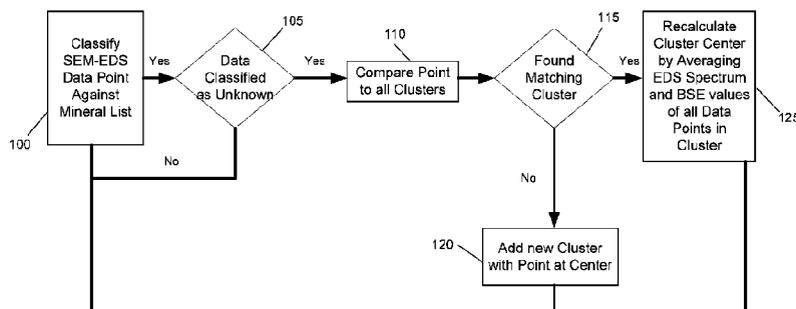




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(54) **Titre : ANALYSE EN GRAPPES DE DONNEES INCONNUES DANS UN ENSEMBLE DE DONNEES SEM-EDS**
 (54) **Titre: CLUSTER ANALYSIS OF UNKNOWNNS IN SEM-EDS DATASET**



(57) **Abrégé/Abstract:**

The present invention discloses a method for determining the mineral content represented by the entire SEM-EDS dataset, including initially unknown data points. SEM-EDS data points are taken and compared to a set of known data points. Any data point that is not sufficiently similar to the known data point is classified as unknown and clustered with like unknown data points. After all data points are analyzed, any clusters of unknown data points with a sufficient number of data points are further analyzed to determine their characteristics. All clusters of unknown data points with an insufficient number of data points to allow further analysis are considered outliers and discarded.

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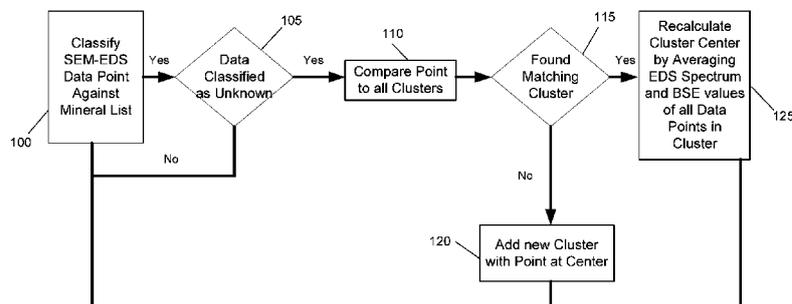
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FIG. 1

(57) **Abstract:** The present invention discloses a method for determining the mineral content represented by the entire SEM-EDS dataset, including initially unknown data points. SEM-EDS data points are taken and compared to a set of known data points. Any data point that is not sufficiently similar to the known data point is classified as unknown and clustered with like unknown data points. After all data points are analyzed, any clusters of unknown data points with a sufficient number of data points are further analyzed to determine their characteristics. All clusters of unknown data points with an insufficient number of data points to allow further analysis are considered outliers and discarded.

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CLUSTER ANALYSIS OF UNKNOWNNS IN SEM-EDS DATASET

Technical Field of the Invention

[0001] The present invention relates generally to methods and structures for identifying minerals using charged particle beam systems and energy dispersive spectroscopy systems.

Background of the Invention

[0002] Mineral analysis systems, such as the QEMSCAN[®] (Quantitative Evaluation of Minerals by Scanning Electron Microscopy) and MLA[™] (Mineral Liberation Analyzer) from FEI Company, the assignee of the present invention, have been used for many years to determine the type and relative quantity of minerals present in a mine. Such systems direct an electron beam toward a sample, typically in the form of small granules fixed in epoxy in a mold, and measure the energy of x-rays coming from the material in response to the electron beam. One such process is called “energy dispersive x-ray analysis” or “EDS,” which can be used for elemental analysis or chemical characterization of a sample. Backscattered electron (BSE) detectors are also used for mineral analysis in conjunction with electron beam columns. The intensity of the BSE signal is a function of the average atomic number of the material under the electron beam, and this relationship can be used to develop a useful mineral identification method.

[0003] EDS systems rely on the emission of X-rays from a sample to perform elemental analysis. Each element has a unique atomic structure, which allows x-rays that are characteristic of an element’s atomic structure to be uniquely identified from one another. To stimulate the emission of x-rays from a sample, a beam of charged particles is focused onto the sample, which causes electrons from inner shells to be ejected. Electrons from outer shells seek to fill this electron void, and the difference in energy between the higher energy

shell and the lower energy shell is released as an x-ray, which can be detected by an EDS detector.

[0004] QEMSCAN[®] comprises a SEM (scanning electron microscope), multiple EDS detectors, and software for controlling automated data acquisition. This technology identifies and quantifies elements within an acquired spectrum and then matches this data against a list of mineral definitions having fixed elemental ranges. The width of the elemental ranges depends on the number of x-rays in the spectrum, so mineral definitions developed for an x-ray spectrum having a first number of x-ray counts cannot be applied to spectra having a different number of x-rays. Thus, it has not been possible to define a universal database for an arbitrary number of x-ray counts. Also, the QEMSCAN[®] defines the unknown sample using the first located match, even if there might be a better match elsewhere in the mineral database. A QEMSCAN[®] comparison to a mineral definition results in either a match or no match, with no indication as to whether the unknown sample composition is in the center of the elemental range, which would indicate a high probability match, or at the edge of the range, which would indicate a lower probability match.

[0005] MLA technology also combines a SEM, multiple EDS detectors, and automated quantitative mineralogy software. MLA computes a probability match between a measured mineral spectrum and a reference mineral spectrum. This method works reasonably, but the numerical value obtained tends to be dominated by the size of the largest peak in the x-ray spectrum.

[0006] The acquisition time of a suitable BSE signal is typically on the order of microseconds per pixel. EDS systems, however, are usually slower and have a longer acquisition time, typically requiring on the order of several seconds per pixel to collect enough x-rays to uniquely identify a sample spectrum. The increased acquisition time substantially reduces the number of pixels that can be measured. EDS systems are typically

insensitive to light atoms. Because of the specific advantages and drawbacks of EDS detectors and BSE detectors, it is sometimes useful to use both BSE and EDS together to accurately identify minerals. This joint detector approach takes longer to perform an analysis, which can make this approach less suitable for some applications.

[0007] A mineral classification system must be capable of comparing each unknown measured spectrum to a library of known mineral spectrums, and then making a selection based on which known mineral is most similar to the measured spectrum. Typically, to find the most similar spectrum requires the use of a metric that represents the degree of similarity between the measured data and the known material.

[0008] Currently, there are various ways to compare two spectrums directly, either by calculating a distance metric or a similarity metric. An example of a method of comparison used in the prior art is to take the sum of the differences between the two spectrums as a distance. The MLA uses a chi-squared statistical test to compare the value at each energy channel of the measured spectrum to the value at the corresponding channel of the known mineral spectrum. These prior art approaches are based around comparing the spectrums on a channel by channel basis. The problem of using a comparison on a channel by channel basis is that there is no guarantee that all required peaks in the mineral spectrum are present in the measured spectrum. It is possible that a measured spectrum appears to be similar to a mineral yet it is missing an element that is required by the definition of that mineral, or has an additional element not found in that definition of a mineral.

[0009] In the XBSE_STD (extended BSE with automated standards collections) measurement mode of the MLA, each data point is compared against a mineral list. If the data point is not similar to any mineral, then a new mineral entry is created and a high quality EDS spectrum is immediately measured from the sample. However, there are several significant limitations of this approach. First, the user is presented with hundreds of

unknown data points and there is no way to distinguish which ones occur most frequently and which ones are outliers. Second, the analysis cannot be performed offline as it requires access to the SEM to collect the high quality data during measurement. Finally, only the raw data is presented to the user and there is no analytical tool to give elemental composition. Thus, there is a need for an improved mineral identification method.

Summary of the Invention

[0010] An object of the invention is to improve the identification of minerals present in a sample.

[0011] The present invention facilitates the determination of the mineral content of sample represented by an SEM-EDS dataset, including samples that did not initially match any of the system mineral definitions.

