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THE MODELING OF AUGER SPECTRA

MODELIRANJE AUGERJEVIH SPEKTROV

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The presented work deals with the process of simulated AES spectra creation. The purpose of virtual spectra creation is to use them as a testing ground for different background-removal and noise-reduction algorithms. Numerous methods for background removal and noise reduction exist already, but there is uncertainty about their performance and the accuracy of the data produced, since it is well known that the raw data is altered any time it undergoes any kind of processing conducted for different purposes. This is due to the fact that the levels of background and noise are at unknown levels in the measured AES spectra. By using simulated spectra the case is different. The levels of background and noise are added by the user, thus their levels are known exactly prior to processing. For this reason, they make a valuable means for assessing the performance of different algorithms intended for background removal and noise reduction.
The article describes the principles of simulation of AES spectra and shows the basic elements of the developed software.

Keywords: AES spectra, data processing, simulation, neural networks, VBA

Predstavljeno delo obravnava proces simulacije Augerjevih spektrov. Osnovni namen generiranja virtualnih spektrov je vzpostavitev okolja, namenjenega preizkušanju različnih algoritmov za odstranjevanje spektralnega ozadja in šuma. Obstaja veliko splošnih metod za odstranjevanje ozadja in šuma, ki pa so bile narejene za druge namene, zato njihov vpliv na interpretacijo sestavin spektra ni znan. Znano je, da vsaka metoda, ki odstranjuje ozadje in šum, neizogibno popači tudi osnovno informacijo. Do sedaj je bilo nemogoče zanesljivo oceniti napake, ki jih povzročajo posamezni algoritmi, ker so bili vedno uporabljeni na merjenih spektrih, za katere ni točno znano, kako so sestavljeni, prav tako tudi ne vemo, kakšno je ozadje in koliko je zares šuma. Pri simuliranih spektrih pa v vsakem primeru posebej natančno vemo, kako so sestavljeni, zato je ocena delovanja metod za odstranjevanje neželenih delov spektra lahko zelo zanesljiva.
Članek opisuje postopke simulacije Augerjevih spektrov in prikazuje osnovne gradnike razvitega programskega orodja.

Ključne besede: Augerjevi spektri, obdelava podatkov, simulacija, nevronski sistemi, VBA

1 INTRODUCTION

The main goal of our work was to design a system which will be able to generate a series of AES (Auger Electron Spectroscopy) spectra with one clear aim – to provide an environment where numerous algorithms for AES spectra analysis can be verified, compared and tested. In order to achieve this goal, we have analyzed the appearance of many measured spectra. The article describes the way the AES spectra were analyzed and finally how the different elements were brought together to produce the artificial AES spectra.

1.1 A brief description of AES

Auger electron spectroscopy is a powerful analytical technique for studying surfaces.[1] AES is a very surface-sensitive technique due to the fact that most of the signal comes from the topmost atomic layers of the surface of the sample.[2] Together with X-ray photo-electron spectroscopy (XPS), it has been extensively used for determining the chemical compositions of thin films of nanometer thicknesses in a large variety of applications.[3] This technique is based on the Auger effect, a phenomenon discovered by both Pierre Auger and Lise Meitner independently in the 1920s, even though Pierre Auger is accredited with the discovery in the scientific community.[4] The Auger effect constitutes the emission of an electron from an atom following the filling of a vacancy in an inner electron shell.[5] Even though the discovery of the phenomenon was made in the early 1920s, it was not until the 1950s that AES became a practical characterization technique for analyzing surface features.[6]

AES involves probing the surface with an electron beam, creating excited states of atoms present in the sample[7] through core-shell ionization, and emitting "Auger electrons" with characteristic energies,[8] which are used to determine the surface chemical composition.[9] Afterwards, these electrons enter the analyzer, where depending on the type of the analyzer used they get deflected to degrees which depend on their kinetic energies, and then electrons with different kinetic energies enter the detector at different locations. With the detector the number of electrons reaching specific locations is measured. At the end of the process we obtain the data plotted on the screen as the number of electrons per second reaching the detector versus their kinetic energy. A simplified diagram of this whole process is represented in **Figure 1**.

After obtaining the spectrum the data needs to be processed in order to derive from it the necessary information. Different tools (programs) are used for processing the AES spectra. During these operations

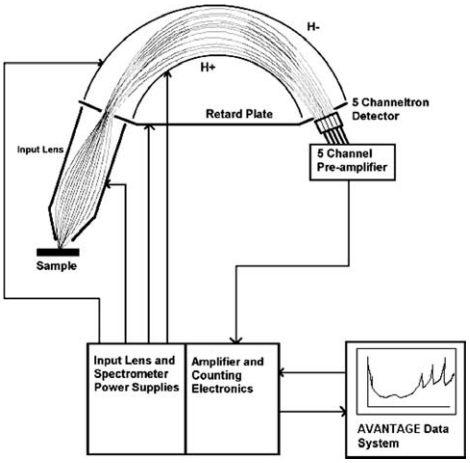

Figure 1: Detection process in Auger Electron Spectroscopy[10]
Slika 1: Proces detekcije pri Augerjevi elektronski spektroskopiji[10]

though, e.g., differentiation of the spectra for quantification, inevitably the raw data is being altered, often at unknown levels to the user. It is important to have information about the influence the program itself has on the data during the processing. In this way the post-processing features observed on the spectra that are not representative of the material, but are due to the influence of the program, will be readily accounted for.

