Factor analysis for the characterization of the nano-surface of the nitroazobenzene-modified glassy carbon electrode

Erdal Dinç*. Dumitru Baleanu**, Ali Osman Solak***, Haslet Ekşi***, and Remziye Güzel****

*Department of Analytical Chemistry, Faculty of Pharmacy, Ankara University, 06100 Tandoğan, Ankara, Turkey (e-mail: dinc@pharmacy.ankara.edu.tr)
** Department of Mathematics and Computer Sciences, Faculty of Arts and Sciences, Çankaya University,06530 Balgat, Ankara, Turkey and National Institute for Laser, Plasma and Radiation Physics, Institute of Space Sciences, Magurele-Bucharest, P.O. Box,MG-23, R 76911, Romania (e-mail: dumitru@cankaya.edu.tr)
***Department of Chemistry, Faculty of Arts and Sciences, Ankara University, 06100, Tandoğan Ankara, Turkey (e-mail: osolak@science.ankara.edu.tr and hsleksi@gmail.com)
****Department of Chemistry, Faculty of Arts and Sciences, Dicle University, 06100, Diyarbakır, Turkey (e-mail: guzel.remziye@gmail.com)

Abstract: Factor analysis with orthogonal varimax rotation was applied to determine the existence of a nanostructure on the nitroazobenze-modified glassy carbon electrode (NAB-GC) system. The NAB-GC electrode systems and benzoic acid-nanofilm (NAB-FILM) were obtained by using electrochemical surface modification experiments. The IR spectra of the bare glassy carbon electrodes (GC), the NAB-GC electrode system and NAB-FILM were recorded. The IR data of the bare GC,BA-GC and BA-FILM were categorized into five series consisting of FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3;FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5, respectively. The factor analysis method was separately applied to each group to extract the factor loadings. The orthogonal varimax rotation technique was used to obtain the rotated factor loadings corresponding to the first two factors. After the estimation of the relationship among and within groups, the results indicate the existence of the NAB-FILM on the NAB modified glassy carbon electrodes.

Keywords**:** Factor analysis, Orthogonal varimax rotation, NAB nanofilm, Characterization.

1. INTRODUCTION

Today new instrumentation techniques give us many additional possibilities for the registration of the signals at different forms for the qualitative and quantitative evaluation for the analysis of samples, chemical structures and material systems. In all cases, one-, two-, three- and high-dimensional data corresponding to the above signals may not give us sufficient results for the qualitative and quantitative analyses such as exploration of chemical structure, classification or reduction of data, screening or transformation of data, definition of relationships. In this context, factor analysis is a multivariate analysis approach that can be applied for the identification, interpretation and characterization of the basic structure of chemical systems or chemical data patterns using variation in data variables [Nigmatullin et al., 2009, 2010a, b].

For electrochemical analyses, preparation of chemically modified electrodes (CME), mostly at the carbonaceous surfaces, have attracted increased interest due to the potential usage of CME in analytical applications and several area of science and industry [Zen et al., 2003]. Electrochemical modifications are based on the preparation of thin films of the selected chemical at the glassy carbon (GC) or metal surfaces to endow desirable properties of the film, preferentially by covalent bonding using aryl diazonium salts. The electrochemical method of diazonium salt reduction was initiated by Pinson's group [Bourdillon et al., 1992] and developed by several researchers [Nigmatullin et al., 2010a,b; Zen et al., 2003; Bourdillon et al., 1992; Üstündağ et al., 2009; Yu et al., 2007; Turan et al., 2009; Pinson et al., 2005]. As it is known the reduction of aryl diazonium salts is performed by a one-electron reduction mechanism on the carbon surfaces, either in aqueous or nonaqueous media. This electrochemical reduction allows the formation of nanofilms defined by the covalent bonds of aryl groups with carbon atoms on the electrode surfaces. These types of modified electrodes can also be used in fabricating molecular junctions to determine a variety of current-voltage responses of molecular junctions, such as rectification, negative differential resistance, conductance switching, photocurrent, and various electron transport mechanisms for microelectronic devices [Solak et al., 2003]. The conductance-switching behavior of several organic nanofilms on carbon surfaces was reported extensively by McCreery's group [Solak et al., 2003; McCreery et al., 2003; Solak et al., 2002]. In that studies the authors concluded that a monolayer of nitroazobenzene, nitrobiphenyl or biphenyl 'switched' from a high-resistance state to one with a factor of ten or more lower resistance, in the presence of the application of a negative voltage between a graphitic conductor and a metallic top contact.

