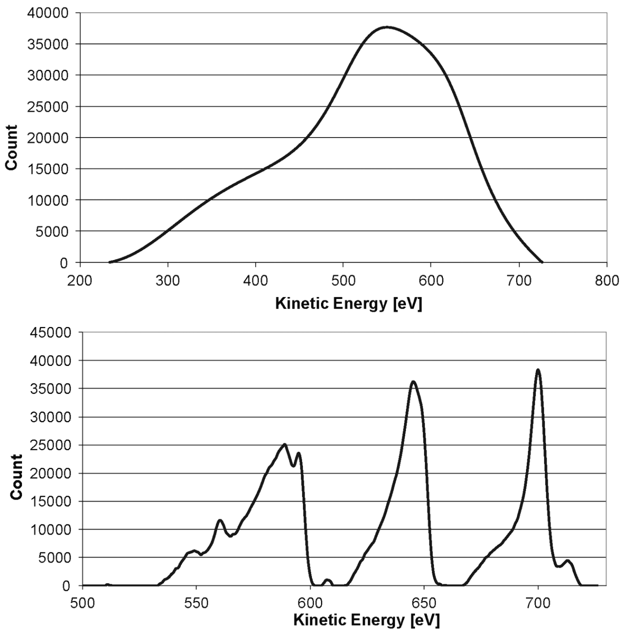

Figure 3: a) The AE spectra peak base and b) spectral peaks
Slika 3: a) Podlaga spektralnih vrhov in b) spektralni vrhovi AE-spektra

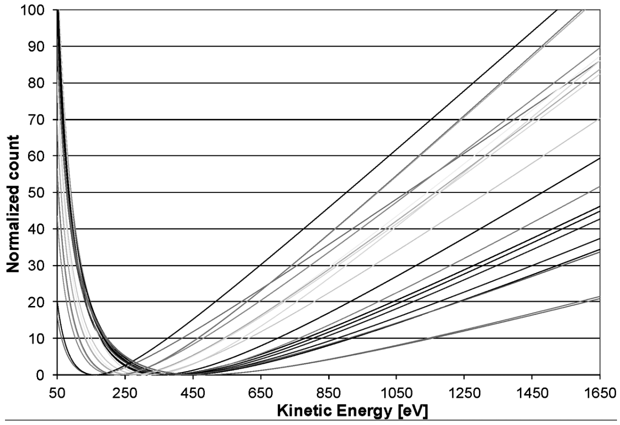

Figure 4: The randomly defined primary backgrounds
Slika 4: Naključno določena primarna ozadja

intended for facilitating the quantitative interpretation of electron spectra (Auger and XPS spectra), and therefore a lot of attention is paid to the detailed physical phenomena related to the excitation and emission of the Auger electron or photoelectron. The database of SESSA contains the data of many physical parameters needed in quantitative electron spectroscopy (AES and XPS).[13] The simulations needed for the purpose discussed in this paper do not require such detailed simulations. The key factor here is that the spectra resemble the real measured ones, and that the values of the different components of the spectra are known before the processing starts. This fact is of utmost importance for the comparison of values of any of the spectral components before and after the processing.

As mentioned in the introduction, smoothing is often used for reducing the noise in Auger electron spectra. For spectra measured with a energy step size 1 eV a 5-point averaging window is recommended.[14] Since most of the measured spectra that were used when building the simulator were of energy step size 1 eV, the same averaging window was used for processing the spectrum

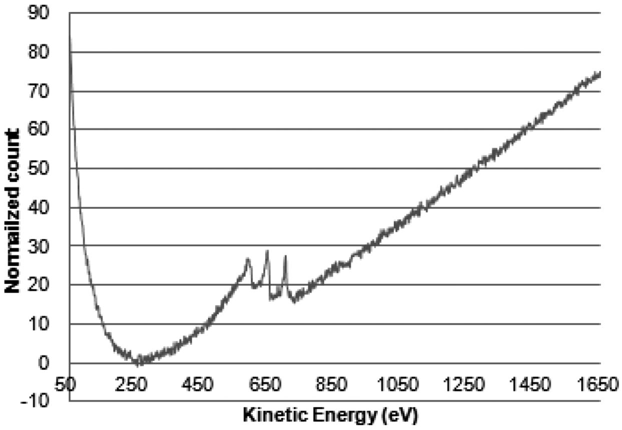

Figure 5: Processed spectrum from **Figure 1** using a 5-point window smoothing in CasaXPS
Slika 5: AE-spekter s **slike 1** po uporabljenem glajenju z oknom širine 5 točk (program CasaXPS)

