



(51) International Patent Classification:

G01J 3/02 (2006.01) G01N 21/63 (2006.01)
G01N 23/20 (2006.01) G02F 1/355 (2006.01)
G01N 23/207 (2006.01)

(21) International Application Number:

PCT/US2016/068837

(22) International Filing Date:

28 December 2016 (28.12.2016)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

62/271,992 28 December 2015 (28.12.2015) US

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(81) Designated States (unless otherwise indicated, for every
kind of national protection available): AE, AG, AL, AM,

AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY,
BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM,
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HN, HR, HU, ID, IL, IN, IR, IS, JP, KE, KG, KH, KN,
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TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every
kind of regional protection available): ARIPO (BW, GH,
GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ,
TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU,
TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE,
DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU,
LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK,
SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
GW, KM, ML, MR, NE, SN, TD, TG).

Published:

- with international search report (Art. 21(3))
- before the expiration of the time limit for amending the
claims and to be republished in the event of receipt of
amendments (Rule 48.2(h))

(54) Title: METHODS FOR ALIGNING A SPECTROMETER

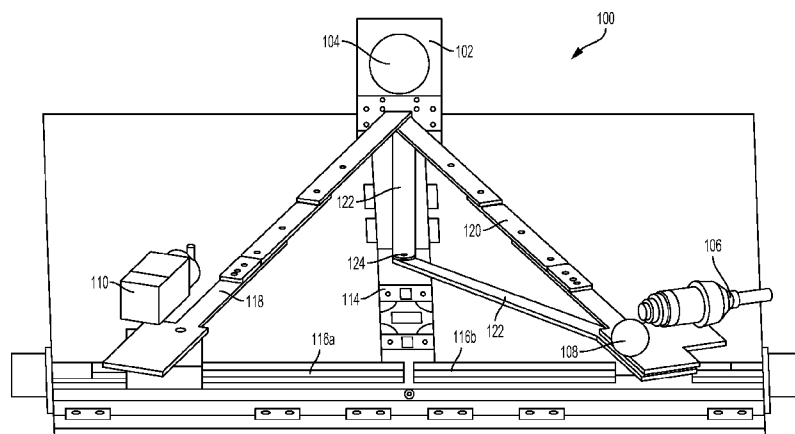


FIG. 1

(57) Abstract: An example method for aligning a spectrometer is described herein. The spectrometer includes a radiation source, a crystal analyzer, and a detector that are all positioned on an instrument plane. The method includes rotating the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane. An origin of the reciprocal lattice vector is located on the axis. The method further includes tilting the crystal analyzer or translating the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source. Example spectrometers related to the example method are also disclosed.

METHODS FOR ALIGNING A SPECTROMETER

CROSS-REFERENCE TO RELATED APPLICATION

[0001] This application claims the benefit of U.S. Provisional Patent Application No. 62/271,992, filed on December 28, 2015, the contents of which are incorporated herein by reference in their entirety.

STATEMENT REGARDING FEDERALLY SPONSORED RESEARCH OR DEVELOPMENT

[0002] This invention was made with government support under Contract Numbers DE-FG02-09ER16106 and DE-SC0008580, awarded by the United States Department of Energy. The government has certain rights in the invention.

BACKGROUND

[0003] Unless otherwise indicated herein, the materials described in this section are not prior art to the claims in this application and are not admitted to be prior art by inclusion in this section.

[0004] Many x-ray spectrometers use a curved crystal analyzer (CCA) to monochromatize x-rays for illumination of a sample or to monochromatize x-rays that are emitted from, or transmitted through, the sample. A CCA is typically fabricated by gluing or bonding a Si or Ge wafer in a concave glass lens or other concave form. The crystallographic orientation of the wafer surface is chosen so that the spacing between crystal planes nominally parallel to the surface is appropriate, via Bragg's law, to generate constructive interference of x-rays within the energy or wavelength range of interest.

[0005] The CCA will generally exhibit a miscut that results in a reciprocal lattice vector of the CCA having a non-zero tilt with respect to the surface vector exposed by the miscut. The non-zero tilt can be corrected via tilting the CCA about two perpendicular axes such that the reciprocal lattice vector of the CCA is properly aligned with respect to the source and the detector. Depending on the spectrometer and on the magnitude of the miscut, using two-tilt correction to align the CCA for proper operation of the spectrometer may take several hours. Two-axis tilt correction is generally accomplished via two sets of motorized micrometers, which adds cost and complexity. Additionally, two-axis tilt correction might be required each time a particular CCA is used.