Several spectroscopic methods including X-ray photo electron spectroscopy (XPS), electron spin resonance (ESR) and, especially, infrared (IR) spectroscopy, as well as electrochemical and electrochemical impedance spectroscopic (EIS) methods, have been used for the analysis of the modified GC surfaces for characterization [McCreery et al., 2003]. In some cases, these conventional analytical characterization methods do not give expected results mainly due to the existence of excessive noise and the complexity related to weak nanofilm signals coming from the structure of surfaces. It is clear that new signal processing tools or signal manipulation algorithms must be used to overcome the above drawbacks to describe the qualitative identification of the nanofilms or nano surfaces.

NAB is an interesting molecule and has been extensively studied by various authors for the modification of GC and metal surfaces to investigate its electrical and spectroscopic studies under the applied potential. [McCreery et al., 2003; Solak et al., 2002; Actis et al., 2008; Anariba et al., 2006]

The main aim of this study is to apply a new powerful factor analysis approach to the IR spectra of the nitroazobenzene modified GC electrode (NAB-GC) surface, bare GC surface and nitroazobenzene diazonium salt (NAB-DAS) for the structural qualitative characterization of the nanofilm, consisting of the surface of the modified NAB-GC electrode system, to verify the existence of the nitroazobenzene molecules on the modified GC surfaces.

In this study the IR data corresponding to NAB-film, GC-NAB, GC were categorized into following sequence; FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5, respectively. Factor analysis tool was applied to the matrix of correlation coefficients obtained from the experimental IR data of the above sequence. After above procedure, the orthogonal varimax rotation technique was applied factor loadings obtain from the correlation coefficient matrix and then we obtain the rotated factor loadings. As a consequence, the plots of bar and line representations of FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5 were indicated an existence of the nanofilms consisting of NAB films on the modified NAB-GC surfaces.

2. Theoretical outline

2.1. Factor analysis

Factor analysis has been applied (1) to *reduce* the number of variables and (2) to *detect structure* in the relationships between variables [R.J. Rummei, 1970]. In some cases, factor analysis (FA) and principal component analysis (PCA) are considered to be synonymous. Both FA and PCA approaches are based on the orthogonal rotation within eigenspace for a data matrix.

Factor analysis may use either correlations or covariances. The covariance covab between two variables, a and b, is their correlation times their two standard deviations: covab = rab sa sb, where rab is their correlation and sa and sb are their standard deviations. Any variable's covariance with itself is its variance—the square of its standard deviation. A correlation matrix can be thought of as a matrix of variances and covariances of a set of variables that have already been adjusted to a standard deviation of 1. Since a correlation or covariance matrix can be translated to one another easily, in many statistical books, authors may use either a correlation or covariance matrix or both to illustrate how factor scores are obtained.

The central theorem of factor analysis, in mathematical terms, is that we can partition a covariance matrix M into a common portion C that is explained by a set of factors, and a unique portion R that is unexplained by those factors. In matrix language, M = C + R, which means that each entry in matrix M is the sum of the corresponding entries in matrices C and R. The explained C can be further broken down into component matrices C 1, C 2, C 3, … and Cx, explained by individual factors. Each of these one-factor components Cx equals the "outer product" of a column of factor loading. A statistical program may rank several matrices Cx if it finds that there is more than one matrix with eigenvalues greater than 1. An eigenvalue is defined as the amount of variance explained by one more factor. Since a component analysis is adopted to summarize a set of data, it would not be meaningful to find another factor that explains less variance than is contained in one variable (eigenvalues of less than 1). Therefore, statistical programs often default this rule selecting factors.

Principal component analysis is commonly used in statistics for factor analysis and was introduced to achieve representation or summarization. It attempts to reduce p variables to a set of m linear functions of those variables that best describe and summarize the original p. Some conditions need to be satisfied to have a set of m factors for the purpose of factor analysis. First, the m factors must be mutually uncorrelated. Second, any set of m factors should include the functions of a smaller set. Third, the squared weights defining each linear function must sum to 1, denoting the total variance explained. By using all p, we get a perfect reconstruction of the original X -scores, while by using the first m (with the greatest eigenvalues), we get the best reconstruction possible for that value of m and the most simplified model for interpretation.