When the spectra are measured, the peaks and noise are superimposed on a slowly varying background.[11] For different purposes, such as the automation of the recognition of AES spectra, data processing like background subtraction and noise reduction is obligatory. Alongside noise, the background is usually regarded as a problem of data processing.[12] In the process of background subtraction and noise reduction through different tools, the spectra are being altered, often at unknown levels to the experimenter.

This work is going to deal with the process of modeling the AES spectra, with the intention of creating simulated spectra to be used later for assessing the performance of the background-removal and noise-reduction algorithms. The advantage of using simulated AES spectra lies in the fact that the levels of background and noise are added by the user, and thus are known prior to the spectra processing. Having prior knowledge about the levels of these two elements of the spectra is a clear advantage, because after processing them through the algorithms for background removal and noise reduction, by comparison the influence the program itself has on the data during the processing can be determined. By taking into account this fact and correcting for it, the uncertainty in the outgoing data will be reduced.

2 EXPERIMENTAL PART

The modeling of the AES spectra involved the careful investigation of numerous real spectra measured from

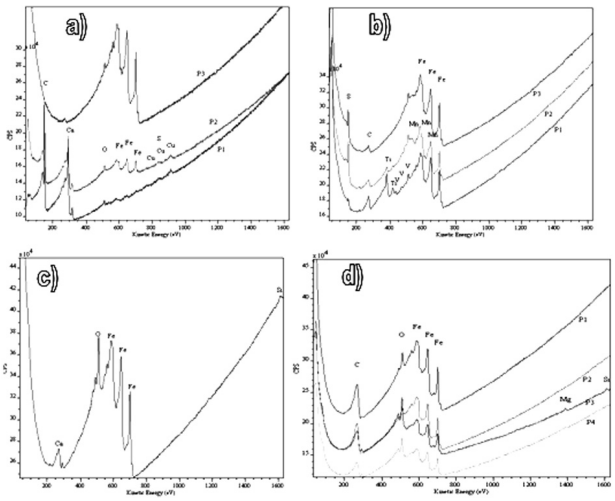

Figure 2: The "Direct" AES spectra used for the determination of the shape of the spectra
Slika 2: Nekaj primerov Augerjevih spektrov, ki so bili uporabljeni za določevanje posameznih sestavnih delov spektra

metallic samples. **Figure 2** represents some typical examples of the measured spectra.

The spectra were taken using the Microlab 310-F spectrometer at the IMT laboratory for surface analysis.

2.1 Approximation of the background

For the purpose of defining the general shape properties of the background, the data were transferred in a digital form from the standard .vms files of CasaXPS into Excel. **Figure 3** represents the digital data already transferred into an Excel file, with the graph of the spectra being drawn from the imported data.

There the number of points representative of the background were taken, and using the graphing tools in Excel the approximate background for a couple of spectra were drawn. **Figure 4** represents such a case.

Those background shapes for a couple of spectra, in the normalized form, were plotted together in order to investigate and possibly reach some conclusions about their shapes. **Figure 5** represents the manually defined background shapes for a number of spectra.

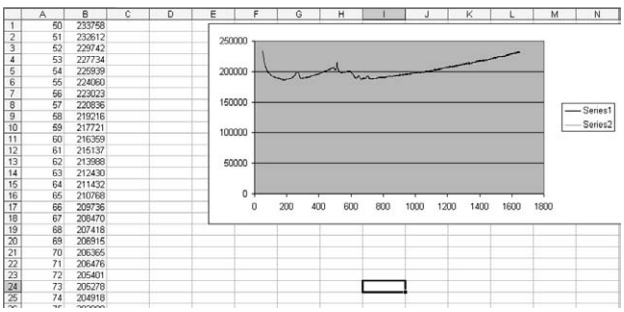

Figure 3: Spectra in digital form transferred from a .vms file and the corresponding graph in Excel
Slika 3: Digitalni zapis spektra, prenesenega z datoteke .vms, ter pripadajoč graf v Excelu