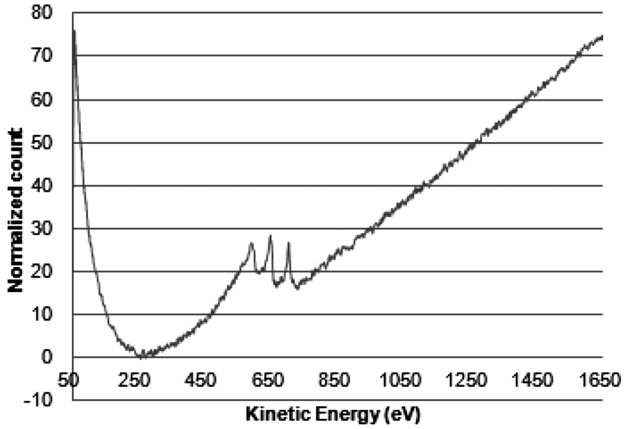

Figure 6: Processed spectrum from **Figure 1** using a notch filter in Audacity
Slika 6: AE-spekter s **slike 1** po uporabi ozkopasovnega filtra (program Audacity)

shown in **Figure 1**. The processing was performed using CasaXPS. The resulting spectrum is given in **Figure 5**.

The same simulated spectrum (**Figure 1**) was processed by applying a notch filter. The threshold frequency was selected arbitrarily for this case, just for a comparison. This procedure was completed using Audacity, where this procedure is used to reduce the noise in sound files. The resulting spectrum is given in **Figure 6**.

3 RESULTS AND DISCUSSION

After applying the smoothing procedures to the simulated spectrum, the noiseless simulated signal ($S_{\text{noiseless}}$) was subtracted from the processed spectrum ($S_{\text{processed}}$), thus obtaining the remaining noise after processing ($N_{\text{remaining}}$):

$$N_{\text{remaining}} = S_{\text{processed}} - S_{\text{noiseless}} \tag{1}$$

Such a procedure was used for obtaining the values of the remaining noise for each data point. These values were then compared to the initial simulated noise, N_{initial}, which is the random noise added to the simulated spectrum, thus obtaining the noise ratios that serve as a measure of the efficiency of the processing software in reducing the noise and bringing the signal closer to the noiseless one:

$$N_{\text{ratio}} = N_{\text{remaining}} / N_{\text{initial}} \tag{2}$$

Figure 7 illustrates the concept behind the use of the noise ratios for this kind of evaluation of the efficiency in noise reduction.

As may be inferred from **Figure 7**, when manipulating the signal for reducing the noise the obtained signal will have a new value with a different deviation from the target point, the noiseless signal. This new difference from the noiseless signal, the remaining noise, will be smaller than, equal to, or greater than that of the initial noise. Thus, for one specific data point a noise ratio of

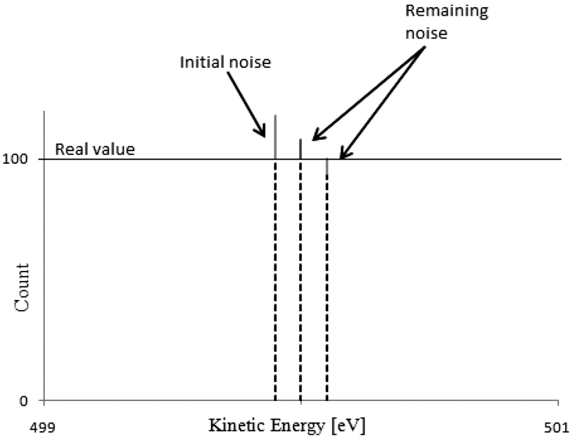

Figure 7: Concept of noise ratios as a measure of the efficiency in noise reduction

Slika 7: Koncept razmerja šumov kot merilo učinkovitosti zmanjševanja šuma

less than one means that the processing was successful in reducing the noise, a noise ratio of one means that the noise level is kept the same, and a noise ratio of more than one means that the noise level is actually increased due to the processing of the spectrum. A graphical plot of the noise ratios would serve as a quick assessment at a glance with respect to the success of the noise-reduction routine, as will be shown later on.

