

Database For Trace Analysis

Trace evidence analysis

Coupled with an Energy Dispersive x-ray System (EDS), the Scanning Electron Microscope (SEM) is often used to analyze trace evidence. Automated identification of gun shot residue is an excellent example of this. The traditional approach has been to mount the unknown in some fashion, insert it in the SEM, and collect an x-ray spectrum from the unknown. Peak positions are then used to determine the elements present, and the peak intensities are related to the amounts present. There are several problems associated with the analysis in this approach, however and, as a consequence, the solution reached may be incorrect.

First, there are typically artifacts associated with the spectrum, such as escape and sum peaks, and often, because of the nature of the sample, relatively poor statistics. An experienced operator can usually overcome these obstacles. Another major problem occurs if the sample being examined is not flat, polished and homogeneous at the micron level. Many typical samples (shards, cosmetics, smears, powders, etc.) do not lend themselves to this form of preparation, and as a consequence meaningful quantitative results can not be obtained, even if the model were perfect and the physical parameters well-defined. Finally, supposing perfect chemical analysis results are obtained,

even an experienced user will have difficulty in reliably identifying the material from the chemical analysis. One could compare the unknown sample results to results obtained from similar materials, if one had some idea of what materials to use in the comparison, but this requires intuitive interpretation.

The computer database

The full extent of the problem is exemplified in a computer program developed and patented by C. E. Fiori and C. R. Swyt at NIST in 1994, which allowed theoretical calculation of a spectrum from a hypothetical sample, under varying conditions, for any reason, such as determining detection limits, comparing the theoretical spectrum to real spectra, etc. In use, the operator could pick any one of several models and parameters from many sources to achieve the calculated spectrum, and as might be anticipated, the resulting spectra varied considerably. In fact, by properly (or improperly) choosing your parameters and model, you could obtain nearly any result you wished. For the forensics scientist this is not an entirely satisfactory solution. The general problem can be greatly simplified by an effective search from an extensive database that would reduce the number of candidate materials to a manageable number.

Today, in most spectroscopies, (e.g. FTIR, RAMAN, XRD) databases of spectra exist, and computer programs are used to compare unknown spectra against a database for a match. In the forensics community, databases exist for ballistics, DNA, fingerprints, etc., and the use of these databases is preferred. Toward this

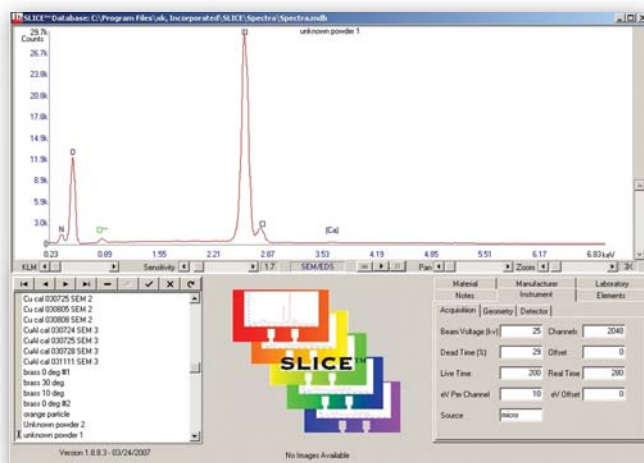


FIGURE 1. Main spectral display window with access to tabbed information on displayed spectrum.

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end, the FBI awarded a contract in 1998 to xk, Incorporated to develop a database and methodology for SEM/EDS analysis. This was completed and developed into the commercial SW package SLICE (Spectral Library for Identification and Classification Explorer).

Since then, SLICE has been extended to include the use of x-ray fluorescence (XRF) spectra. In use, physical parameters that characterize the materials stored in the database are also included. Characteristics such as warp, fill, thickness gauge, color, refractive index, chemistries, instrumental conditions, laboratory, manufacturer, lot number, etc. are included in the truly relational database, and can become a part of the search as well as the degree of fit between the spectrum from the unknown and those in the database, to more fully refine and identify the trace evidence.