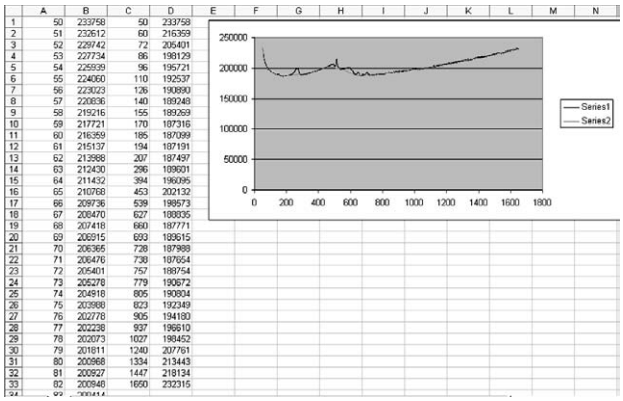

Figure 4: Manually defined background for one spectrum
Slika 4: Ročno določevanje ozadja spektra

From **Figure 5** it is obvious that the AES spectra background is very much variant. Nevertheless, some distinctive features can be observed there, like the "low-energy part" – the descending part where the background shows a rapid decrease in the signal with the kinetic energy increase; the "mid-energy part" – the central part where the increase of the background is observed, which is again followed by the decrease; and the "high-energy part" – the raising part where the background is steadily increasing.

The manual background definition is a very time-consuming process, as much as it is not very reliable.

2.2 Neural network system for background AES approximation

In order to produce a more reliable impression of the background, where a larger amount of AES spectra can be checked with regard to the shape of the background, we have developed a method capable of approximating the background shape. For this purpose, a feedforward neural network was used.

For our purposes, we have used the neural networks for data modeling or function approximation. Neural networks are model-less approximators, meaning they are capable of accomplishing the approximation tasks regardless of any knowledge of the nature of the modeled

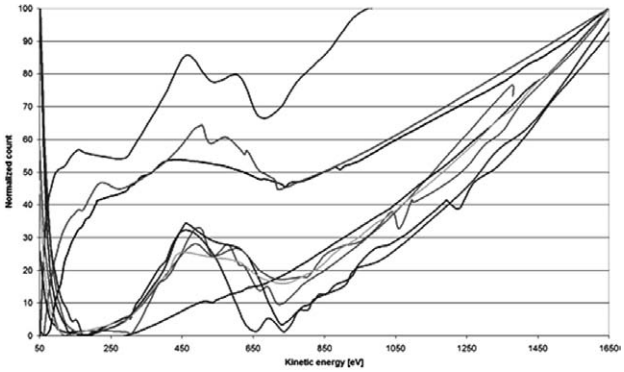

Figure 5: Manually defined background in normalized form
Slika 5: Ročno določeno ozadje v normirani obliki

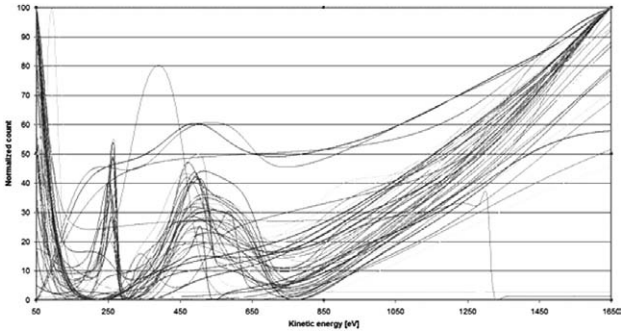

Figure 6: The curves of AES spectra backgrounds for various measured spectra as approximated by the neural network.
Slika 6: Krivulje ocenjenih ozadij za Augerjeve spektre. Ozadje je bilo ocenjeno z nevronskim sistemom.

system. For classical approximation techniques, it is often necessary to know the basic mathematical model of the approximated problem.

The most important property of neural networks is their ability to learn the model from the data presented. This means that the user needs only to be sure that a causal relation between the presented parameters really exists. Almost no further knowledge of the system behavior is needed. When the neural network builds the model, the dependences among the parameters are included in the model.

For implementing the neural networks we used the Neuralyst (Cheshire Ltd.), which is a supplement to Microsoft Excel and VBA (Visual Basic for Accessories), to be able to make the best use of Neuralyst.

The backgrounds for 63 measured AES spectra were approximated using an error backpropagation neural network[13,14]. Since the cumulative AES spectra count values differ in magnitudes significantly, and we have been interested in the comparison of the shape of the spectra, all the samples were normalized prior to the approximation by the neural network. **Figure 6** represents the outcome of the neural network formation of the background for all 63 measured spectra.

From **Figure 6** we can see the same characteristics as was the case with the method where the background was determined manually (**Figure 5**).

2.3 Modeling the background shape

After obtaining a general visual impression for the shape of the backgrounds of the spectra and investigating them, we went to the next level of finding a representative function that would best fit that shape, and the function of which would be used later to simulate the background.