By using Equation (1), first the values for the remaining noise were found for each data point, and then by dividing at the respective data points according to Equation (2), the noise ratios were found and recorded in the data sheet, as shown in **Table 1** for the spectrum processed in CasaXPS, and in **Table 2** for the spectrum processed in Audacity.

By plotting the obtained noise ratios for each data point according to Equation (2), the graph obtained will give, at a glance, an indication of the improvement with regards to the noise. **Figure 8** shows such graphs for the two processing routes discussed in this paper.

Table 1: Data sheet with the noise ratios from the 5-point smoothed Auger spectrum

Tabela 1: Razmerja amplitud šumov pri glajenju spektra s 5-točkovnim povprečenjem

	A	B	C	D	E	F	G	H	I
1	Kinetic Energy	Fe Peaks	Simulated Background	Noiseles AE spectrum	Initial Noise	Complete AE spectrum	5 Point Smoothed	Remaining Noise (G-D)	Noise Ratios (H/E)
2	50	0	85.521594	85.52159	-1.29378	84.22782	84.3649	-1.1566939	0.89404339
3	51	0	83.178313	83.17831	0.421041	83.59935	83.225	0.04668741	0.11088572
4	52	0	80.927765	80.92777	-0.41938	80.50839	80.5747	-0.3530651	0.84188131
5	53	0	78.764702	78.7647	-0.88762	77.87708	78.6823	-0.0824024	0.09283547
6	54	0	76.684264	76.68426	1.545949	78.23021	77.389	0.70473584	0.45585978
7	55	0	74.681944	74.68194	0.384103	75.06605	75.3379	0.65595638	1.70776009
8	56	0	72.753556	72.75356	-0.69507	72.05849	72.2577	-0.4958559	0.71339476
9	57	0	70.89521	70.89521	-0.83461	70.0606	69.9403	-0.9549098	1.14414195
10	58	0	69.103282	69.10328	-1.16494	67.93834	67.9807	-1.1225824	0.96364053
1595	1643	0	74.301336	74.30134	-1.60146	72.69988	74.4497	0.14836413	-0.09264303
1596	1644	0	74.366858	74.36686	1.49713	75.86399	74.1172	-0.249658	-0.16675773
1597	1645	0	74.432383	74.43238	-1.13928	73.29311	74.7135	0.28111716	-0.24675032
1598	1646	0	74.49791	74.49791	0.11125	74.60916	73.6919	-0.8060105	-7.24505201
1599	1647	0	74.563441	74.56344	-1.35235	73.21109	73.6805	-0.8829409	0.65289337
1600	1648	0	74.628974	74.62897	-1.08518	73.5438	73.7001	-0.928874	0.85596404
1601	1649	0	74.69451	74.69451	0.224889	74.9194	74.6885	-0.0060099	-0.02672388
1602	1650	0	74.760049	74.76005	0.410064	75.17011	75.2536	0.49355147	1.20359684

Table 2: Data sheet with the noise ratios from the AE spectrum processed using a notch filter

Tabela 2: Razmerja amplitud šumov pri filtriranju spektra z ozkopasovnim filtrom

	A	B	C	D	E	F	G	H	I
1	Kinetic Energy	Fe Peaks	Simulated Background	Noiseles AE spectrum	Initial Noise	Complete AE spectrum	Audacity Smoothed	Remaining Noise (G-D)	Noise Ratios (H/E)
2	50	0	85.5215939	85.52159	-1.294	84.22782	19.85671	-65.664886	50.7543595
3	51	0	83.1783126	83.17831	0.421	83.59935	45.33394	-37.844375	-89.882924
4	52	0	80.9277651	80.92777	-0.419	80.50839	64.56315	-16.364618	39.0213159
5	53	0	78.7647024	78.7647	-0.888	77.87708	68.37446	-10.390246	11.7057686
6	54	0	76.6842642	76.68426	1.5459	78.23021	75.32746	-1.3568018	-0.8776499
7	55	0	74.6819436	74.68194	0.3841	75.06605	73.34811	-1.3338349	-3.4725938
8	56	0	72.7535559	72.75356	-0.695	72.05849	75.92464	3.1710817	-4.5622793
9	57	0	70.8952098	70.89521	-0.835	70.0606	71.43866	0.5434543	-0.6511494
10	58	0	69.1032824	69.10328	-1.165	67.93834	72.58164	3.4783531	-2.9858672
11	59	0	67.3743966	67.3744	-1.086	66.28791	68.05102	0.6766247	-0.622762
12	60	0	65.7054003	65.7054	-0.177	65.52819	69.1224	3.4169989	-19.281932
1598	1646	0	74.4979105	74.49791	0.1112	74.60916	74.49698	-0.0009344	-0.0083989
1599	1647	0	74.5634409	74.56344	-1.352	73.21109	73.67407	-0.8893705	0.6576478
1600	1648	0	74.628974	74.62897	-1.085	73.5438	74.11458	-0.5143922	0.47401608
1601	1649	0	74.6945099	74.69451	0.2249	74.9194	73.63111	-1.0633957	-4.7285443
1602	1650	0	74.7600485	74.76005	0.4101	75.17011	74.74124	-0.0188118	-0.0458752