[0012] In a preferred embodiment, SEM-EDS data points are collected and compared to a set of known data points. Any data point that is not sufficiently similar to the known data point is classified as unknown and clustered with similar unknown data points. After all the data points are analyzed, any clusters of unknown data points with a sufficient number of data points are further analyzed to determine their characteristics.

[0013] Embodiments of the invention differentiate unknown data points that are simply outliers, from data points that represent a genuine mineral that is occurring in the sample. The clustering analysis can be performed offline, online, or in real time, and re-processed anytime. The results presented to the operator are typically elemental compositions, average atomic number, or other characteristics that are measured by the analysis. The raw EDS and BSE spectrums may also be presented, as well as the raw data of any other tests done.

[0014] The foregoing has outlined rather broadly the features and technical advantages of the present invention in order that the detailed description of the invention that follows may

be better understood. Additional features and advantages of the invention will be described hereinafter. It should be appreciated by those skilled in the art that the conception and specific embodiments disclosed may be readily utilized as a basis for modifying or designing other structures for carrying out the same purposes of the present invention. It should also be realized by those skilled in the art that such equivalent constructions do not depart from the spirit and scope of the invention as set forth in the appended claims.

Brief Description of the Drawings

[0015] For a more thorough understanding of the present invention, and advantages thereof, reference is now made to the following descriptions taken in conjunction with the accompanying drawings, in which:

[0016] FIG. 1 shows a flow chart of the method to classify all unknown data points into clusters; and

[0017] FIG. 2 shows the analysis of all clusters to determine if they contain only outlier data points or if the mineral definition list needs updating.

[0018] FIG. 3a-3j are example spectra obtained by energy dispersive x-ray spectroscopy.

[0019] FIGS. 4A and 4B are x-ray spectra of quartz and pyrite, respectively.

[0020] FIG. 5 is a scanning electron microscope system with EDS capability.

Detailed Description

[0021] Embodiments of the present invention are directed to a method and apparatus for efficiently and easily classifying data points. A “data point” is a group of data, such as an EDS spectrum and/or backscattered electron (“BSE”) value. A data point typically corresponds to a mineral. Characteristics of data points corresponding to known minerals are compared to the characteristics of the measured data points. If the characteristics are identical or very similar, the data point is labeled as a known or similar data point. However,

if the characteristics of the data point are not similar to the characteristics of the known data points, the data point is labeled as an unknown or dis-similar data point. Any unknown or dissimilar data points will enter into the clustering analysis.

[0022] A beam is directed toward a sample surface and emissions generated from the surface by the beam impact are detected. The primary beam can comprise, for example, electrons, ions, photons (e.g., a laser beam or x-rays), or atoms. The beam is typically focused to a point on the sample and the point is scanned across the sample. Particles (used herein to include photons and scattered primary particles) that are emitted, backscattered, or transmitted through the sample in response to the primary beam are detected. Different emissions from the sample, such as x-rays, backscattered electrons, secondary electrons, Auger electrons, transmitted electrons, or photons, are detected in various analysis modalities. The invention is not limited to any particular analytical technique.

[0023] The different modalities may provide different information about properties of the sample, such as contour information, compositional information, topographical information, or chemical state information. For example, backscattered electron data may be acquired at the same time as x-ray data, with the x-rays being placed at the correct location in the backscattered electron image to produce a spectrum cube. In some embodiments, the different analysis modalities include detecting emissions generated by different beams at different times.

[0024] In some embodiments, an electron beam is directed toward a sample and scanned across regions having different characteristics, such as different mineral compositions. A first detector may provide information about contour, topography, or atomic number, for example, by detecting backscattered electrons, while a second detector may provide information about composition, for example, by detecting characteristic x-rays.

[0025] Cluster analysis, or clustering, is the task of assigning a set of objects into groups,

also called clusters, so that the objects in the same cluster are more similar to each other than to those in other clusters. Cluster analysis groups objects based on the information found in the data describing the objects or their relationships. The goal is that the objects in a group will be similar to one another and different from the objects in other groups. The greater the similarity within a group, and the greater the difference between groups, the “better” or more distinct the clustering.

[0026] Cluster analysis itself is not one specific algorithm, but is a general approach to assigning minerals identifications. It can be achieved by various algorithms that differ significantly in their notion of what constitutes a cluster and how to efficiently find them. Clustering can therefore be formulated as a multi-objective optimization problem. The appropriate clustering algorithm and parameter settings, including values such as the distance function to use, a density threshold or the number of expected clusters, depend on the individual data set and intended use of the results. Cluster analysis is typically an iterative process of knowledge discovery or interactive multi-objective optimization that involves trial and error. It will often be necessary to modify preprocessing and parameters until the result achieves the desired properties.

[0027] Any standard clustering technique, such as Agglomerative, Single-Pass or K-Means, may be used for the analysis of the present invention. For example, one possible distance metric takes the sum of the differences between the EDS Spectrum channel values.

[0028] As shown in FIG. 1, the first step in the process is to classify every data point in the SEM-EDS data set, 100, as a known or unknown, 105. A data point is “known” if its spectrum matches the known spectrum of a mineral within a predetermined limit. For example, one measurement of how well spectra match is the Cosine Similarity metric analysis as given in Equation 1,

$$\text{similarity} = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|} = \frac{\sum_{i=1}^n A_i \times B_i}{\sqrt{\sum_{i=1}^n (A_i)^2} \times \sqrt{\sum_{i=1}^n (B_i)^2}} \quad \text{Equation (1)}$$

where “i” represents each measurement parameter, such as each normalized energy channel height, average atomic number from back-scattered electron analysis, or other measurement parameter, and the values of data points each spectrum is summed over all the energy channels and other measurements. In some embodiments, a spectrum is considered a match to a reference spectrum when the similarity metric of the two is greater than 90%.

[0029] After excluding known data points, all unknown data points are compared to the clusters of unknown data points, 110. If the unknown data point’s characteristics are similar to another cluster, that is, the similarity metric is greater than a pre-determined amount, the unknown data point is placed in that cluster, 115. If the unknown data point is not similar to other clusters, a new cluster is created, 120. The average value of every cluster for each energy channel is recalculated after the addition of each new data point to further refine the cluster’s characteristics and differentiate each cluster from the others, 125.

[0030] The results of the clustering analysis will be several clusters, with each cluster containing least one “unknown” data point. As shown in FIG. 2, once the SEM-EDS data set is reduced to known data points and clusters of unknown data points, the clusters are sorted by the number of data points in the clusters, 200. This list can be reduced to only those clusters that matched a significant number of data points, 205, for example the top 20 clusters, although analysis of all or fewer clusters is possible. As used herein matching means unknown data points are clustered or grouped together when the characteristics of each data point are identical or similar to the characteristics of the other data points in the cluster or group. In one embodiment, the characteristics of each data point in a group should

be within at least three percent of the average value of the all data points in the group. The matching criteria can be tightened if more precise measurements are needed.

[0031] Once all clusters have been sorted, it is determined whether or not there are any clusters remaining, 210. If there are no clusters remaining after removal of those with few data points, the remaining clusters are outliers, 215, and the process is complete.

[0032] However, if there are clusters remaining, it means that there is a mineral in the sample that has not been identified. The remaining clusters then undergo quantitative EDS analysis to give the elemental composition of the unknown minerals, 220, and a BSE analysis to determine the average atomic number of the minerals, 225. The average EDS spectrum and BSE value is calculated from each cluster, by averaging all the data points within a cluster. This gives a high quality EDS spectrum that can be further analyzed to give accurate elemental composition and atomic numbers based on BSE data.

[0033] Once all data is analyzed and placed in the appropriate cluster, the analyzed cluster data is presented to the operator, 230, who may make use of the data to expand the list of mineral definitions to minimize the unknown data points, 235, eliminate clusters with minimal data points, 205, and/or determine that all “unknown” data points are outliers and can be ignored, 215. If desired the operator can instruct the analysis to be repeated so as to rerun the sample with an updated known data point list which will produce fewer unknown data points.

