Different approaches for SiO_2 inelastic electron scattering cross section spectra dissolving

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Different approaches for SiO_2 inelastic electron scattering cross section spectra dissolving

A Yu Igumenov and T A Andryushchenko

Reshetnev Siberian State University of Science and Technology, 31 Krasnoyarskii rabochii prospekt, Krasnoyarsk, 660037, Russia

E-mail: igumenovau@mail.ru

Abstract. Inelastic electron scattering cross section spectra (Kλ-spectra) of SiO_2 were dissolved into bulk-loss and surface-loss components using factor analysis and Tougaard functions approximation. Primary electron energy dependences of various components intensities were received. It was shown that joint using of factor analysis and Tougaard functions approximation allows receiving more reliable results in inelastic electron scattering cross section spectra studies.

1. Introduction

Silicon dioxide is widely used for the development of micro- and nanoelectronics. SiO_2 is the most common gate dielectric for creating devices based on metal-dielectric-semiconductor (MOSFET) structures. Currently, various SiO_2-based materials are developing to achieve a higher band gap value. Accordingly, the elemental composition and chemical bonds analyzing methods, including electron spectroscopy methods, are in demand.

In this paper inelastic electron scattering cross section spectra ($K\lambda$-spectra) of SiO_2 were investigated by dissolving it into bulk-loss and surface-loss components by factor analysis (FA) [1-5] and Tougaard functions approximation [5-10].

2. Experimental

This paper presents the results of SiO_2 $K\lambda$-spectra investigation. Inelastic electron scattering cross section spectra ($K\lambda$-spectra) [11-13] are the product of the inelastic mean free path λ and the differential inelastic scattering cross section K (E_0, E_0 - E), where E_0 and E are the energies of primary and reflected electrons, $T = E_0 - E$ are electron energy losses. The spectra were analyzed at the primary electron energies of 300, 600, 1200, 1900, and 3000 eV.

Factor analysis allows processing the original set of spectra as a single array. Factor analysis identifies trends in spectra shape evolution with primary electron energy variation. It determines the number of independent components (Principal component analysis) from each other and divides them. As usually, these energy-loss components have bulk-loss and surface-loss origin.

Figure 1 shows the factor analysis stages. The original spectra is decomposed into the linear combination of most intense contributions. Components shape are optimized to reach Tougaard peak [11] shape using multiplying factor axes by the rotating matrix R (1) (Target transformation):

$$R = \begin{bmatrix} cos\varphi & sin\varphi \\ -sin\varphi & cos\varphi \end{bmatrix}, \quad (1)$$

where φ is the angle of factors rotation.

After that the original spectra are represented as a linear combination of factors.

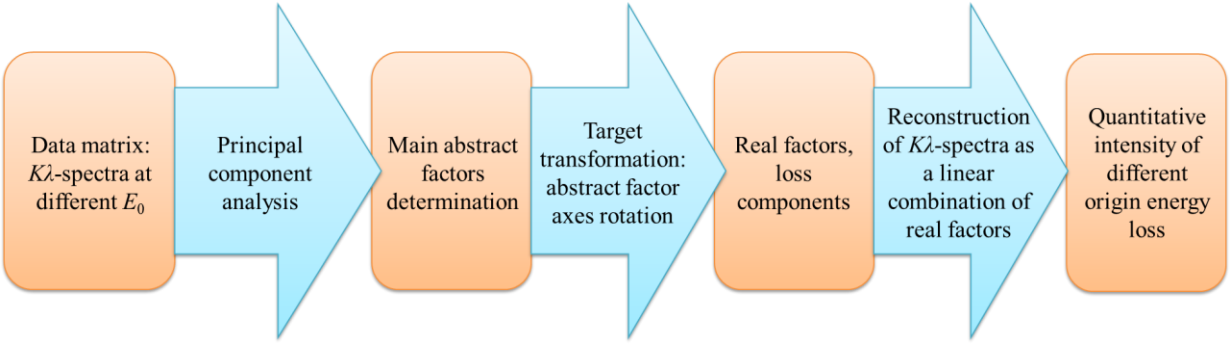


Figure 1. The factor analysis stages.