Statistical programs allow researchers to select how many factors will be chosen. Ideally, we want to identify a certain number of factors that would explain or represent all the relevant variables. However, the use of factor analysis is not just to find all the statistically "significant" factors; rather,

those factors identified should be meaningful to the researchers and interpreted subjectively by them. If the factors generated are meaningless in terms of the compositions of variables, such a factor analysis is not useful. In general, researchers may use exploratory factor analysis to find statistically significant factors (eigenvalues > 1) if they do not have prior knowledge of what factors may be generated from a number of variables. Therefore, it is very common that two different researchers would have two sets of factors even though they used an identical dataset. It is not about who is right or wrong, but whether researchers can adopt a group of factors that lead to better interpretation of the data. If researchers have prior knowledge (e.g., theories) of those factors, they can limit the number of factors to be generated in statistical programs rather than allowing statistical programs to generate them. In other words, researchers determine if the proposed variables are grouped into factors as suggested by the theory.

Researchers may use the rotation of a factor-loading matrix to simplify structure in factor analysis. Consider a set of p multiple regressions from p observed variables, wherein each regression predicts one of the variables from all m factors. The standardized coefficients in this set of regressions form a $p \times m$ matrix called the factor-loading matrix. We may replace the original factors with a set of linear functions of those factors for the same predictions as before, but with a different factor-loading matrix. In practice, this rotated matrix is expected to be used with simpler structures to better serve researchers' subjective interpretations.

3. Experimental section

3.1. *Chemicals and reagents*

Nitroazobenzene diazonium salt (NAB DAS) was synthesized from 4-amino-4′-nitrobenzene (Aldrich) (PANAB) as a precursor. Approximately 0.5 g of PANAB was weighed into a three-necked 50-mL round-bottom flask; then 10 mL of 50% fluoroboric acid (Riedel-de Haën) was added and the resultant mixture stirred with a magnetic stirring bar. A 4:1 molar ratio of $NaNO_2$ was weighed into a separate container, dissolved at room temperature, and the solution was cooled to 0°C. The cold $NaNO_2$ solution was added dropwise to the cooled content of the three-necked flask by keeping the temperature below 0°C. Following the complete addition of $NaNO_2$, the mixture was stirred extra 30 min in the ice bath. The insoluble diazonium salt was filtered and the product was recrystallized by dissolving in cold (0°C) acetonitrile followed by slow addition of cold anhydrous ether to recover the diazonium tetrafluoroborate salt.

Ultra pure quality of water with a resistance of 18.3 [MΩ·cm], obtained from HumanPower 1+ purification system, was used in all experiments. In all experiments, the solutions were thoroughly deoxygenated by bubbling with purified argon gas (99.999%) for 10 min prior to the voltammetric measurements and an argon gas blanket was maintained over the solutions during the electrochemical experiments to keep the oxygen away from the solution.

3.2. *Instrumentation*

Electrochemical Measurements: A classical three-electrode cell system was used in all electrochemical experiments. Ag/Ag^+ (0.01 M in 0.1 M TBATFB in acetonitrile) reference electrode was used in non aqueous solutions during modification. The Ag/Ag+ reference electrode was calibrated to ferrocene standard solution and a Pt wire counter electrode was employed. BAS Model MF-2012 and Tokai GC-20 glassy carbon electrodes were used as working electrodes. The NAB modified GC electrode is designated as NAB-GC electrode with a geometric area of 0.071 cm^2. CV technique was performed with a BAS CV-50W electrochemical analyzer (Bioanalytical Systems, West Lafayette, IN, USA) equipped with C3 Cell Stand.

IR Measurements: The FTIR spectra of NAB films on the GC surface and bare GC surface were obtained using a Bruker Tensor 27 spectrometer (Bruker Optics Inc., Ettlingen, Germany) at room temperature. The spectrometer is equipped with a Ge crystal attenuated total reflectance (Ge-ATR) accessory and a DTGS detector. All spectra were collected in the region 4000 – 600 cm^{-1} with 256 scans at 4 cm^{-1} resolutions. The IR spectra of solid NAB-DAS were taken after they were accumulated on GC surface.