[0034] The following example shows an analysis of 10 different samples having spectra show in FIGS. 3a-3j. The spectra of the ten samples are being compared to spectra of known minerals in a mineral list. In this example, the mineral list has only two minerals, quartz and pyrite, having spectra as shown in FIGS. 4a and 4b. Each of the spectra of a sample represents a data point. In this example, the data point does not include backscattered electron data. After obtaining the spectra corresponding to the ten points, each data point is

analyzed for its similarities with known spectra, for example, by using a cosine comparison on multiple energy channels. Table 1 shows the results of the comparison, and the classification shows the result of the analysis. The known data points are Quartz and Pyrite.

Table 1: Sample Data and Cluster Analysis

Number	Similarity With Quartz	Similarity With Pyrite	Similarity with Unknown_1	Similarity with Unknown_2	Classification
1	99.2%	4.3%	-	-	Identified as quartz
2	3.73%	54.19%	-	-	New cluster added 'Unknown_1'
3	3.04%	98.18%	-	-	Identified as Pyrite
4	5.77%	43.08%	8.63%	-	New Cluster added 'Unknown_2'
5	4.54%	47.81%	95.37%	10.43%	Matches cluster 'Unknown_1'
6	98.96%	4.7%	4.16%	7.22%	Identified as Quartz
7	6.45%	44.89%	10.72%	91.70%	Matches cluster 'Unknown_2'
8	8.96%	43.72%	11.03%	92.81%	Matches cluster 'Unknown_2'
9	6.02%	43.03%	11.67%	92.42%	Matches cluster 'Unknown_2'
10	9.04%	43.93%	11.45%	93.16%	Matches cluster 'Unknown_2'

[0035] In this example, a spectrum is considered a match when the similarity between samples is greater than ninety percent (90%). As seen in Table 1, samples 1 and 6 have a 99.2% match and 98.96% match, respectively, with the known values of Quartz, thus the software will designate those samples as Quartz. Sample 2 does not match with either Quartz or Pyrite to a degree of greater than 90%, so it is classified as an unknown sample and placed in unknown cluster one. Sample 3 has a match of 98.18% with the known value of Pyrite, thus the software will classify this sample as Pyrite. Sample 4 does not match any of the known samples, and does not match closely with the first unknown sample, sample 3, so it is classified as a second unknown sample and placed in unknown cluster two. Sample 5 has a greater than 90% match to Sample 2 and is placed in unknown cluster one. Samples 7-10 have a greater than 90% match to sample 4, therefore these samples are placed in unknown cluster two. At this point the operator can evaluate the samples in unknown clusters one and

two to determine if further analysis is needed, additional known data sets should be added to the software, or if the unknown clusters are simply outlier data points that can be ignored.

Thus it can be seen that the current method can quickly and easily cluster unknown samples for more efficient handling.

[0036] FIG. 5 is an example of a scanning electron beam system 500 with an x-ray detector 540 suitable for analyzing samples prepared according to the present invention. A scanning electron microscope 541, along with power supply and control unit 545, is provided with system 500. An electron beam 532 is emitted from a cathode 553 by applying voltage between cathode 553 and an anode 554. Electron beam 532 is focused to a fine spot by means of a condensing lens 556 and an objective lens 558. Electron beam 532 is scanned two-dimensionally on the specimen by means of a deflection coil 560. Operation of condensing lens 556, objective lens 558, and deflection coil 560 is controlled by power supply and control unit 545.

[0037] A system controller 533 controls the operations of the various parts of scanning electron beam system 500. The vacuum chamber 510 is evacuated with ion pump 568 and mechanical pumping system 569 under the control of vacuum controller 532.

[0038] Electron beam 532 can be focused onto sample 502, which is on movable X-Y stage 504 within lower vacuum chamber 510. When the electrons in the electron beam strike sample 502, the sample gives off x-rays whose energy correlated to the elements in the sample. X-rays 532 having energy inherent to the elemental composition of the sample are produced in the vicinity of the electron beam incident region. Emitted x-rays are collected by x-ray detector 540, preferably an energy dispersive detector of the silicon drift detector type, although other types of detectors could be employed, which generates a signal having an amplitude proportional to the energy of the detected x-ray.

[0039] Output from detector 540 is amplified and sorted by the processor 520, which

counts and sorts the total number of x-rays detected during a specified period of time, at a selected energy and energy resolution, and a channel width (energy range) of preferably between 10-20 eV per channel. Processor 520 can comprise a computer processor; operator interface means (such as a keyboard or computer mouse); program memory 522 for storing data and executable instructions; interface means for data input and output, executable software instructions embodied in executable computer program code; and display 544 for displaying the results of a multivariate spectral analysis by way of video circuit 542.

[0040] Processor 520 can be a part of a standard laboratory personal computer, and is typically coupled to at least some form of computer-readable media. Computer-readable media, which include both volatile and nonvolatile media, removable and non-removable media, may be any available medium that can be accessed by processor 520. By way of example and not limitation, computer-readable media comprise computer storage media and communication media. Computer storage media include volatile and nonvolatile, removable and non-removable media implemented in any method or technology for storage of information such as computer-readable instructions, data structures, program modules or other data. For example, computer storage media include RAM, ROM, EEPROM, flash memory or other memory technology, CD-ROM, digital versatile disks (DVD) or other optical disk storage, magnetic cassettes, magnetic tape, magnetic disk storage or other magnetic storage devices, or any other medium that can be used to store the desired information and that can be accessed by processor 520.

[0041] Program memory 522 can include computer storage media in the form of removable and/or non-removable, volatile and/or nonvolatile memory and can provide storage of computer-readable instructions, data structures, program modules and other data. Generally, the processor 520 is programmed by means of instructions stored at different times in the various computer-readable storage media of the computer. Programs and operating systems

are typically distributed, for example, on floppy disks or CD-ROMs. From there, they are installed or loaded into the secondary memory of a computer. At execution, they are loaded at least partially into the computer's primary electronic memory. The invention described herein includes these and other various types of computer-readable storage media when such media contain instructions or programs for implementing the steps described below in conjunction with a microprocessor or other data processor. The invention also includes the computer itself when programmed according to the methods and techniques described herein.

[0042] An x-ray spectrum obtained as described above can be stored in a portion of memory 522, such as the measured spectra memory portion 523. Data template memory portion 524 stores data templates, such as definitions of known spectra of elements or, in some embodiments, known diffraction patterns of materials.

[0043] While the embodiment shown includes a scanning electron microscope, related embodiment could use a transmission electron microscope or a scanning transmission electron microscope to generate x-rays from the sample. An x-ray fluorescence system could also be used to generate x-rays from the sample. Other embodiments may detect other characteristic radiation, such as gamma rays, from a sample.

[0044] According to some embodiments of the present invention, a method for determining the mineral content of a sample comprises directing an electron beam toward multiple points of unknown composition; detecting x-rays emitted as a result of the electron beam impacting the sample to acquire an x-ray spectrum, the information comprising a data point; classifying the data point from a sample by comparison to a set of known data points as a classified data point, wherein said classified data point is classified as a similar data point if the characteristics of the classified data point are similar to the characteristics of a known data point and alternatively the classified data point is classified as a dissimilar data point if the characteristics of the classified data point are not similar to a known data point; placing the

data point into a group wherein the characteristics of the data points within the group have characteristics similar to that of the classified data point; repeating the previous steps until all data points are classified data points and are placed in groups with similar characteristics; and analyzing the groups with dissimilar data points for use in processing the mineral sample.

[0045] In some embodiments, the method further comprises removing all groups of dissimilar data points except the twenty groups with the most number of dissimilar data point before analyzing the groups with the dissimilar data points to determine the mineral content of the groups with dissimilar data points. In some embodiments, the method further comprises removing all groups of dissimilar data points with five or less dissimilar data points before analyzing the groups with dissimilar data points to determine the mineral content of the groups with dissimilar data points.