SUMMARY

[0006] In one example, a method for aligning a spectrometer is provided. The spectrometer includes a radiation source, a crystal analyzer, and a detector that are all positioned on an instrument plane. The method includes rotating the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane. An origin of the reciprocal lattice vector is located on the axis. The method further includes tilting the crystal analyzer or translating the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source.

[0007] In another example, a non-transitory computer readable medium stores instructions that, when executed by a computing device, cause the computing device to perform functions. The functions include rotating, via a motor, the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane. An origin of the reciprocal lattice vector is located on the axis. The functions further include tilting, via a motor, the crystal analyzer or translating, via a motor, the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source.

[0008] In yet another example, a computing device includes one or more processors and a non-transitory computer readable medium storing instructions that, when executed by the one or more processors, cause the computing device to perform functions. The functions include rotating, via a motor, the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane. An origin of the reciprocal lattice vector is located on the axis. The functions further include tilting, via a motor, the crystal analyzer or translating, via a motor, the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source.

[0009] In yet another example, a spectrometer includes a stage configured to hold a crystal analyzer. The stage is rotatable about a first axis that is within an instrument plane of the spectrometer, the stage is rotatable about a second axis that is within the instrument plane or perpendicular to the instrument plane, and the stage is rotationally fixed about a third axis that is perpendicular to both the first axis and the second axis. The spectrometer further includes a

radiation source that is located on the instrument plane and (i) aligned to emit radiation toward the stage or (ii) aligned to emit radiation toward a sample, thereby causing radiation to be emitted toward the stage. The spectrometer further includes a detector that is located on the instrument plane and configured to detect radiation that is scattered by the crystal analyzer.

[0010] In yet another example, a spectrometer includes a stage configured to hold a crystal analyzer. The stage is rotatable about a first axis that is within an instrument plane of the spectrometer, the stage is rotationally fixed about a second axis that is perpendicular to the first axis, and the stage is rotationally fixed about a third axis that is perpendicular to both the first axis and the second axis. The spectrometer further includes a radiation source that is located on the instrument plane and (i) aligned to emit radiation toward the stage or (ii) aligned to emit radiation toward a sample, thereby causing radiation to be emitted toward the stage. The spectrometer further includes a detector that is located on the instrument plane and configured to detect radiation that is scattered by the crystal analyzer. The spectrometer further includes a mechanism configured to translate the detector within the instrument plane such that the detector is positioned to detect radiation scattered by the crystal analyzer.

[0011] When the term “substantially” or “about” is used herein, it is meant that the recited characteristic, parameter, or value need not be achieved exactly, but that deviations or variations, including for example, tolerances, measurement error, measurement accuracy limitations and other factors known to those of skill in the art, may occur in amounts that do not preclude the effect the characteristic was intended to provide. In some examples disclosed herein, “substantially” or “about” means within +/- 5% of the recited value.

[0012] Various embodiments disclosed herein may be discussed in further detail in “Robust optic alignment in a tilt-free implementation of the Rowland circle spectrometer,” by Devon R. Mortensen and Gerald T. Seidler, which is hereby incorporated by reference in its entirety (available at <http://www.sciencedirect.com/science/article/pii/S0368204816301025>).

[0013] These, as well as other aspects, advantages, and alternatives will become apparent to those of ordinary skill in the art by reading the following detailed description, with reference where appropriate to the accompanying drawings. Further, it should be understood that this summary and other descriptions and figures provided herein are intended to illustrate the invention by way of example only and, as such, that numerous variations are possible.

BRIEF DESCRIPTION OF THE DRAWINGS

[0014] Figure 1 depicts a spectrometer, according to an example embodiment.

[0015] Figure 2 depicts a spectrometer, according to an example embodiment.

[0016] Figure 3 depicts a stage mounted on a bracket, according to an example

embodiment.

[0017] Figure 4 depicts some components of a spectrometer, according to an example embodiment.

[0018] Figure 5 is a block diagram of an example method, according to an example embodiment.

[0019] Figure 6 depicts rotation of a crystal analyzer, according to an example embodiment.

[0020] Figure 7 depicts a location of a reciprocal lattice vector of a crystal analyzer and locations of components of a spectrometer, according to an example embodiment.