As can be seen in **Figures 8a** and **8b**, in both cases most of the points representing the noise ratios occupy the region between –1 and 1, while some of the peaks lie outside these boundaries. If the ratio of the remaining noise to the initial noise is less than 1, this indicates that the new signal after processing is actually closer to the real signal than the one before processing, thus indicating an improvement with respect to the noise. The noise ratios whose values lie outside the [–1,1] interval

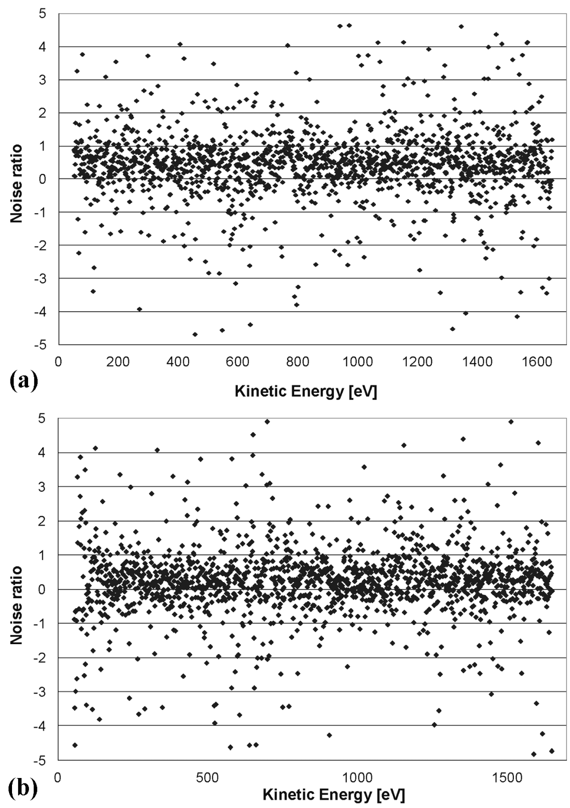

Figure 8: Noise ratios from: a) the 5-point smoothed spectrum and b) the spectrum smoothed using a notch filter

Slika 8: Razmerja amplitud šumov pri: a) filtriranju spektra s 5-točkovnim povprečenjem in b) pri filtriranju spektra z ozkopasovnim filtrom indicate that for those specific data points the processing has actually worsened the situation with respect to the noise. Plotting these noise ratios for all the data points in the spectrum offers a convenient way to see at a glance whether there is an improvement in terms of the noise or not, as well as for comparing different processing techniques for this purpose. Again, the usefulness of the simulated spectra must be stressed in this regard, because no such comparison can be made if the values for the noise are not known at the beginning, as it is in the case of the measured spectra.

4 CONCLUSIONS

Simulated spectra have been used to assess the performance of two noise-reduction techniques. A simple idea of using the noise ratios as a measure of the efficiency of the noise-reduction routines was presented. By applying this idea on a simulated spectrum, which was processed using two different procedures, the values for the noise ratios at each data point were found for the respective procedures. Plotting the noise ratios provided a convenient way to assess, at a glance, the efficiency of the processing route in reducing the noise. The noise ratios for the majority of the data points lie in the [–1,1] interval, indicating an improvement with respect to the noise.

The only way in which the values of the noise ratios can be obtained is if the values of the noise and the noiseless signal are known before and after the processing. Such a condition can be fulfilled if simulated spectra are used in the assessment stage, as shown in this paper.

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