[0046] In some embodiments, the method further comprises removing all groups of dissimilar data points with twenty or less dissimilar data points before analyzing the groups with dissimilar data points to determine the mineral content of the groups with dissimilar data points. In some embodiments, the groups with dissimilar data points are analyzed to determine the mineral content of the groups with dissimilar data points by conducting a quantitative energy dispersive x-ray spectroscopy to determine the elemental composition of the group of dissimilar data points. In some embodiments, the set of known data points are altered based on the results of the energy dispersive x-ray spectroscopy analysis and the sample is processed again with the altered set of known data points.

[0047] In some embodiments, the groups with dissimilar data points are analyzed to determine the average atomic number of the groups with dissimilar data points by conducting a backscattered electron detector analysis. In some embodiments, the set of known data points are altered based on the results of the backscattered electron detector analysis and the sample is processed again with the altered set of known data points.

[0048] In some embodiments, each group of classified data points has an average value which is recalculated with the addition of each classified data point. In some embodiments, the characteristic of each classified data point is within three percent of the average characteristic value of the group it is placed in. In some embodiments, the characteristic of each classified data point is within one percent of the average characteristic value of the group it is placed in. In some embodiments, the characteristic of each classified data point is within 0.01 percent of the average characteristic value of the group it is placed in.

[0049] In some embodiments, a newly classified data point is placed in a separate group if there are no previously classified data points with characteristics similar to the newly classified data points.

[0050] According to some embodiments, a scanning electron microscope x-ray spectroscopy device comprises a source of a charged particle beam or photon beam and means for directing the beam towards a mineral sample; a detector for detecting emissions from the sample in response to the beam and for forming a data set comprising multiple data points; a processor for controlling the scanning electron microscope; and a computer readable data storage storing computer instruction to classify an x-ray spectroscopy data point taken from the sample by comparison to a set of known data points as a classified data point wherein said classified data point is classified as a similar data point if the characteristics of the classified data point are similar to the characteristics of a known data point and alternatively the classified data point is classified as a dissimilar data point if the characteristics of the classified data point are not similar to a known data point; placing the x-ray spectroscopy data point into a group wherein the characteristics of the data points within the group have characteristics similar to that of the classified data point; repeating the previous steps until all x-ray spectroscopy data points are classified data points and are placed in groups with similar characteristics; and analyzing the groups with dissimilar data points for

use in processing the mineral sample.

[0051] Further, whenever the terms “automatic,” “automated,” or similar terms are used herein, those terms will be understood to include manual initiation of the automatic or automated process or step. Whenever a scan or image is being processed automatically using computer processing, it should be understood that the raw image data can be processed without ever generating an actual viewable image. In the following discussion and in the claims, the terms "including" and "comprising" are used in an open-ended fashion, and thus should be interpreted to mean "including, but not limited to”

[0052] It should be recognized that embodiments of the present invention can be implemented via computer hardware or software, or a combination of both. The methods can be implemented in computer programs using standard programming techniques—including a computer-readable storage medium configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner—according to the methods and figures described in this specification. Each program may be implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language can be a compiled or interpreted language. Moreover, the program can run on dedicated integrated circuits programmed for that purpose.

[0053] Further, methodologies may be implemented in any type of computing platform, including but not limited to, personal computers, mini-computers, main-frames, workstations, networked or distributed computing environments, computer platforms separate, integral to, or in communication with charged particle tools or other imaging devices, sensors, and the like. Aspects of the present invention may be implemented in machine readable code stored as memory on a storage medium or device, whether removable or integral to the computing

platform, such as a hard disc, optical read and/or write storage mediums, RAM, ROM, and the like, so that it is readable by a programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. Moreover, machine-readable code, or portions thereof, may be transmitted over a wired or wireless network. The invention described herein includes these and other various types of computer-readable storage media when such media contain instructions or programs for implementing the steps described above in conjunction with a microprocessor or other data processor. The invention also includes the computer itself when programmed according to the methods and techniques described herein.

[0054] Computer programs can be applied to input data to perform the functions described herein and thereby transform the input data to generate output data. The output information is applied to one or more output devices such as aberration correctors or to a display monitor. In preferred embodiments of the present invention, the transformed data represents physical and tangible objects, including producing a particular visual depiction of the physical and tangible objects on a display.

[0055] Preferred embodiments of the present invention may make use of a particle beam apparatus, energy beam apparatus, or apparatus using a physical probe tip in order to image a sample. Such beams or physical probes used to image a sample inherently interact with the sample resulting in some degree of physical transformation. Further, throughout the present specification, discussions utilizing terms such as “calculating,” “determining,” “measuring,” “generating,” “detecting,” “forming,” “resetting,” “reading,” “subtracting,” “detecting,” “comparing,” “acquiring,” “mapping,” “recording,” “transforming,” “changing,” or the like, also refer to the action and processes of a computer system, a sensor, or similar electronic device, that manipulates and transforms data represented as physical quantities within the computer system into other data similarly represented as physical quantities within the

computer system or other information storage, transmission or display devices.

[0056] The invention has broad applicability and can provide many benefits as described and shown in the examples above. The embodiments will vary greatly depending upon the specific application, and not every embodiment will provide all of the benefits and meet all of the objectives that are achievable by the invention. Particle beam systems suitable for carrying out some embodiments of the present invention are commercially available, for example, from FEI Company, the assignee of the present application.

[0057] To the extent that any term is not specially defined in this specification, the intent is that the term is to be given its plain and ordinary meaning. The accompanying drawings are intended to aid in understanding the present invention and, unless otherwise indicated, are not drawn to scale. Although the present invention and its advantages have been described in detail, it should be understood that various changes, substitutions and alterations can be made herein without departing from the spirit and scope of the invention as defined by the appended claims. Moreover, the scope of the present application is not intended to be limited to the particular embodiments of the process, machine, manufacture, composition of matter, means, methods and steps described in the specification. As one of ordinary skill in the art will readily appreciate from the disclosure of the present invention, processes, machines, manufacture, compositions of matter, means, methods, or steps, presently existing or later to be developed that perform substantially the same function or achieve substantially the same result as the corresponding embodiments described herein may be utilized according to the present invention. Accordingly, the appended claims are intended to include within their scope such processes, machines, manufacture, compositions of matter, means, methods, or steps.

[0058] We claim as follows:

WHAT IS CLAIMED IS:

1. A method for determining the mineral content of a sample, said method comprising:

directing an electron beam toward multiple points of the sample;

detecting x-rays emitted as a result of the electron beam impacting the sample to acquire an x-ray spectrum data point;

providing the data point to a computer and by the computer:

classifying the data point from the sample by comparing the data point to a set of known data points, wherein the data point is classified as a similar data point if the characteristics of the data point are similar to the characteristics of a known data point of a set of known data points and, alternatively, the data point is classified as a dissimilar data point if the characteristics of the data point are not similar to the characteristics of any data points of the set of known data points;

for the data point classified as the similar data point, designating a mineral content corresponding to the known data point;

for the data point classified as the dissimilar data point, placing the data point into a group of a plurality of groups with dissimilar data points, wherein the characteristics of the data points within the group have characteristics similar to the characteristics of the data point;

repeating the previous steps until all data points are classified and are placed in groups with similar characteristics; and

analyzing the groups with dissimilar data points to determine a mineral content of the groups with dissimilar data points.

2. The method of claim 1, further comprising removing all groups of dissimilar data points except for twenty groups with the most number of dissimilar data points before analyzing the groups with dissimilar data points to determine the mineral content of the groups with dissimilar data points.

3. The method of claim 1 or claim 2, further comprising removing all groups of dissimilar data points with five or less dissimilar data points before analyzing the groups

with dissimilar data points to determine the mineral content of the groups with dissimilar data points.

4. The method of any one of claims 1 – 3, further comprising removing all groups of dissimilar data points with twenty or less dissimilar data points before analyzing the groups with dissimilar data points to determine the mineral content of the groups with dissimilar data points.

5. The method of any one of claims 1 – 4 wherein the groups with dissimilar data points are analyzed to determine the mineral content of the groups with dissimilar data points by conducting a quantitative energy dispersive x-ray spectroscopy to determine the elemental composition of the groups with dissimilar data points.