According to the characteristics observed in **Figures 5 and 6** the ideal function for the AES spectra background was proposed to be:

$$f_{\mathrm{B}} = A\left(\frac{1}{px_{\mathrm{e}}} + bx_{\mathrm{e}} + c\right) + B \qquad (1)$$

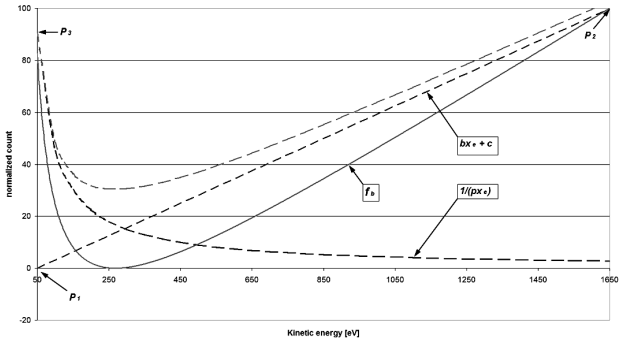

Figure 7: The construction of the background function
Slika 7: Konstrukcija funkcije, ki opisuje ozadje spektra

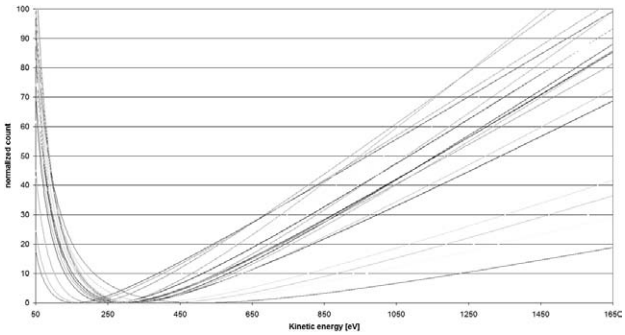

Figure 8: The randomly chosen backgrounds for the simulated AES spectra
Slika 8: Naključno izbrana ozadja za simulirane Augerjeve spektre

Where:
f_B: represents the background function
x_e: the kinetic energy
A, B, p, b, c: parameters which define the shape of the background

The construction of the background function is shown in **Figure 7**.

The construction of the randomly shaped background function starts with the random selection of the parameters of the linear part

$$f_{\text{lin}} = bx_{\text{e}} + c \tag{2}$$

where the points $\mathbf{P_1}$ and $\mathbf{P_2}$ (**Figure 7**) are randomly selected. The point $\mathbf{P_1}$ is the zero crossing of the linear part, and $\mathbf{P_2}$ is the value of the normalized count for the kinetic energy of 1650 eV. The random generator generates the values for $\mathbf{P_1}$ in the range [0, 1000], and $\mathbf{P_2}$ in the range [60, 140]. The limits for both values were defined experimentally, by observing the behavior of real spectra.

From the known points $\mathbf{P_1}$ and $\mathbf{P_2}$ the coefficients $\boldsymbol{b}$ and $\boldsymbol{c}$ of the linear part are defined.

$$\begin{gathered} y = bx_{\text{e}} + c \\ b = \frac{P_{2y}}{P_{2x} - P_{1x}};\ P_{2y} = 1650\ ;\ P_{1y} = 0 \\ c = -bP_{1x} \end{gathered} \tag{3}$$

Then follows the definition of the non-linear part

$$f_{\text{nlin}} = \frac{1}{px_{\text{e}}} \tag{4}$$

For this part the random generator generates the value of the non-linear part for the kinetic energy of 50 eV. In figure 8 this point is denoted by $\mathbf{P_3}$. The random generator selects the values from the interval [20, 500]. Again the border values were taken experimentally. Finally the value for the parameter $\boldsymbol{p}$ is set.

$$P = \frac{1}{P_{3x} \cdot P_{3y}} \tag{5}$$

Parameters A and B are set in the scaling process, where the minimal part of the background function is set close to 0, and the maximal part close to 100.

By using equation 1 as a model function and having the computer randomly generate the necessary parameters within the previously set limiting values, some simulated primary background shapes were obtained. **Figure 8** represents a number of the simulated shapes of the primary background.

2.4 Completing the simulation

To complete the simulation we also had to gather information about the characteristic peaks of elements. For that purpose the characteristic elemental AES spectra of Al, C, Co, Cu, Fe, Au, Ni, O, Si, Ag, Ti, and Va were gathered from Compro10, a database easily accessible on the net.

Generally, we suppose that the measured spectra are constructed according to equation 6.

$$S = f_i(a_i s_i) + P_{\text{B}} + N \tag{6}$$

where S represents the measured AES spectra, f_i is some non-linear function binding the standardized spectra into the composed elements of the spectra, a_i is the amount of i-th element in the spectra, s_i the i-th pure element represented in the AES spectra, P_B is the primary background, and N is the noise.

In the case of synthesis of the artificial AES spectra, the non-linear dependence of the various standardized spectra is assumed to be linear, thus producing equation 7.

$$S = \sum_{i=1}^{M} (a_i s_i) + P_{\text{B}} + N \tag{7}$$

where the symbol M denotes the number of all the spectra in the database.