[0021] Figure 8 depicts tilting of a crystal analyzer, according to an example embodiment.

[0022] Figure 9 depicts tilting of a crystal analyzer, according to an example embodiment.

DETAILED DESCRIPTION

[0023] As mentioned above, one approach for addressing spectrometer alignment errors caused by a crystal analyzer formed from a miscut wafer is to use two-axis tilt correction. Other approaches for alleviating alignment errors are disclosed herein. These approaches involve rotating the crystal analyzer about an axis that is within an instrument plane (*e.g.*, a Rowland circle) of the spectrometer. By finding a maximum intensity of diagnostic signals corresponding respectively to various rotational positions of the crystal analyzer, one can determine a first rotational position at which a reciprocal lattice vector of the crystal analyzer is within the instrument plane. Alternatively, by finding a minimum intensity of diagnostic signals corresponding respectively to various rotational positions of the crystal analyzer, one can determine a second rotational position at which a projection of the reciprocal lattice vector upon the plane of rotation is perpendicular to the instrument plane.

[0024] From the first rotational position, the reciprocal lattice vector of the crystal analyzer can be tilted within the instrument plane to bisect a line segment that is bounded by a detector of the spectrometer and a radiation source of the spectrometer. This constitutes proper alignment of the spectrometer that satisfies the Rowland circle condition. Instead of tilting the crystal analyzer after the rotation, the detector can be translated into a position such that the reciprocal lattice vector of the crystal analyzer bisects the (changed) line segment that is bounded by the detector and the radiation source. This also constitutes proper alignment of the spectrometer that satisfies the Rowland circle condition.

[0025] From the second rotational position, the reciprocal lattice vector of the crystal analyzer can be tilted into the instrument plane to bisect a line segment that is bounded by the detector and the radiation source.

[0026] Referring now to the Figures, Figure 1 is a partially upward looking view of a spectrometer 100. The spectrometer 100 includes a stage 102, a crystal analyzer 104, a radiation source 106, a sample 108, a detector 110, a frame 114, a rail 116a, a rail 116b, an arm 118, an arm 120, and a hinged arm 122. The hinged arm 122 includes a hinge 124.

[0027] The stage 102 is configured to hold the crystal analyzer 104 in place during operation of the spectrometer 100. Various embodiments of the stage 102 may include clips and/or slots that operate to hold the crystal analyzer 104 in place. The stage 102 is shown in more detail in Figure 3.

[0028] The crystal analyzer 104 is composed of a crystalline material such as silicon or germanium, for example. The crystal analyzer 104 may take the form of a spherically curved crystal analyzer or a doubly-curved crystal analyzer having at least one axis of rotational symmetry. The crystal analyzer 104 is configured to receive radiation (*e.g.*, x-rays) that are emitted by, or transmitted through, the sample 108. The crystal analyzer 104 may operate by selectively scattering, via Bragg reflection, radiation within a particular wavelength/energy band based on the lattice spacing of the crystal analyzer 104 and orientation of the crystal analyzer 104 with respect to the sample 108 or based on the orientation of the crystal analyzer 104 with respect to the radiation source 106.

[0029] The radiation source 106 may take the form of an x-ray source (*e.g.*, an x-ray tube), but other examples are possible. The radiation source 106 may be configured to emit x-rays or other radiation towards the sample 108. In a particular emission mode, the radiation impacting the sample 108 may cause the sample 108 to emit further radiation toward the crystal analyzer 104. In some transmission mode configurations, some of the radiation emitted by the radiation source 106 transmits through the sample 108 toward the crystal analyzer 104.

[0030] In other examples, the sample 108 is positioned near the detector 110 instead of the radiation source 106, contrary to what is shown in Figure 1. The radiation source 106 may be aligned to emit radiation (*e.g.*, x-rays) directly toward the crystal analyzer 104, and the crystal analyzer 104 may monochromatize radiation received directly from the radiation source 106. The monochromatized radiation may then illuminate the sample 108 and radiation that is either transmitted through or emitted from the sample 108 may be received by the detector 110.

[0031] The sample 108 may generally include any material sample of interest.