The Tougaard functions approximation is applied to each spectra separately and usually allows to bring out a larger number of components in spectra, then FA. It is possible to directly control the number of peaks, its width, position, and intensity. The three-parameter Tougaard function has the following form (2) [13]:

$$\lambda K = \frac{BT}{\left(C - T^2\right)^2 + DT^2}, \tag{2}$$

B, *C*, *D* are fitting parameters and have special values for different elements. The peak intensity depends on parameter *B*, peak energy depends on parameter *C* but does not correspond to it explicitly, peak width and, indirectly, peak energy depend on parameter *D*. Tougaard functions (universal classes of inelastic electron scattering cross section) are used to describe inelastic electron scattering cross section spectra.

The Tougaard three-parameter function has been modified (3):

$$\lambda K = \frac{BT}{\left(\left(T_p\left(-T_p + \sqrt{4T_p^2 + D}\right)\right) - T^2\right)^2 + DT^2}, \tag{3}$$

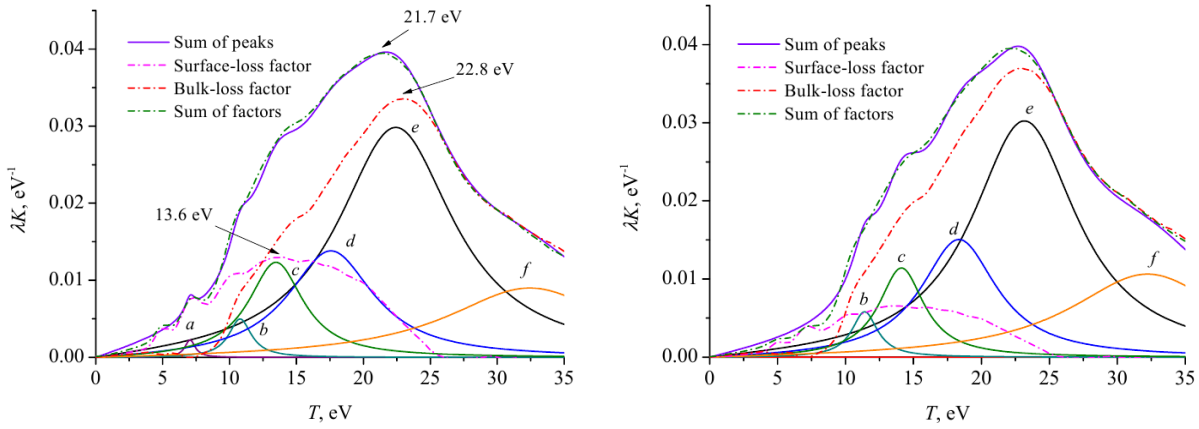
where the parameter T_p corresponds to the position of the peak maximum in absolute units.

3. Results and discussion

The original $K\lambda$-spectra were dissolved into 6 peaks (*a*-*f*) with using Tougaard function approximation. This number of components makes it possible to describe the original spectra with sufficient accuracy. It is possible to divide the contributions of different origin, which are bulk and surface plasmons, electron transitions combining certain peaks.

Using factor analysis two contributions were received. These contributions describe the different origin of electron excitations in a solid. The energy loss of the surface-loss factor which corresponds to the excitation of surface plasmon is 13.6 eV; the maximum of the bulk-loss factor is describing the excitation of bulk plasmon and located at energy loss 22.8 eV. The energy of the bulk-loss factor maximum is close to the bulk plasmon energy in SiO_2 [14].

The peaks and factors at primary electron energies 600 and 1900 eV are shown in figure 2.



(a) (b)

Figure 2. SiO_2 spectra dissolving at primary electron energies (a) 600 and (b) 1900 eV.

The Tougaard function approximation and factor analysis represent close to each other cumulative spectra. The fitting spectra shape is identical to the original $K\lambda$-spectra shape. This suggests that it is possible to accurately describe the original inelastic electron scattering cross section spectra and identify different origin contributions using both methods.