For the purpose of creating the so-called standard spectra database, the elementary spectra were analyzed. **Figure 9** shows the spectra of pure Fe.

From visually inspecting **Figure 9** we can see that the AES spectra consist of the three distinctive elements:
1. The primary background,
2. The peaks base,
3. The peaks.

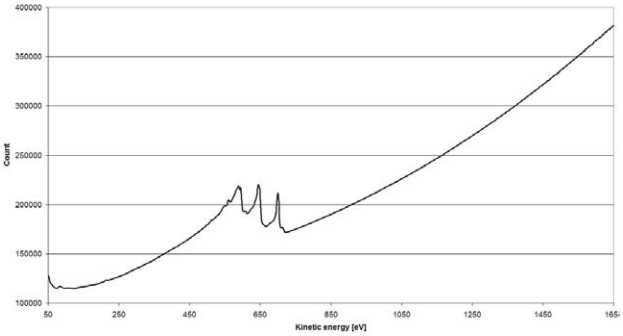

Figure 9: The AES spectrum of Fe
Slika 9: Augerjev spekter Fe

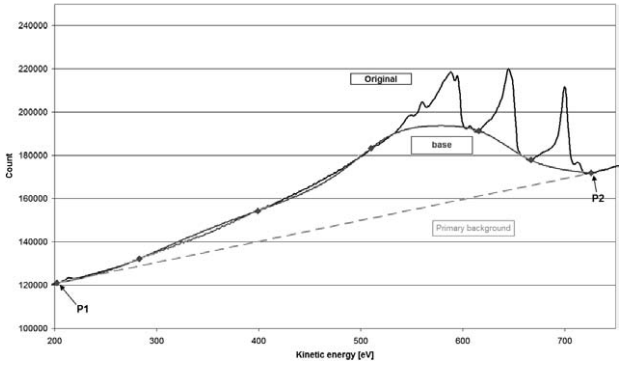

Figure 10: The AES spectra elements
Slika 10: Elementi Augerjevega spektra

Figure 10 illustrates these distinctive parts. For the purpose of extraction of the three spectra elements, several steps were introduced as follows:

1. Two points $\mathbf{P_1}$ and $\mathbf{P_2}$ (**Figure 10**) were selected. They are common to all three curves.
2. The line that represents the primary background through $\mathbf{P_1}$ and $\mathbf{P_2}$ was constructed. We are aware that in the measured spectra the primary background is nowhere linear, but the use of the line is close enough for the intended purpose.
3. On the part of the AES spectra between $\mathbf{P_1}$ and $\mathbf{P_2}$ the set of points describing the base of the peaks was selected (**Figure 10**). Typically, the number of selected points was up to 10.

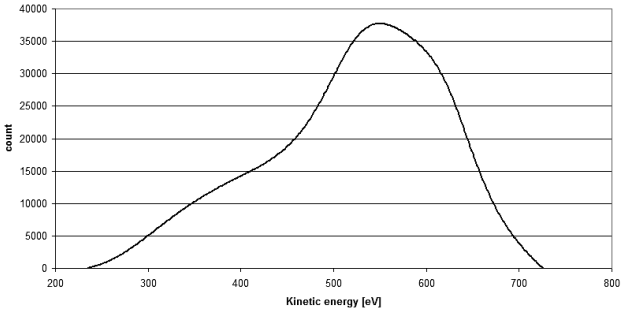

Figure 11: The approximated function of the base of the peaks for the Fe AES spectrum
Slika 11: Aproksimirana funkcija podlage vrhov za Augerjev spekter Fe

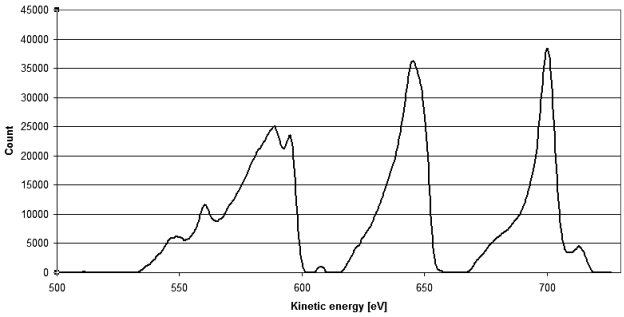

Figure 12: The extracted peaks of Fe AES spectra
Slika 12: Izločeni vrhovi za Augerjev spekter Fe

The shape of the base function was approximated by the four-layer neural network (configuration 1-4-8-1). The approximated function was stored in a table containing the Kinetic energy and count values for the area between $\mathbf{P_1}$ and $\mathbf{P_2}$ (**Figure 11**).

4. Once the base function is known it is subtracted from the original spectra, thus obtaining the shape of the extracted peaks (**Figure 12**).