6. The method of claim 5, further comprising altering the set of known data points based on results of the energy dispersive x-ray spectroscopy analysis and the sample is processed again with the altered set of known data points.

7. The method of any one of claims 1 – 5 wherein the groups with dissimilar data points are analyzed to determine an average atomic number of the groups with dissimilar data points by conducting a backscattered electron detector analysis.

8. The method of claim 7 wherein the set of known data points is altered based on the results of the backscattered electron detector analysis and the sample is processed again with the altered set of known data points.

9. The method of any one of claims 1 – 8 wherein each of the groups of classified data points has an average characteristic value which is recalculated with the addition of each classified data point.

10. The method of claim 9 wherein the characteristic of each classified data point is within three percent of the average characteristic value of the group it is placed in.

11. The method of claim 9 or claim 10 wherein the characteristic of each classified data point is within one percent of the average characteristic value of the group it is placed in.

12. The method of any one of claims 9 – 11 wherein the characteristic of each classified data point is within 0.01 percent of the average characteristic value of the group it is placed in.

13. The method of any one of claims 1 – 12 wherein a newly classified data point is placed in a separate group if there are no previously classified data points with characteristics similar to the newly classified data point.

14. The method of claim 1, further comprising displaying the analyzed groups with dissimilar data points to an operator.

15. A scanning electron microscope x-ray spectroscopy device comprising:
a source of a charged particle beam or a photon beam and means for directing the beam towards a mineral sample;

a detector for detecting emissions from the sample in response to the beam and for forming a data set comprising multiple data points;

a processor for controlling the scanning electron microscope; and

a computer readable data storage storing computer instructions to:

classify an x-ray spectroscopy data point taken from the sample by comparing the data point to a set of known data points, wherein said data point is classified as a similar data point if the characteristics of the data point are similar to the characteristics of a known data point and, alternatively, the data point is classified as a dissimilar data point if the characteristics of the data point are not similar to the characteristics of any data points of the set of known data points;

for the data point classified as the similar data point, designating a mineral content corresponding to the known data point;

for the data point classified as the dissimilar data point, placing the data point into a group of a plurality of groups with dissimilar data points, wherein the characteristics of the data points within the group are similar to the characteristics of the data point;

repeating the previous steps until all data points are classified and are placed in groups with similar characteristics; and

analyzing the groups with dissimilar data points to determine mineral content of the groups with dissimilar data points.

16. A method for determining the mineral content of a sample, said method comprising:

directing an electron beam toward multiple points of the sample;

obtaining a sample data point comprising spectral information by detecting x-rays emitted as a result of the electron beam impacting the sample to acquire an x-ray spectrum, the x-ray spectrum comprising the spectral information;

providing the sample data point to a computer and by the computer:

comparing the sample data point to a set of known data points;

classifying the sample data point as a similar data point if characteristics of the sample data point are similar to characteristics of a data point of the set of known data points and, alternatively, classifying the sample data point as a dissimilar data point if the characteristics of the sample data point are not similar to the characteristics of any data point in the set of known data points;

for the sample data point classified as the similar data point, designating a mineral content corresponding to the known data point;

for the sample data point classified as the dissimilar data point, placing the sample data point into a group of a plurality groups with dissimilar data points, wherein the characteristics of the data points within the group have characteristics similar to characteristics of the sample data point;

obtaining additional sample data points and repeating the previous steps for each of the additional sample data points until all of the sample data points have been classified and placed in groups with similar characteristics;

determining, for each group of dissimilar data points, an averaged data point, the averaged data point being the average of the dissimilar data points of the group; and

analyzing the averaged data point of each group of dissimilar data points to determine the mineral contents corresponding to the groups of dissimilar data points.

17. The method of claim 16 wherein analyzing the averaged data point of each group of dissimilar data points to determine the mineral contents of the groups of dissimilar data points includes conducting a quantitative energy dispersive x-ray spectroscopy analysis on each of the averaged data points to determine the elemental compositions of the group of dissimilar data points.

18. The method of claim 17 further comprising:

altering the set of known data points based on the results of the quantitative energy dispersive x-ray spectroscopy analysis; and

repeating the steps of directing an electron beam, obtaining sample data points, comparing the sample data points to a set of known data points, classifying the sample data points, placing the sample data points into groups, determining averaged data points for each group of dissimilar data points, and analyzing the averaged data points, wherein:

repeating the step of comparing the sample data points to a set of known data points comprises comparing the sample data points to the altered set of known data points; and

repeating the step of classifying the sample data points comprises classifying the sample data points using the comparison of the sample data points to the altered set of known data points.

19. The method of claim 16 or claim 17 wherein the groups of dissimilar data points are analyzed to determine the average atomic number of the groups of dissimilar data points by conducting a backscattered electron detector analysis.

20. The method of claim 19 further comprising:

altering the set of known data points based on the results of the backscattered electron detector analysis; and

repeating the steps of directing an electron beam, obtaining sample data points, comparing the sample data points to a set of known data points, classifying the sample data points, placing the sample data points into groups, determining averaged data points for each group of dissimilar data points, and analyzing the averaged data points, wherein:

repeating the step of comparing the sample data points to a set of known data points comprises comparing the sample data points to the altered set of known data points;
and

repeating the step of classifying the sample data points comprises classifying the sample data points using the comparison of the sample data points to the altered set of known data points.

21. The method of any one of claims 16-20 wherein the averaged data point for each group of dissimilar data points is recalculated with the addition of each dissimilar data point to the group.

22. The method of claim 21 wherein a characteristic of each classified sample data point is within three percent of the average value of the characteristic for the group the classified sample data point is placed in.

23. The method of claim 22 wherein the characteristic of each classified sample data point is within one percent of the average value of the characteristic for the group the classified sample data point is placed in.

24. The method of claim 21 wherein the characteristic of each classified sample data point is within 0.01 percent of the average value of the characteristic for the group the classified sample data point is placed in.

25. The method of any one of claims 16-24 wherein a newly classified sample data point is placed in a separate group if there are no previously classified sample data points with characteristics similar to the newly classified sample data point.

26. A scanning electron microscope x-ray spectroscopy device comprising:
a source of a charged particle beam or a photon beam and means for directing the beam towards a mineral sample;
a detector for detecting emissions from the sample in response to the beam and for forming a data set comprising multiple mineral sample data points;

a processor for controlling the scanning electron microscope x-ray spectroscopy device; and

a computer readable data storage storing computer instructions, which when executed on the processor, carry out the method of any one of claims 16-25.