As it stands, the components intensity is changing with primary electron energy increasing. As can be seen in figure 2, the peak *a* disappears in the high primary electron energy spectra. Its position and behavior indicate that it belongs to the surface contribution group of the spectra. Figure 3 illustrates the primary electron energy dependences of peaks and factors positions.

Peak *a* is absent in the high primary electron energy spectra. The position of other peaks is almost unchanged that is an indicator of low mathematical uncertainty of these dissolving. The factor maximums energies remain constant when primary electron energy changes because the factors were obtained with using the entire array of source spectra, and its positions are determined from the general analysis. The position of the surface-loss factor is close to the position of Tougaard peak *c* from approximation set. The bulk-loss factor energy corresponds to peak *e* position. Figure 2 shows that these Tougaard peaks are the most intense. Thus, peaks *c* and *e* are interpreted as surface and bulk plasmons, and peaks *a*, *b*, *d*, and *f* are electron transitions.

The surface origin contribution intensity decreases and the bulk origin contribution intensity increases with an increasing of primary electron energy. This is well illustrated by the integral intensities (area) of factors or combinations of Tougaard peaks depending on the primary electron energy, as shown in figure 4. The combination of peaks *a*, *b*, and *c* describes the surface origin contribution in the inelastic electron scattering cross section spectra. Peaks *d*, *e*, and *f* belong to the bulk origin group of peaks.

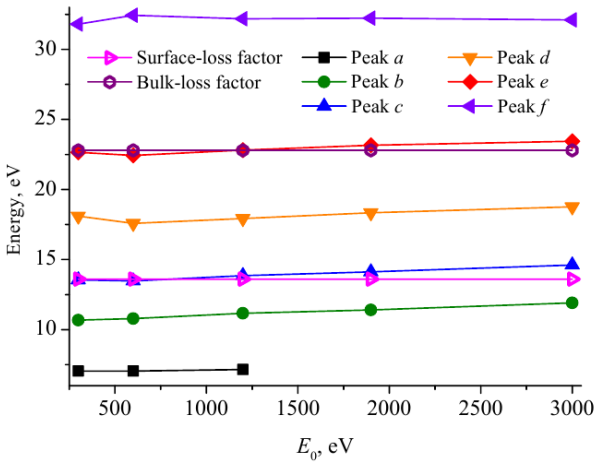


Figure 3. Primary electron energy dependences of peaks and factors positions.

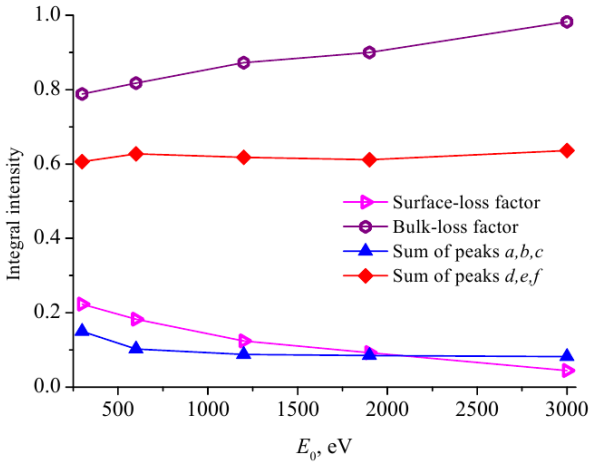


Figure 4. Primary electron energy dependences of peaks and factors area.

The behavior of peaks *a*, *b*, and *c* areas combination is similar to the dependence which is obtained for the surface-loss factor. This confirms the agreement of results that were obtained by different methods. Peaks *d*, *e* and *f* areas combination and the bulk-loss factor have an increasing character of the primary electron energy dependence that confirms its origin.

4. Conclusions

It is shown that the combined application of factor analysis and Tougaard function approximation allows obtaining more reliable and detailed information about the electron energy loss processes, determining peak energies, intensities and divide the bulk and surface contributions. The energies and integral intensities of surface and bulk plasmons and electron transitions are determined. The fitting peaks and factors energies are consistent with the electron energy loss literature data. Primary electron energy dependences of peaks and factors intensity indicate bulk and surface origin of excitations.

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