2.5 The virtual AES spectra generator

The system for the random generation of AES spectra was developed under Microsoft Excel using Visual Basic for Applications and consists of six distinctive elements:

1. The generator Console
2. The Files control center
3. The Primary background generator
4. The Noise generator
5. The standard elements peaks database
6. The standard elements peak base database.

2.5.1 The generator Console

The generator console is the central part of the AES spectra generator. It provides the basic constituent data regarding the generated AES spectra. The following are data provided on the Console datasheet:

- The generator mode of operation. Two modes are currently possible: "ONE AES" producing only one randomly generated AES spectra without the saving to the file; "SAVE TO FILE" option, which generates random AES spectra and stores the data to the files.
- The number of elements provided in the standard spectra database. Currently, the standard spectra database contains 11 spectra of standard elements. Additional spectra are very easily included in the database.
- The number of actual AES spectra constituents. Although the number of standard spectra is provided, the process of random AES spectra generation can be limited to the lower number of actual constituents. The number is specified by the user.
- The graphical representation of the randomly generated spectra. The generated spectra are joined with

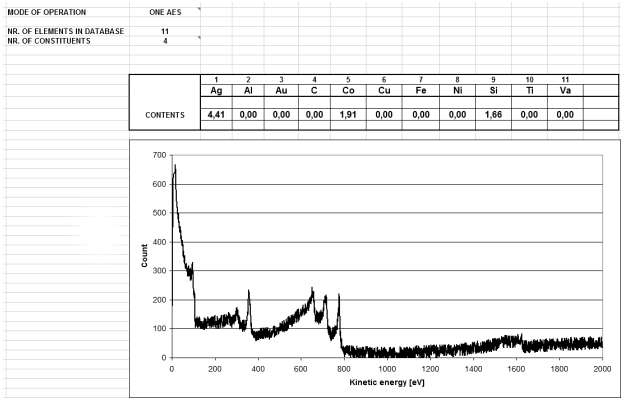

Figure 13: The AES spectra generator main console
Slika 13: Osrednji del generatorja Augerjevih spektrov

the primary background as well as with the noise. The result of the multiple random generation is graphically presented. The additional information is provided on the table where the amounts of the constituents are given (**Figure 13**).

2.5.2 The Files control center

The Files control center defines the way in which the randomly generated AES spectra are stored. The user defines the name of the files where the spectra are to be stored. The provided name is joined by the subsequent number of the generated spectra and stored in the directory, the name of which has already been provided by the user. It is also necessary to specify the number of generated AES spectra that are to be saved in the separate file.

The data contained in each file are:

- The sum of all the peaks contained in the generated AES spectra
- The sum of all the base elements that are part of each standard spectra
- The randomly generated primary background
- The noise
- The AES spectra construction data

2.5.3 The Primary background generator

The primary background generator controls the process of AES spectra primary background generation. The user must define the intervals for the primary background parameters. The AES spectra generator uses the given intervals to randomly re-shape the basic primary background equation. **Figure 14** represents the graphical user interface for the AES spectra primary background generation.

2.5.4 The Noise generator

The noise generator provides the random noise that is to be added to the AES spectra. The user can define the upper limit for the AES spectra noise. The noise

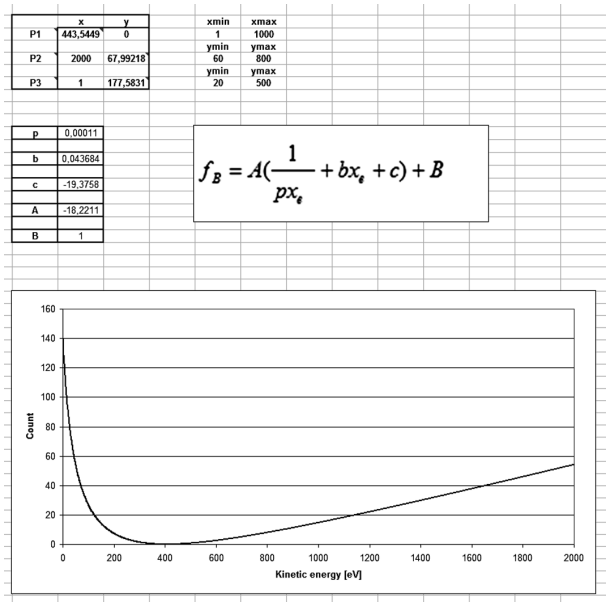

Figure 14: The AES spectra primary background generation
Slika 14: Generiranje osnovnega ozadja Augerjevega spektra

generator then forms the noise according to the given boundary. The generated noise is bipolar, providing that the AES spectra fluctuations affect the spectra both as the addition and subtraction to the signal (**Figure 15**). In the literature, the noise level is understood to be in a non-linear dependence with the kinetic energy. In the first stage of the AES signal modeling we opted to use the linear dependence of the noise amplitude over the kinetic energies used.[15]

2.5.5 The standard-elements peaks database

The standard-elements peaks database contains the data on the pure – standard – elements that are the basis of the AES spectra generation. So far, 11 elements have been added to the database. This database contains only the peaks data (**Figure 16**). Other parts are stored elsewhere.