Polishing and Cleaning of Glassy Carbon Electrodes. Glassy carbon (GC) electrodes (Bioanalytical Systems, 0.071 cm^2) were polished successively in 0.3 μm and 0.05 μm alumina slurries (Baikowski Int.Corp.). Nanopure water (18 MΩ cm) on Buehler polishing microcloth. Polished GC electrodes were sonicated in Nanopure water and then in a mixture of 50:50 (v/v) 2-propanol (IPA) (Riedel-de Haën)/acetonitrile (Aldrich) combined with an equal volume of Norit A activated carbon. Electrodes were rinsed with acetonitrile, which had been purified with activated carbon, and then with Nanopure water, dried with an argon gas stream, and derivatized immediately.

Derivatization of GC with Diazonium Tetrafluoroborate Salt. The electrochemical derivatization procedure was adapted from published procedures [Solak et al., 2003]. Surface derivatization of GC was performed using 1 mM solutions of the NAB-DAS 0.1 M TBATFB in acetonitrile. The diazonium salt solutions were deaerated with argon for at least 10 min before derivatization. Derivatization of the surfaces was performed using cyclic voltammetry with a scan rate of 200 mV/s for 10 complete cycles between +0.4 and -0.8 V versus Ag^+/Ag.

4. Results and Discussion

One of the main problems of nanostructured materials or electrochemical modification of electrode surfaces is the qualitative and quantitative chractarizations of nano systems

or nano layers on the modified electrode systems. Todays's instrumentaion techniques namely X-ray photo electron spectroscopy (XPS), electron spin resonance (ESR) and, especially, infrared (IR) spectroscopy, as well as electrochemical and electrochemical impedance spectroscopic (EIS) methods do not provide desirable analytical results for the identification or characterization of structural nano systems. For these kinds of signals the presence of noise complicates the procedure how to read these signals and implicitly how to identify existence of nanofilm.

In this study a factor analysis application was performed to identify the nanostructured NAB on the NAB-modified GC electrode systems. The extraction of loading factors representing the symmetric data matrix obtained from IR spectra of GC electrodes and their NAB-modified GC electrodes and NAB-nanofilms (obtained as a difference between GC and modified systems) were performed by the factor analysis in order to classify and detect the difference of the modified and unmodified electrode systems for monitoring the nanofilms.

In this study the IR spectra defined by FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5, were used as an input for the factor analysis procedure. In the first step, a dispersion matrix consisting of correlation coefficients obtained from IR data of FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5 was computed by means of the written M-file window in Mathlab 7.10 software. The out of the above procedure was illustrated in Table 1. The eigenvalues and their corresponding eigenvectors were calculated from a dispersion matrix consisting of correlation coefficients. Eigenvalues with cumulative percent contrubution for each factor were depicted in the second part of the Table 1 for FILM, GC-NAB and GC sequences, repectively. The eigenvectors coresponding to the above eigenvalues for each factor were shown in Table 2.

By comparing the cumulative contribution of the all factors mentioned in the last part of the Table 1 for FILM, GC-NAB and GC sequences, respectively we decided that the first two factors (cumulative % contribution is 96.63 for Table 1 are sufficient for our purposes via factor loadings.

Table 1. The matrix of the correlation coefficeients obtained from the IR data and the corresponding extracted eigenvalues with cumilative percent contrubution for each factor