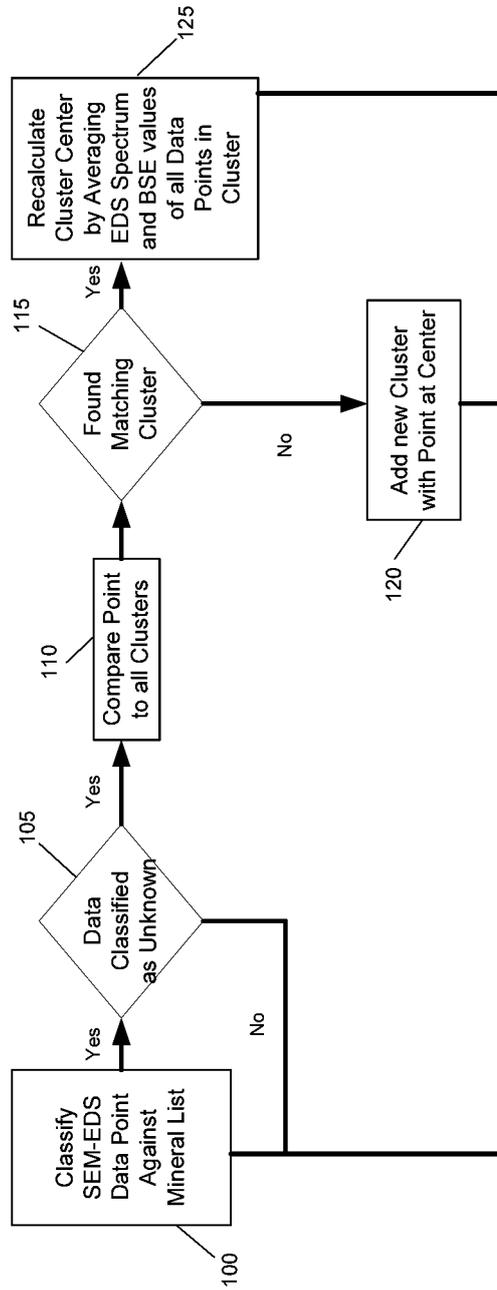


FIG. 1

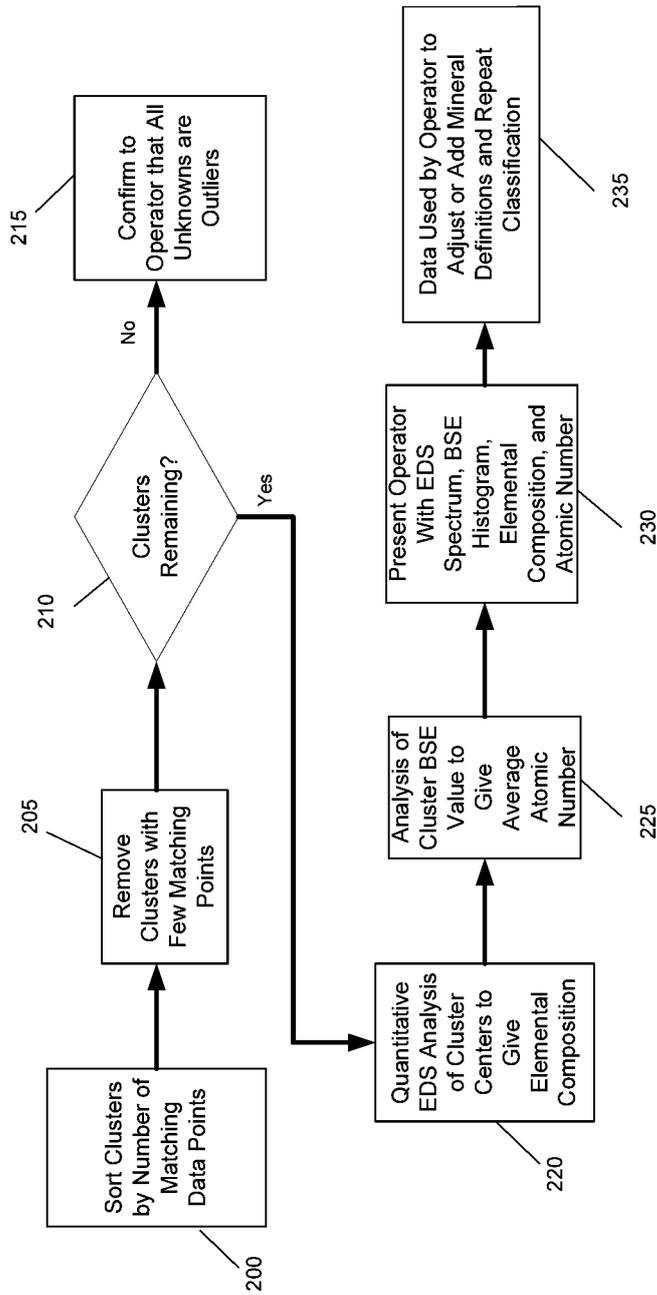
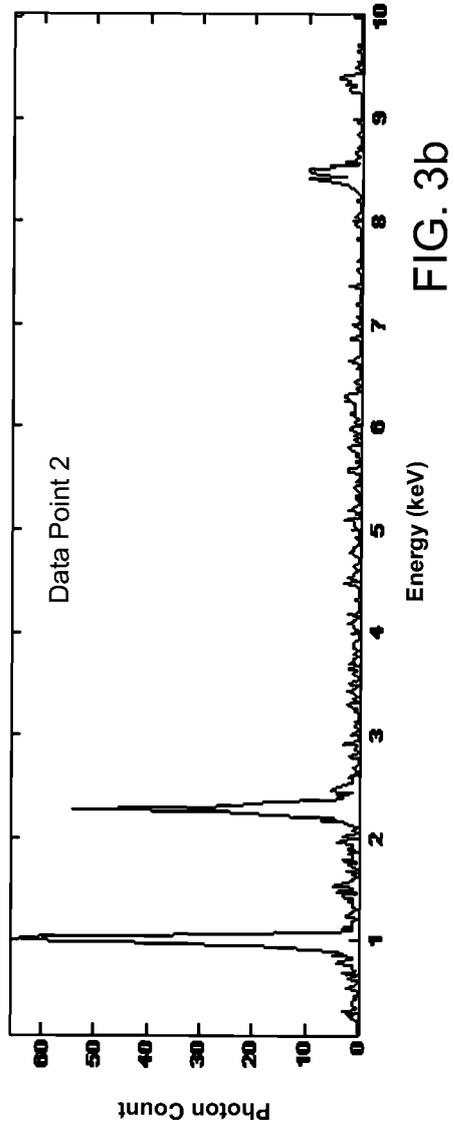
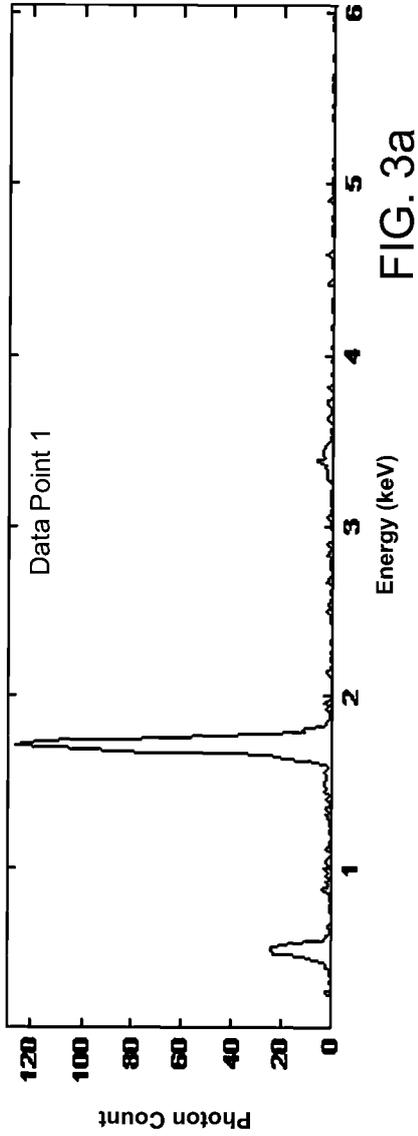