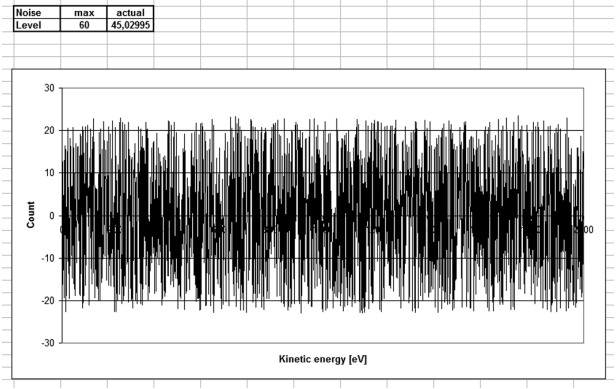

Figure 15: The AES spectra noise
Slika 15: Dodan šum Augerjevemu spektru

1	kinetic energy	1	2	3	4	5	6	7	8	9	10	11
2	eV	Ag	Al	Au	C	Co	Cu	Fe	Ni	Si	Ti	Va
3	1	1,458843405	0	7,235415428	0	0	0	0	0	18,66672	0	0
4	2	13,05296682	0	27,75620573	0	0	0	0	0	36,03436	0	0
5	3	35,48330814	0	41,54103022	0	0	0	0	0	54,8241	0	0
6	4	58,46859806	0	47,53857699	0	0	0	0	0	57,28049	0	0
7	5	76,71293879	0	54,25447137	0	0	0	0	0	57,29505	0	0
8	6	89,29555989	0	59,53721244	0	0	0	0	0	58,0645	0	0
9	7	96,61959806	0	64,71527927	0	0	0	0	0	59,73892	0	0
10	8	99,47087319	0	69,15421532	0	0	0	0	0	60,40827	0	0
11	9	98,74896727	0	71,94161693	0	0	0	0	0	59,88531	0	0
12	10	95,70511617	0	74,92995569	0	0	0	0	0	58,55592	0	0
13	11	91,79740617	0	79,02207872	0	0	0	0	0	56,70751	0	0
14	12	88,2460202	0	81,66399413	0	0	0	0	0	53,71709	0	0
15	13	85,36093567	0	83,16791941	0	0	0	0	0	49,76669	0	0
16	14	83,46246275	0	85,68449827	0	0	0	0	0	45,53661	0	0
17	15	82,46752056	0	89,17851854	0	0	0	0	0	41,25068	0	0
18	16	81,69311916	0	91,44918029	0	0	0	0	0	37,18716	0	0
19	17	80,43557563	0	92,35993849	0	0	0	0	0	33,58462	0	0
20	18	78,70487734	0	92,83098686	0	0	0	0	0	30,51096	0	0
21	19	77,12125287	0	93,42641841	0	0	0	0	0	27,83945	0	0
22	20	75,74640215	27,8054921	93,86783997	0	0	0	0	0	25,42721	44,80378	66,75417
23	21	74,6213415	26,12997675	93,83923199	0	0	0	0	0	23,29018	49,32057	66,32416
24	22	73,71469132	25,34905323	93,93946216	0	0	0	0	0	21,33561	51,66256	65,56686
25	23	72,9640523	24,73814092	94,02046234	0	0	0	0	0	19,61832	54,48296	64,44257
26	24	72,43115629	24,41516886	93,73441915	0	0	0	0	0	18,28778	58,49928	62,61042
27	25	71,92951862	24,49805434	92,81171391	0	0	0	0	0	17,14695	60,5726	58,75256
28	26	71,18993246	24,73523148	91,81367054	0	0	0	0	0	16,24494	55,50723	54,08659
29	27	70,2328273	25,26689923	90,90211325	0	0	0	0	0	15,53258	37,43392	49,57564
30	28	68,95454874	25,94502211	89,95807279	0	0	0	0	0	14,98766	15,73928	46,69808
31	29	67,59280517	26,88024767	88,97263855	0	0	0	0	0	14,74438	6,549249	44,74163
32	30	66,04402769	27,55508533	88,0614388	0	0	0	0	0	14,63863	2,698981	40,66067
33	31	64,46327704	28,28727126	87,16354756	0	0	0	0	0	14,68496	0,715552	31,56831
34	32	62,98498525	29,2024048	86,28757821	0	0	0	0	0	14,97334	0,081542	17,77097
35	33	61,61953012	29,90135524	85,65934112	0	0	0	0	0	15,31742	0,015882	7,780719
36	34	60,35667178	30,70203676	85,28467722	0	0	0	0	0	15,74066	0	3,201487
37	35	59,26898855	31,36806067	85,19555086	0	0	0	0	0	16,20544	0	0,840073
38	36	58,2326169	32,83084564	85,16632658	0	0	0	0	0	16,55251	0	0
39	37	57,18583253	34,01159817	85,19147464	0	0	0	0	0	17,03891	0	0
40	38	56,02562137	35,339304	85,03103188	0	0	0	0	0	17,6038	0	0,41539
41	39	54,71111167	36,6812686	84,60145118	0	0	0	0	0	18,23121	0	0,857178
42	40	53,24288739	37,72011431	83,61949681	0	0	0	0	0	18,98108	0	1,427221
43	41	51,77576068	37,49077117	82,07706238	0	0	0	0	0	19,83697	0	1,632147