	FILM1	GC-NAB1	GC1	FILM 2	GC-NAB2	GC2	FILM 3	GC-NAB3	GC3	FILM 4	GC-NAB4	GC5	FILM 5	GC-NAB5	GC5
FILM1	1	0.1977	0.1560	0.7620	0.1827	0.1154	0.8503	0.1695	0.1254	0.8386	0.1966	0.1671	0.8183	0.1875	0.1608
GC-NAB1	0.1977	1	0.9986	0.3124	0.9996	0.9957	0.2416	0.9985	0.9963	0.4122	0.9993	0.9992	0.2797	0.9992	0.9987
GC1	0.1560	0.9986	1	0.2833	0.9993	0.9990	0.2051	0.9989	0.9993	0.3826	0.9990	0.9999	0.2476	0.9993	1.0000
FILM2	0.7620	0.3124	0.2833	1	0.3073	0.2548	0.8384	0.3064	0.2642	0.9093	0.3169	0.2911	0.9316	0.3101	0.2881
GC-NAB2	0.1827	0.9996	0.9993	0.3073	1	0.9972	0.2317	0.9992	0.9978	0.4070	0.9996	0.9997	0.2732	0.9997	0.9995
GC2	0.1154	0.9957	0.9990	0.2548	0.9972	1	0.1690	0.9977	0.9999	0.3498	0.9961	0.9983	0.2154	0.9969	0.9988
FILM3	0.8503	0.2416	0.2051	0.8384	0.2317	0.1690	1	0.2244	0.1790	0.8766	0.2447	0.2155	0.9216	0.2362	0.2106
GC-NAB3	0.1695	0.9985	0.9989	0.3064	0.9992	0.9977	0.2244	1	0.9983	0.3997	0.9988	0.9990	0.2699	0.9991	0.9991
GC3	0.1254	0.9963	0.9993	0.2642	0.9978	0.9999	0.1790	0.9983	1	0.3600	0.9970	0.9988	0.2255	0.9977	0.9992
FILM4	0.8386	0.4122	0.3826	0.9093	0.4070	0.3498	0.8766	0.3997	0.3600	1	0.4195	0.3914	0.9231	0.4117	0.3877
GC-NAB4	0.1966	0.9993	0.9990	0.3169	0.9996	0.9961	0.2447	0.9988	0.9970	0.4195	1	0.9994	0.2849	0.9999	0.9992
GC5	0.1671	0.9992	0.9999	0.2911	0.9997	0.9983	0.2155	0.9990	0.9988	0.3914	0.9994	1	0.2567	0.9996	0.9999
FILM5	0.8183	0.2797	0.2476	0.9316	0.2732	0.2154	0.9216	0.2699	0.2255	0.9231	0.2849	0.2567	1	0.2773	0.2529
GC-NAB5	0.1875	0.9992	0.9993	0.3101	0.9997	0.9969	0.2362	0.9991	0.9977	0.4117	0.9999	0.9996	0.2773	1	0.9996
GC5	0.1608	0.9987	1.0000	0.2881	0.9995	0.9988	0.2106	0.9991	0.9992	0.3877	0.9992	0.9999	0.2529	0.9996	1
Factor	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Eigenvalue	10.5934	3.9016	0.2585	0.1353	0.0658	0.0424	0.0013	0.0011	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
% Contrubution	70.62	96.63	98.36	99.26	99.70	99.98	99.99	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 2. The eigenvectors extracted from the matrix of the correlation coefficeients obtained from the IR data

	Eigenvectors														
	F(I)	F(II)	F(III)	F(IV)	F(VI)	F(VII)	F(VIII)	F(X)	F(XI)	F(XII)	F(XIII)	F(XIV)	F(XV)	F(XVI)	F(XVII)
FILM 1	0.0996	0.4292	-0.7701	-0.3704	-0.2551	-0.0707	-0.0666	-0.0103	0.0272	-0.0155	-0.0055	0.0049	-0.0017	0.0018	-0.0010
GC-NAB1	0.3032	-0.0792	-0.0509	0.0058	-0.0522	0.0107	0.6882	-0.1434	0.2838	0.3816	0.3302	-0.2245	0.1019	-0.0773	0.0088
GC1	0.3014	-0.0980	-0.0119	0.0038	-0.0079	-0.0014	-0.0699	0.2512	0.0987	0.4039	-0.2323	0.2122	-0.7253	-0.0221	-0.1814
FILM 2	0.1392	0.4169	0.5447	-0.3856	-0.4432	0.4050	0.0008	0.0310	-0.0096	-0.0015	-0.0005	-0.0016	0.0024	-0.0008	0.0014
GC-NAB2	0.3029	-0.0840	-0.0202	0.0055	-0.0131	0.0035	0.3748	-0.0515	0.0086	-0.7786	-0.0761	-0.0067	-0.3027	0.1991	-0.1184
GC2	0.2989	-0.1164	0.0249	0.0036	-0.0085	-0.0122	-0.3218	-0.0034	0.5634	-0.0973	-0.4218	-0.4665	0.1949	-0.1796	0.0047
FILM 3	0.1169	0.4416	-0.1371	0.7815	-0.0321	0.3990	-0.0314	0.0007	0.0216	-0.0048	0.0001	0.0010	-0.0018	0.0013	0.0012
GC-NAB3	0.3025	-0.0875	0.0161	0.0105	-0.0397	-0.0073	-0.1649	-0.8648	-0.2418	0.1242	-0.1588	0.1562	-0.0102	0.0067	-0.0121
GC3	0.2997	-0.1111	0.0234	0.0022	-0.0015	-0.0126	-0.4461	0.0055	0.2397	-0.1644	0.7430	0.1778	-0.0887	-0.0846	0.1221
FILM 4	0.1686	0.4051	0.0801	-0.2581	0.8494	0.1041	0.0188	-0.0314	0.0230	0.0150	0.0015	0.0015	0.0015	0.0020	0.0016
GC-NAB4	0.3036	-0.0773	-0.0319	0.0075	0.0066	0.0022	0.0023	0.2149	-0.5102	-0.0741	0.0408	-0.1114	0.1592	-0.6605	-0.3363
GC5	0.3020	-0.0929	-0.0216	0.0069	-0.0099	-0.0006	0.1519	0.2160	0.0630	-0.0258	-0.2706	0.6261	0.3464	-0.1065	0.4781
FILM 5	0.1308	0.4428	0.2798	0.1906	-0.1058	-0.8126	0.0179	0.0168	0.0011	0.0030	0.0013	0.0003	-0.0001	-0.0010	-0.0028
GC-NAB5	0.3032	-0.0817	-0.0251	0.0068	0.0022	-0.0041	-0.0942	0.1806	-0.4536	0.0985	0.0208	-0.4653	-0.0910	0.3192	0.5628
GC5	0.3017	-0.0953	-0.0117	0.0062	-0.0033	-0.0025	-0.1150	0.1950	-0.0665	0.1293	0.0252	0.1001	0.4151	0.6041	-0.5286