FIG. 2



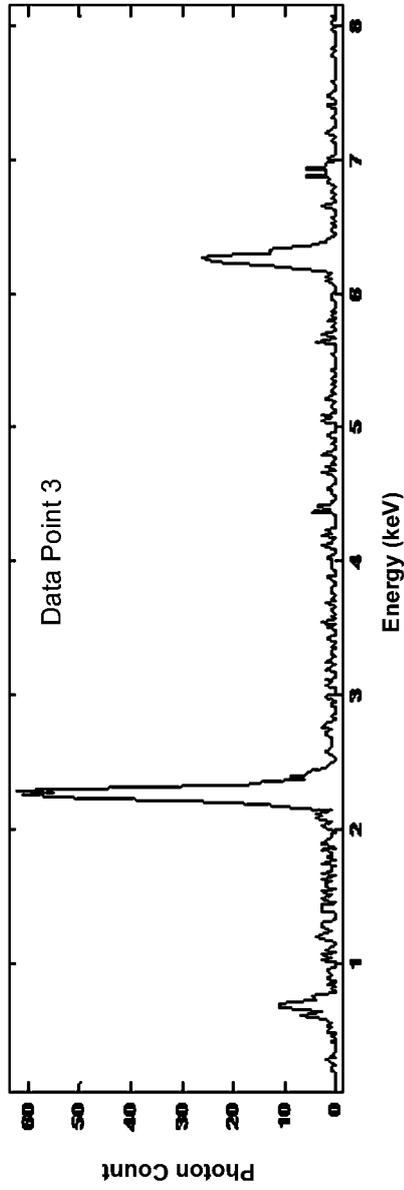


FIG. 3c

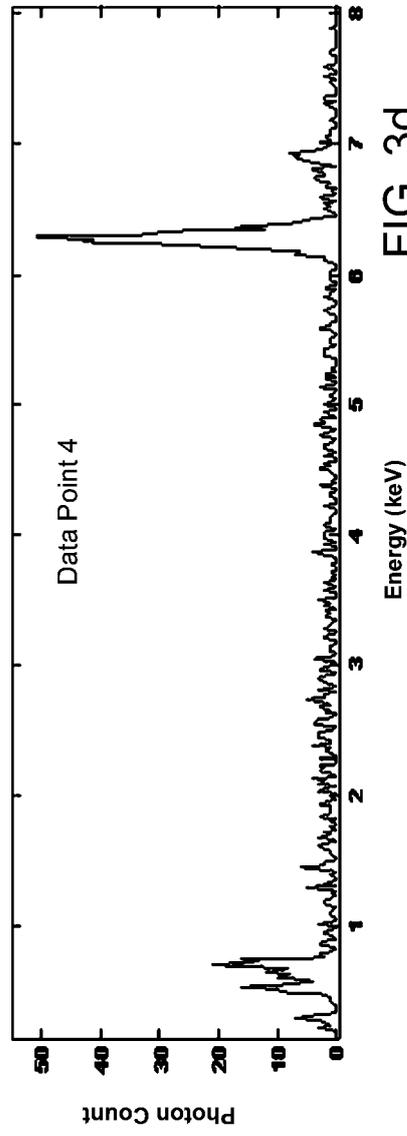


FIG. 3d

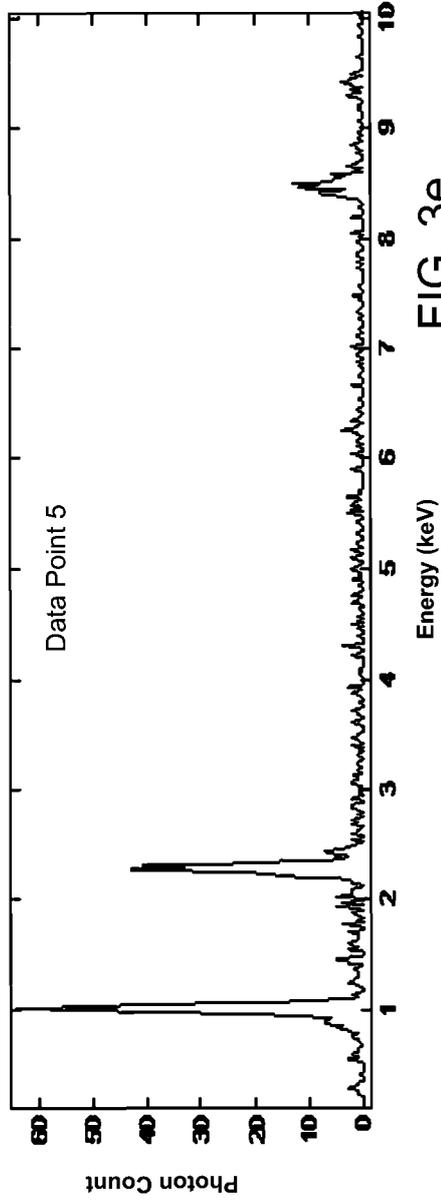


FIG. 3e

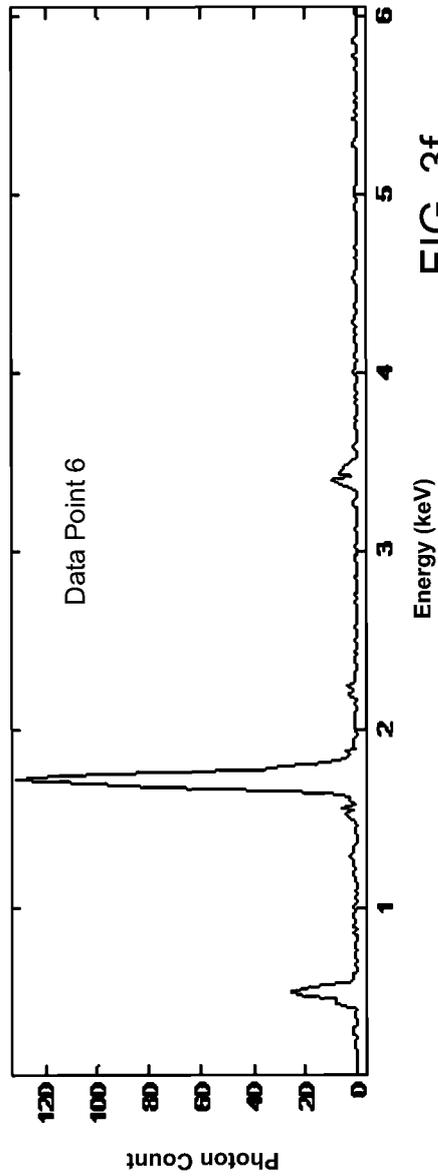
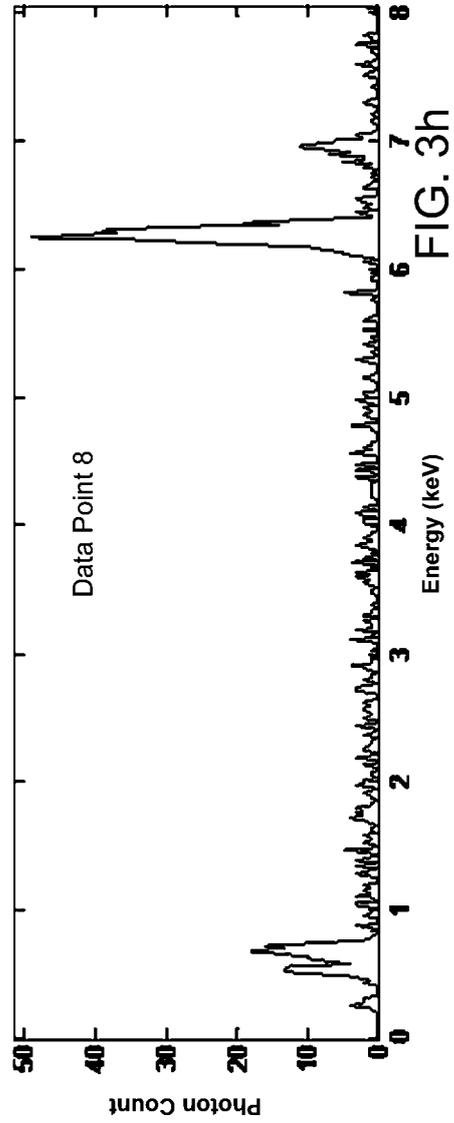
