A DIFFERENTIATION OF GLASS MICROTRACES OF THE SAME QUALITATIVE COMPOSITION

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ABSTRACT: Analysis of glass microtraces by means of SEM-EDX method provides an information about their main elemental content. The lack of information on the trace elements becomes a difficulty in the case of differentiation of glass objects revealing a similar chemical contents, e.g. vehicle windows and ordinary window sheets. Moreover, chemometric analysis of the analytical results obtained with this method for several glass microtraces originating from the same glass item usually does not allow to treat it as a homogenous object.

A satisfactory solution of the problem of differentiation of two glass objects revealing the same qualitative contents determined with SEM-EDX method was obtained when considering the following model.

Several fragments were selected from two glass items of the same qualitative composition being compared. Mean values of the elements concentration were determined for each fragment. Each of the microtraces was treated as a point in a multidimensional space, described by the mean values of the elements concentrations. Distances between defined in this manner points were calculated. It was assumed that microtraces originating from the same glass item created one cluster. Distances between points in such cluster were smaller than distances between points (microtraces) originating from the two compared items. The formulated in this way problem was statistically tested.

KEY WORDS: SEM-EDX; Glass microtraces differentiation; Multivariable analysis.

Problems of Forensic Sciences, vol. XLVII, 2001, 144–146 Received 26 Februar 2001; accepted 15 September 2001

INTRODUCTION

Comparative examination of samples is one of the main tasks in the field of criminalistics. It usually concerns objects of a similar elemental composition and similar physical properties. Glass as evidence material often occurs in very small quantities. Thus, investigations of glass samples require sensitive analytical methods providing satisfactory results from small amounts of the examined material. One of these methods is the quantitative elemental analysis using a scanning electron microscope with an energy dispersive X-ray spectrometer (SEM-EDX) [3].

It is a method that allows to determine elements present at concentrations at least 0.1% by weight, however it does not provide information on traces elements. Nevertheless, SEM-EDX is useful for examination of very small objects [1, 2].

METHODOLOGY AND DISCUSION

The subject of the study were results of SEM-EDX analysis of glass objects revealing the same qualitative composition. The following model was considered for the differentiation of these glass objects. An object A (e.g. "an evidence sample") and an object B ("a comparative sample") were compared. Several microtraces were taken from each object and the elemental composition was determined for each microtrace. Each sample could be described by 5 or more features because at least 5 elements were determined for each microtrace. Thus, the microtraces could be treated as points in the multidimensional space. In this situation it is necessary to answer the following question: "Do these points create one or two clusters?". The following attempt was used to solve this problem.

Distances between these points were calculated. The "cord" distance {1} was applied as there was not necessary to perform any normalisation of raw data before calculating the distances. For objects, e.g. A1 and B2 the cord distance can be expressed as the following formula:

$$d_{A1-B2} = \sqrt{2 \left(1 - \frac{\sum_{k=1}^{n} c_{A1_{k}} \cdot c_{B2_{k}}}{\sqrt{\sum_{k=1}^{n} c_{A1_{k}}^{2} \cdot \sum_{k=1}^{n} c_{B2_{k}}^{2}}} \right)}$$

$$\{1\}$$

where: c - a concentration of k-th element for compared microtraces A1 and B2; n - a number of the considered elements.

The obtained distances were included in the range from 0 to 1.44. On the base of the obtained results the following values were calculated:

- the mean value of distances between microtraces taken from the same object (d_{int}) was calculated;
- the mean value of distances between microtraces taken from the different objects (d_{ext}) was calculated.

When three microtraces originated from sample A and three microtraces originated from sample B were considered than formulas $\{2\}$ and $\{3\}$ were used for calculating d_{int} and d_{ext} .

$$d_{\rm int} = \frac{d_{A1-A2} + d_{A1-A3} + d_{A2-A3} + d_{B1-B2} + d_{B1-B3} + d_{B2-B3}}{6};$$
(2)

$$d_{ext} = \frac{d_{A1-B1} + d_{A1-B2} + d_{A1-B3} + d_{A2-B1} + d_{A2-B2} + d_{A2-B3} + d_{A3-B1} + d_{A3-B2} + d_{A3-B3}}{9}.$$
 (3)

The following assumptions were considered:

- when the value of d_{int} is lower than d_{ext} than considered microtraces came from different objects;
- when the value of $d_{\rm int}$ was equal to d_{ext} than considered microtraces came from the same object.

In order to check these assumptions the null hypothesis {4} was tested.

$$H_0: d_{int} \le d_{ext}.$$

$$\{4\}$$

The t-Student test was used in order to calculate the probability of acceptance of the null hypothesis (*p*).

In the case when microtraces A_i and B_i were taken from the same object, p was higher than 0.3. In the opposite case the p value was lower than 0.3 (for most of the cases between 0.1–0.15).

CONCLUSION

The differentiation of glass objects revealing the same qualitative elemental composition (determined with SEM-EDX method) can be achieved using the presented approach based upon a cluster analysis.

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