As we mentioned before we retain the first two eigenvectors corresponding the the first two eingenvalues. As shown in Table 3 (for FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5), the factor loadings posses negative values and this fact implies that the chemical meaning is hidden. In order to make the results with chemical interpretation we used so called rotated factor loadings. This rotation is based on the orthogonal varimax rotation technique. The obtained positive results are illustrated in Table 4 (for FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5, respectively).

By starting two columns from Table 3, the plot of the original factor loadings for the first two factors was shown on Figure 1. Due to the negative numerical values in Table 3, this plot given in Figure 1 gives us a restruction knowlege for the interpretion of the results to characterize the nanofilms (NAB-FILMs) on the modified GC-NAB electrodes.

Table 3. The factor loadings matrix obtained by the application of factor analysis of the IR data

	Factor loadings														
	F(I)	F(II)	F(III)	F(IV)	F(VI)	F(VII)	F(VIII)	F(X)	F(XI)	F(XII)	F(XIII)	F(XIV)	F(XV)	F(XVI)	F(XVII)
FILM 1	0.3240	0.8477	-0.3915	-0.1362	-0.0654	-0.0145	-0.0024	-0.0003	0.0006	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB1	0.9869	-0.1565	-0.0259	0.0021	-0.0134	0.0022	0.0243	-0.0047	0.0064	0.0048	0.0012	-0.0007	0.0002	-0.0001	0.0000
GC1	0.9810	-0.1937	-0.0061	0.0014	-0.0020	-0.0003	-0.0025	0.0082	0.0022	0.0051	-0.0008	0.0007	-0.0011	0.0000	-0.0002
FILM 2	0.4530	0.8235	0.2769	-0.1418	-0.1137	0.0834	0.0000	0.0010	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB2	0.9859	-0.1659	-0.0103	0.0020	-0.0034	0.0007	0.0133	-0.0017	0.0002	-0.0098	-0.0003	0.0000	-0.0005	0.0003	-0.0001
GC2	0.9730	-0.2299	0.0127	0.0013	-0.0022	-0.0025	-0.0114	-0.0001	0.0127	-0.0012	-0.0015	-0.0014	0.0003	-0.0002	0.0000
FILM 3	0.3805	0.8723	-0.0697	0.2874	-0.0082	0.0821	-0.0011	0.0000	0.0005	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB3	0.9844	-0.1728	0.0082	0.0039	-0.0102	-0.0015	-0.0058	-0.0283	-0.0054	0.0016	-0.0006	0.0005	0.0000	0.0000	0.0000