An integral part of SLICE is its ability to function nearly independently of operational conditions, and to fully utilize the additional information in the database. The qualitative and quantitative aspects of the analysis are minimized, while the comparative and query aspects have been enhanced to facilitate comparisons and subsequent identification. Currently, the

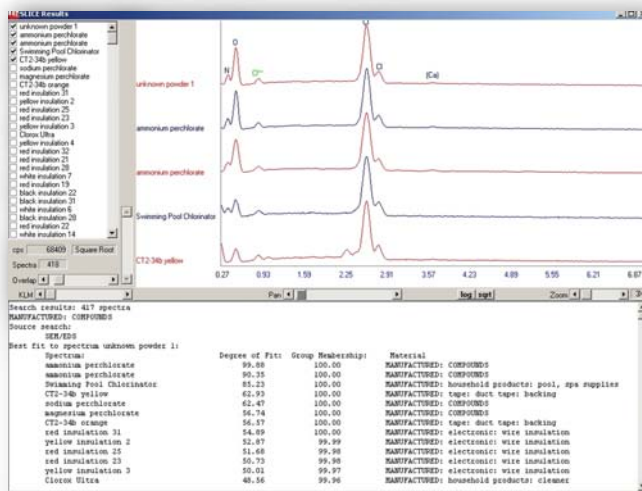


FIGURE 2. Search results window.

database contains approximately 5000 spectra and users can add their own spectra. The database includes spectra for: firearms, GSR, biological materials, paint, glass, explosives, fireworks, alloys, minerals, cosmetics, household products, food supplements, documents, art products, adhesives, personal products and others.

An analysis

The main window of SLICE is shown in Figure 1. The spectrum from an unknown “white powder” is displayed. The Tabs present on this page contain various parameters associated with the

origin of the spectrum and its analysis. There is a notes section that may contain any descriptive information not addressed by the remaining entries. All information may be utilized as part of the query, in addition to the best overall spectral fit. A tree is used to classify materials into categories such as Manufactured:Tapes:Duct Tape:Adhesive, or Natural:Biological:Human: Bone, etc., which are utilized to focus the search.

In this example, a Search was initiated utilizing only best fit, with no other qualifiers, and the results

are shown in Figure 2. The results of the search indicate strongly that the unknown is ammonium perchlorate, even though the spectra from the materials contained in the database were acquired on different microscopes, and not under identical conditions. Just as importantly, the search illustrates that the white powder is dissimilar to a large array of other white powders. Without SLICE, the effectiveness of this determination will be heavily controlled by the experience and skill of the user. Different users might very well obtain different results.

The spectra are compared here using the square root of the spectra, to visibly enhance differences and similarities. In practical use, the user may choose to overlap any number of spectra, in linear, log or square root mode, and with minimal or maximum overlap. A cursor display can be invoked which will normalize all spectra about the point of the cursor for ease in determining similarities and differences. By selecting any spectrum in the display, an information window, which is a duplicate of the Tabs on the main page, may be displayed to enable the user to determine properties of the chosen spectrum. Such a window is shown in Figure 3, displaying the notes tab. If there are internet links displayed, and an active internet connection is available, the linked pages can be accessed and displayed. The overlap, original spectra, notes, etc. can all be copied and pasted into MS Word, or other documents files. Images, PDF files, etc may be related to the spectra, and displayed with the spectrum. Properties and chemistries may be tabulated. The current database contains approximately 5000 spectra and it is expected that it will continue to grow in the future.

More information regarding the SLICE database is available from:
EDAX, Inc., 201-529-6121
www.edax.com

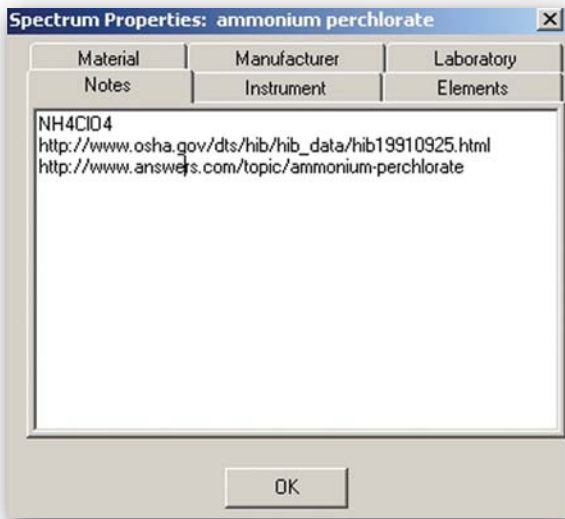


FIGURE 3. Information display window for selected spectrum.