OSAC RESEARCH NEEDS ASSESSMENT FORM

Title of research need: Cross-validation of current and new micro-XRF technology for the the forensic analysis of modern glass.

Keyword(s): Glass, X-ray Fluorescence, validation, databases, elemental analysis

Submitting subcommittee(s): Materials/Trace **Date Approved:** 9/24/18

(If SAC review identifies additional subcommittees, add them to the box above.)

Background Information:

1. Description of research need:

The elemental analysis of glass provides valuable information in the comparison of glass evidence. Micro X-ray Fluorescence has shown to be a valid analytical technique for the comparison of the elemental composition of glass, and a standard test method is now available to forensic examiners.

LA-ICP-MS and micro- XRF are recognized as the most informative tools for forensic glass comparisons. Nonetheless, the most extensive existing glass databases have been built primarily with ICP data (ICP-MS, ICP-OES, and LA-ICP-MS). It will be useful for the XRF-users to generate larger collection datasets that include modern glass compositions to expand the current knowledge on XRF-elemental profiles of glass, evaluate the potential of sharing databases among laboratories, and use alternative probabilistic interpretation approaches.

Moreover, in recent years modern micro-XRF systems are employing SDD detectors instead of the traditional SiLi detectors as they are anticipated to be more sensitive and precise. The comparison among systems currently available at crime laboratories will provide an essential body of knowledge to evaluate the performance of SiLi and SDD detectors under the current ASTM standard method E2926-17.

2. Key bibliographic references relating to this research need:

1. Almirall J, Trejos T. Advances in the Forensic Analysis of Glass Fragments with a Focus on Refractive Index and Elemental Analysis. Forensic Science Review 2006,18(2):73–96.
2. Almirall J, Trejos T. Analysis of Glass Evidence. In: Siegel JA, editor. Forensic Chemistry Fundamentals and Applications. Chichester, UK: John Wiley & Sons, Ltd, 2015; 228–72.
3. ASTM E2330-12. Standard Test Method for Determination of Concentrations of Elements in Glass Samples Using Inductively Coupled Plasma Mass Spectrometry (ICP-MS) for Forensic Comparisons, ASTM International, Vol 14.02
4. ASTM E2926-17. Standard Test Method for Forensic Comparison of Glass Using Micro X-ray Fluorescence (μ-XRF) Spectrometry, ASTM International, Vol 14.02
5. ASTM E2927-16. Standard Test Method for Determination of Trace Elements in Soda-Lime Glass Samples Using Laser Ablation Inductively Coupled Plasma Mass Spectrometry for Forensic Comparisons, ASTM International, Vol 14.02
6. Becker S, Gunaratnam L, Hicks T, Stoecklein W, Warman G. The differentiation of float glass using refractive index and elemental analysis: Comparisons of techniques. Problems of Forensic Science, Vol. 47, 2001, 80-92.
7. Corzo, R, Hoffman, T, Weis, P, Franco-Pedroso, J, Ramos D, Almirall J. The use of LA-ICP-MS databases to calculate likelihood ratios for the forensic analysis of glass evidence. Talanta, 186, 2018, 655-661.
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forensic glass evidence. Science & Justice 38(1), 1998, 15–21.
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12. Duckworth DC, Baynes CK, Morton SJ, Almirall JR. Analysis of variance in forensic glass analysis by ICP-MS: Variance within the method. Journal of Analytical Atomic Spectrometry, Vol. 15, 2000, 821-828.
13. Duckworth DC, Morton S, Baynes C, Koons, RD, Montero S, Almirall JR. Forensic glass analysis by ICP-MS: A multi-element assessment of discriminating power via analysis of variance and pairwise comparisons, Journal of Analytical Atomic Spectrometry, Vol. 17, 2002, 662-668.
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15. Evett IW, Buckleton J. The interpretation of glass evidence: A practical approach. Journal of the Forensic Science Society, Vol. 30, 1990, 215-223.
16. Hicks T, Monard Sermier F, Goldmann T, Brunelle A, Champo C, Margot P. The classification and discrimination of glass fragments using non-destructive energy dispersive X-ray μ fluorescence. Forensic Science International, Vol. 137, 2003, 107-118.
17. Koons RD, Peters CA, Rebbert PS. Comparison of refractive index, energy dispersive X-ray fluorescence and inductively coupled plasma atomic emission spectrometry for forensic characterization of sheet glass fragments. Journal of Analytical Atomic Spectrometry, Vol. 6, 1991, 451-456.
18. Naes BE, Umpierrez S, Ryland S, Barnett C, Almirall JR. A comparison of laser ablation inductively coupled plasma mass spectrometry, micro X-ray fluorescence spectroscopy, and laser induced breakdown spectroscopy for the discrimination of automotive glass. Spectrochimica Acta Part B: Atomic Spectroscopy
19. Ryland SG. Discrimination of flat (sheet) glass specimens having similar refractive indices using micro X-ray fluorescence spectrometry. Journal of the American Society of Trace Evidence Examiners, Vol. 2, 2011, 2-12.
20. Suzuki Y, Sugita R, Suzuki S, Marumo Y. Forensic discrimination of bottle glass by refractive index measurement and analysis of trace elements with ICP-MS. Analytical Sciences, Vol. 16, 2000, 1195-1198.
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22. Trejos T, Koons R, Becker S, et al. Cross-validation and evaluation of the performance of methods for the elemental analysis of forensic glass by μ-XRF, ICP-MS, and LA-ICP-MS. Anal. Bioanal. Chem. 405, 2013, 5393-5409.
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24. Trejos T, Almirall, JR. Sampling strategies for the analysis of glass fragments by LA-ICP-MS Part I. Micro-homogeneity study of glass and its application to the interpretation of forensic evidence, Talanta, Vol. 67, Issue 2, 2005, 388-395.
25. Trejos T, Montero S, Almirall JR. Analysis and comparison of glass fragments by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) and ICP-MS. Anal. Bioanal. Chem., 376 (8), 2003, 1255–64.
26. Walsh KA, Buckleton J, Triggs CM. A practical example of the interpretation of glass evidence. Science and Justice, Vol. 36, 1996, 213-218.
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28. Zadora G, Ramos D. Evaluation of glass samples for forensic purposes — An application of likelihood ratios and an information–theoretical approach. Chemometrics and Intelligent Laboratory Systems 2010;102(2), 63–83.