GC3	0.9754	-0.2194	0.0119	0.0008	-0.0004	-0.0026	-0.0158	0.0002	0.0054	-0.0021	0.0026	0.0005	-0.0001	-0.0001	0.0001
FILM 4	0.5488	0.8002	0.0407	-0.0949	0.2178	0.0214	0.0007	-0.0010	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB4	0.9881	-0.1526	-0.0162	0.0028	0.0017	0.0004	0.0001	0.0070	-0.0115	-0.0009	0.0001	-0.0003	0.0002	-0.0009	-0.0003
GC5	0.9829	-0.1834	-0.0110	0.0025	-0.0025	-0.0001	0.0054	0.0071	0.0014	-0.0003	-0.0010	0.0019	0.0005	-0.0001	0.0004
FILM 5	0.4257	0.8746	0.1423	0.0701	-0.0271	-0.1673	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB5	0.9867	-0.1614	-0.0128	0.0025	0.0006	-0.0008	-0.0033	0.0059	-0.0102	0.0012	0.0001	-0.0014	-0.0001	0.0004	0.0005
GC5	0.9821	-0.1882	-0.0060	0.0023	-0.0009	-0.0005	-0.0041	0.0064	-0.0015	0.0016	0.0001	0.0003	0.0006	0.0008	-0.0005

Table 4. The rotated factor loadings matrix provided by applying the varimax rotation to the factor loadings matrix

							Rotated factor loadings								
	F(I)	F(II)	F(III)	F(IV)	F(VI)	F(VII)	F(VIII)	F(X)	F(XI)	F(XII)	F(XIII)	F(XIV)	F(XV)	F(XVI)	F(XVII)
FILM 1	0.0479	0.8787	-0.4746	0.0191	0.0029	0.0029	0.0002	0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB1	0.9867	0.1590	-0.0225	0.0014	-0.0001	0.0046	0.0264	0.0006	0.0000	-0.0008	0.0003	0.0001	0.0000	0.0000	0.0000
GC1	0.9923	0.1232	-0.0006	-0.0051	0.0092	0.0014	-0.0022	0.0076	0.0010	0.0061	-0.0009	0.0006	-0.0016	-0.0001	0.0000
FILM 2	0.1687	0.9357	0.1345	-0.2394	-0.0728	0.1240	0.0004	-0.0002	-0.0003	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB2	0.9884	0.1508	-0.0061	-0.0029	0.0083	0.0023	0.0107	0.0012	-0.0024	-0.0126	-0.0001	0.0001	-0.0001	0.0000	0.0000
GC2	0.9957	0.0874	0.0188	-0.0130	0.0075	-0.0003	-0.0078	0.0005	0.0151	0.0016	-0.0008	-0.0007	0.0004	-0.0003	-0.0002
FILM 3	0.0912	0.9468	-0.0175	0.2974	-0.0650	0.0481	0.0003	0.0000	-0.0003	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB3	0.9889	0.1450	0.0107	-0.0101	0.0000	0.0013	-0.0006	-0.0296	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC3	0.9947	0.0981	0.0175	-0.0127	0.0094	-0.0006	-0.0137	-0.0013	0.0091	0.0017	0.0035	-0.0001	0.0001	0.0000	0.0000
FILM 4	0.2674	0.9311	-0.0163	-0.0483	0.2424	0.0099	-0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB4	0.9863	0.1637	-0.0115	0.0012	0.0133	0.0013	-0.0040	0.0046	-0.0121	-0.0007	-0.0005	-0.0007	0.0007	-0.0005	-0.0008
GC5	0.9910	0.1332	-0.0054	-0.0022	0.0088	0.0013	0.0039	0.0080	-0.0013	-0.0009	-0.0008	0.0024	0.0000	0.0000	0.0003
FILM 5	0.1295	0.9722	0.0868	-0.0178	-0.0605	-0.1628	0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GC-NAB5	0.9877	0.1552	-0.0081	-0.0009	0.0119	0.0003	-0.0062	0.0031	-0.0099	0.0021	-0.0007	-0.0019	0.0004	-0.0002	0.0006
GC5	0.9916	0.1288	-0.0004	-0.0041	0.0101	0.0009	-0.0049	0.0051	-0.0016	0.0029	-0.0001	0.0002	0.0003	0.0011	0.0001