Figure 16: The standard-elements peaks database
Slika 16: Podatkovna baza standardnih spektrov

2.5.6 The standard-elements peaks base database.

The standard-elements peaks base database is formatted in exactly the same way as in the case of the standard-elements peaks database.

3 RESULTS AND DISCUSSION

Comparing **Figure 17** with **Figure 2** it is obvious that the randomly simulated AES spectra adequately resemble the measured AES spectra. The variations of the backgrounds are sufficient to produce a set of quite different spectra that will allow a thorough analysis of the background- and noise-removal algorithms.

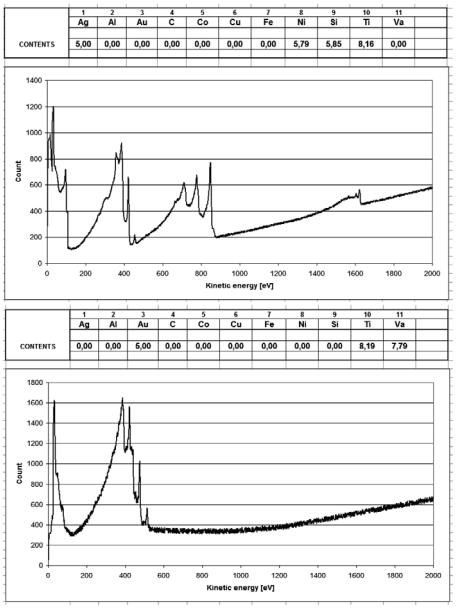

Figure 17: Two cases of simulated AES spectra with their corresponding data
Slika 17: Primera simuliranega Augerjevega spektra

The process of construction of the complete AES spectra starts with the selection of the parameters that control the process. The steps are the following:

1.) The number of constituent elements that are to be joined in the spectra is selected by the user. In our case the user can select 12 different elements. This number can be easily changed by adding the new spectra for additional elements.
2.) The random generator selects the constituent elements (from the number provided by the user in the previous step) and sets the relative amplitude for each selected element (parameter a_i from equation 6).
3.) The primary background is created.
4.) One by one the spectra of the selected elements are added to the primary background.
5.) The randomly generated noise is added.
6.) The normalized form of the simulated spectra is scaled to receive the "realistic" count values.
7.) The created spectrum is stored in a separate file, which will later represent the testing and validation ground for different background- and noise-removal techniques and algorithms. Each file contains detailed data on how the concrete spectra were constructed, so the background and the noise are known in detail. Therefore, a very exact basis for the further analysis is set.

Figure 17 represents two cases of simulated AES spectra, with the corresponding data given alongside in the table.

It is very important to note that the simulated AES spectra do not necessarily have to represent the spectra of real materials. The only condition that has to be fulfilled is for them to resemble the real AES spectra, i.e., to consist of the same constituent parts.

4 CONCLUSIONS

AES is a technique capable of deriving information from the topmost atomic layers of the surface. It is able to identify a very wide range of elements present at solid surfaces, and sometimes it can be used to obtain information about the chemical environment and bonding of surface species.[16] As knowledge about the properties of surfaces and their composition is increasing in importance, so is the need to get accurate information about them through techniques such as AES. An inevitable step after performing a measurement with this technique is the data processing that follows in order to harvest the desired information out of the spectra already taken. Background and noise are two undesired elements that are present alongside the characteristic peaks of elements in measured AES spectra. The background must be removed and the noise reduced to continue with the proper treatment of the data, but being at unknown levels in the raw data and knowing that any data treatment inevitably alters them to some extent, there is uncertainty as to the quality of the outgoing information.

The highlight of this work is the ability to have prior knowledge about the levels of background and noise before the processing of the spectra by various means takes place. Having this in mind, after the processing is done the pre-processed and the post-processed data can be compared to learn how much error the background-subtraction and noise-reduction techniques are introducing into the results that we read. By correcting for this factor the accuracy of the obtained information from the background-removal and noise-reduction tools is greatly improved.

It is of utmost importance to know that the presented work serves only one purpose, i.e., to provide the environment where various algorithms for noise reduction and background removal can be tested and evaluated. Such algorithms can afterwards be used on measured spectra, but with a thorough understanding of the consequences they have for the phase of data processing.

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