3a. In what ways would the research results improve current laboratory capabilities?

LA-ICP-MS and micro- XRF are recognized as the most informative tools for forensic glass comparisons. Although LA-ICP-MS is considered the "gold standard" due to its superior performance, relatively more crime laboratories have access to XRF instrumentation compared to LA-ICP-MS systems due to lower costs of acquisition, ease of use, and straightforward data processing, while still providing high discrimination among glass sources.

Expanding current research on micro- XRF will provide greater support to forensic examiners to defend their results in court. In particular, a useful body of knowledge can be provided by 1) expanding current studies on the variation of XRF elemental composition of glass in modern formulations (within sources, between sources and instrumental variation) and 2) extending studies to evaluate the analytical performance of novel XRF detection technology.

3b. In what ways would the research results improve understanding of the scientific basis for the subcommittee(s)?

At the subcommittee level, these types of research would provide additional support to the interpretation and report writing guidelines that are being developed for glass evidence and trace materials in general.

3c. In what ways would the research results improve services to the criminal justice system?

Increasing the existing body of knowledge on micro-XRF technology for the forensic analysis of glass would allow more efficient use of resources at crime laboratories, and the future application of probabilistic interpretation approaches to support the examiner's opinion in court.

4. Status assessment (I, II, III, or IV): IV

	Major gap in current knowledge	Minor gap in current knowledge
No or limited current research is being conducted	I	III
Existing current research is being conducted	II	IV

This research need has been identified by one or more subcommittees of OSAC and is being provided as an informational resource to the community.

Approvals:

Subcommittee Approval date: 9/24/18

(Approval is by majority vote of subcommittee. Once approved, forward to SAC.)

SAC

1. Does the SAC agree with the research need? Yes [x] No [ ]
2. Does the SAC agree with the status assessment? Yes [x] No [ ]

If no, what is the status assessment of the SAC: [ ]

Approval date: 12/19/18

(Approval is by majority vote of SAC. Once approved, forward to NIST for posting.)