However, the plot of the rotated factor loadings for the first two factors was given in Figure 2. In addition, as it can be clearly seen from Figure 3 (3 dimensional plot for FILM1, GC-NAB1, GC1; FILM2, GC-NAB2, GC2; FILM3, GC-NAB3, GC3; FILM4, GC-NAB4, GC4; FILM5, GC-NAB5, GC5), the calculated loading factors provide us a reach information about the existence of the nanofilms (FILM1,...,FILM 5).
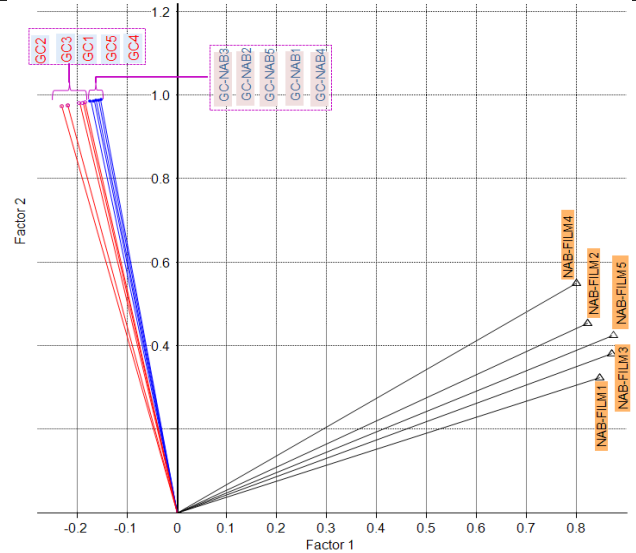

Fig 1. The original factor loadings obtained from the IR data provided by applying varimax rotation technique for the the GC electrode, modified NAB-GC electrode and corresponding nanofilm with two factors retained in the model

From Table 4 and Figure 1-3, we concluded that the data and graphical results of the factor analysis with the orthogonal

varimax rotation technique indicate the exsistance of FILMs (NAB-FILMs) on the modified NAB-GC electrode systems.
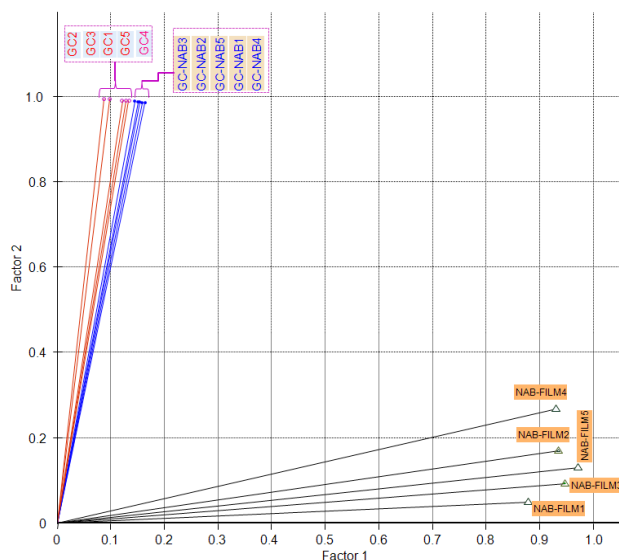

Fig 2. The rotated loadings provided by applying varimax rotation technique for the the GC electrode, modified NAB-GC electrode and corresponding nanofilm with two factors retained in the model

5. Conclusions

The quantitative characterization of the nanostructured systems is one of the fundamental issues for the electrochemical modification studies of electrode surfaces and the related domains. In this study, the factor analysis approach with a varimax orthogonal rotation technique was successful applied to the qualitative identification of the NAB
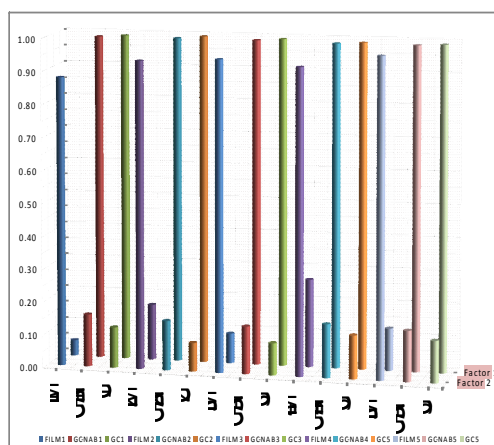
Fig 3. 3D-Bar representations of the rotated first factor loadings obtained by applying varimax rotation to the original factor loadings provided from the IR spectra of the GC electrode, modified NAB-GC electrode and corresponding nanofilm (GC-NAB)

nano films on the modified GC electrodes. We conclude that the factor analysis is a powerful mathematical tool for the extraction of the latent information from the modified electrode systems. As a result, the proposed technique can extract the expected information even in the cases when the classical analytical instrumentation approaches cannot provide the required results. This approach is rapid, simple and gives a better resolution to characterize complex nanostructures without additional experimental studies and sophisticated analytical instrumentations.

Acknowledgments

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