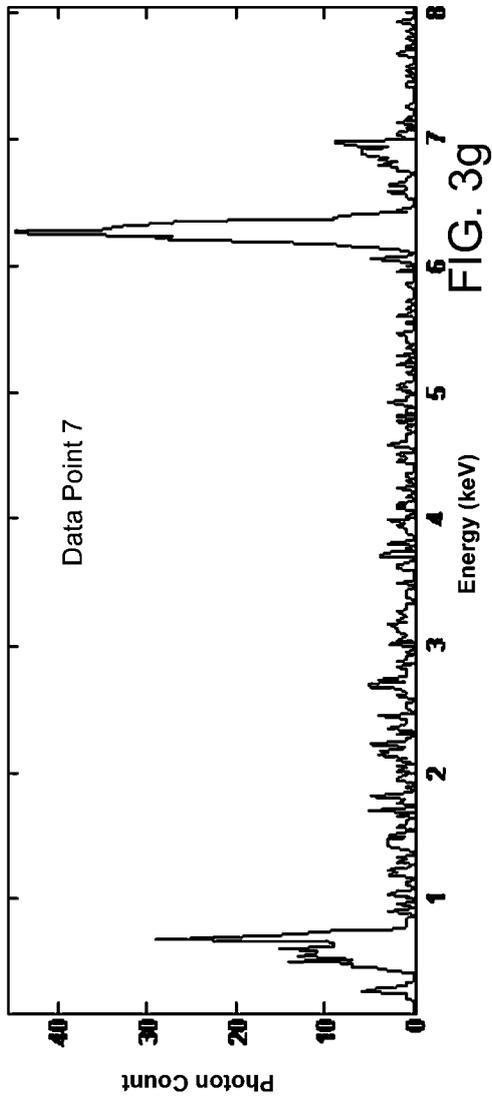
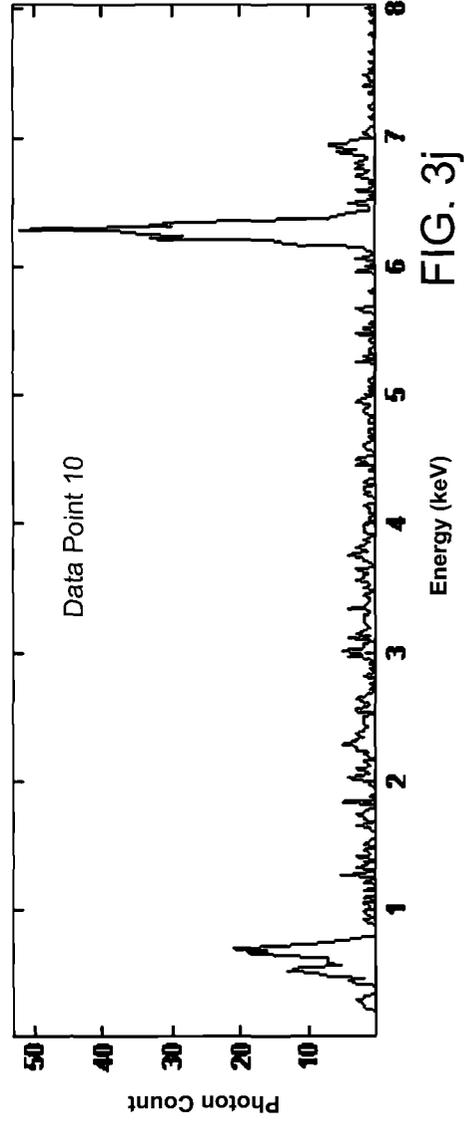
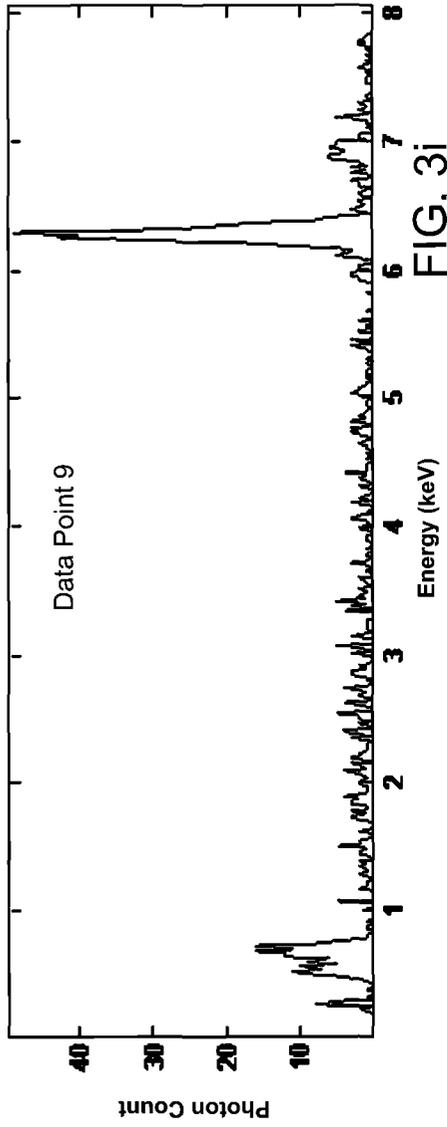
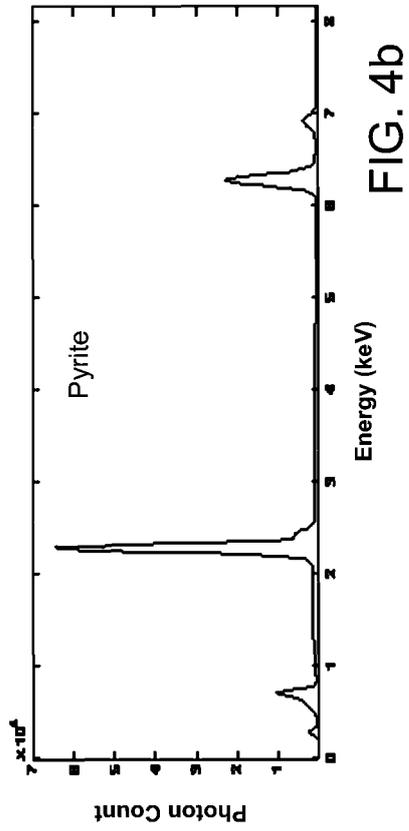
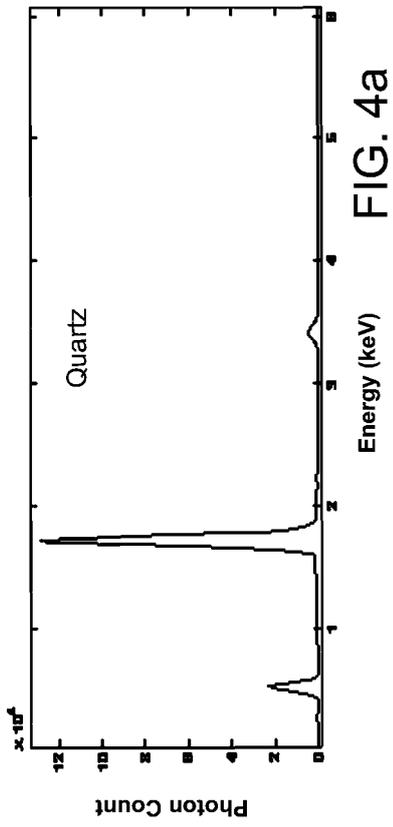


FIG. 3f







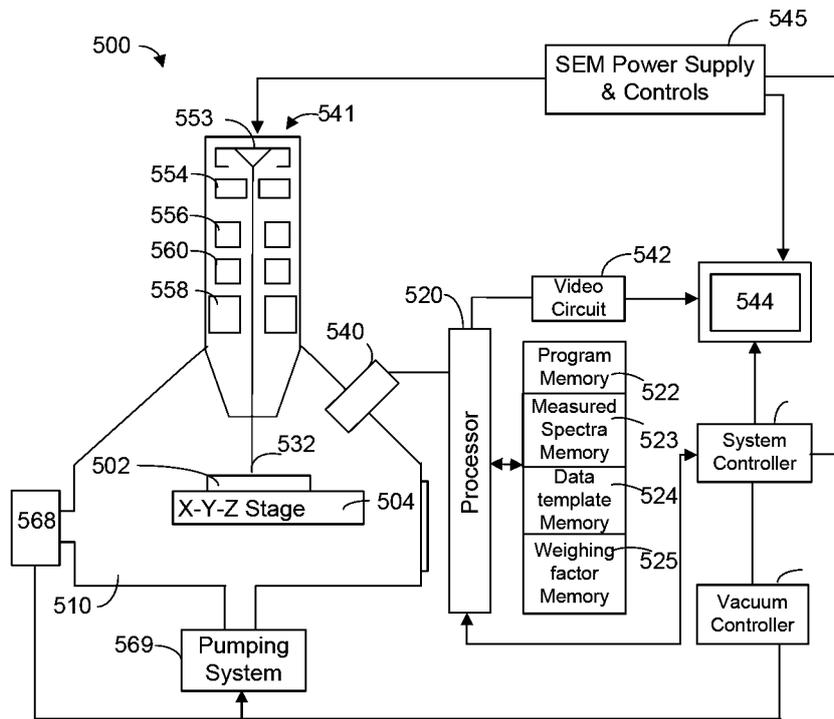


FIG. 5