[0032] The detector 110 may take the form of any camera, line detector, or point detector configured to detect counts, intensity, and/or energy/wavelength of radiation (*e.g.*, x-rays) that are scattered by the crystal analyzer 104 and/or absorbed by, transmitted by, or emitted from the sample 108. The detector 110 may also include a mechanism (*e.g.*, one or more motorized

or non-motorized micrometers) configured to move the detector 110 relative to the crystal analyzer 104 and/or the radiation source 106.

[0033] The frame 114 may be made of metal or other materials and provide structural support for other components of the spectrometer 100.

[0034] The radiation source 106 is coupled to the rail 116b to allow movement of the radiation source 106 along the rail 116b. Similarly, the detector 110 is coupled to the rail 116a to allow movement of the detector 110 along the rail 116a. In various examples, the rails 116a and 116b are collinear or non-collinear.

[0035] The arm 118 couples the detector 110 to the stage 102. More specifically, the arm 118 is configured to track and aim the detector 110 at the crystal analyzer 104 as the detector 110 is moved along the rail 116a.

[0036] The arm 120 couples the radiation source 106 to the stage 102. More specifically, the arm 120 is configured to track and aim the radiation from the radiation source 106 (in direct illumination) or from the sample (in x-ray emission) to impinge on the crystal analyzer 104 as the radiation source 106 and/or the sample 108 are moved along the rail 116b. The arm 120 maybe extensible, *e.g.*, telescoping as shown in Figure 1 and Figure 2, or might otherwise not constrain the distance between various components of the spectrometer 100.

[0037] The hinged arm 122 has two sections of length each approximately equal to the radius of the Rowland circle. The two sections are connected at the hinge 124. The hinged arm 122 functions so that the hinge 124 serves as the center of the Rowland circle and the crystal analyzer 104 necessarily tracks the motion of the Rowland circle as determined by the location of the radiation source 106 and/or the detector 110.

[0038] Figure 2 is a top view of the spectrometer 100, with x, y, and z axes labeled for reference. The crystal analyzer 104 is obscured in the view of Figure 2 because its face is normal to the illustration plane.

[0039] The stage 102 may be configured to rotate the crystal analyzer 104 about one, two, or three axes (x, y, z) depending on the implementation. In some examples, the stage 102 includes one, two, or three sets of motorized or non-motorized micrometers that can be used to rotate or tilt the crystal analyzer 104 about any of the x, y, or z axes. Herein, the y-z plane may be referred to as the instrument plane and the x-z plane may be referred to as the rotation plane. The radiation source 106, the sample 108, the crystal analyzer 104, and the detector 110 may all be positioned within the instrument plane.

[0040] The arm 118, the arm 120, and the rails 116a and 116b are further configured to restrict movement of the stage 102, the detector 110, and the radiation source 106 such that the

stage 102, the detector 110, and the radiation source 106 remain positioned on a circle 119.

[0041] The hinged arm 122 restricts movement of the stage 102 such that the stage 102 remains at a fixed distance from the center of a circle 119 (e.g., the hinge 124). The hinged arm 122 restricts movement of the radiation source 106 such that the radiation source 106 also remains at the fixed distance from the center of the circle 119 (e.g., the hinge 124).

[0042] Figure 3 is a close up view of the crystal analyzer 104 mounted to a bracket 126 via the stage 102. The bracket 126 is mountable to the frame 114. The bracket 126 may take the form of a right-angle bracket. In this example, the stage 102 does not include capabilities for tilt or rotating the crystal analyzer 104, aside from rotating the crystal analyzer 104 within the stage 102 when the stage 102 is loosened.

[0043] Figure 4 depicts select components of the spectrometer 100. The radiation source 106, the crystal analyzer 104, and the detector 110 are all positioned on the y-z instrument plane of the spectrometer 100. The sample 108 is omitted from Figure 4 for simplicity. As shown, an ideal crystal analyzer 104 (not having a miscut) would scatter radiation received from the radiation source 106 (e.g., directly or via the sample 108) to a point 111 within the y-z instrument plane. However, the crystal analyzer 104 will generally be imperfect due to a miscut error, resulting in a reciprocal lattice vector 109 that is not aligned with the point 111. As the crystal analyzer 104 is rotated about the y-axis, the reciprocal lattice vector 109 traces a circle 112 having a center at the point 111.

[0044] Figure 5 is a block diagram of an example method 500 for aligning a spectrometer. A radiation source, a crystal analyzer, and a detector of the spectrometer are all positioned on an instrument plane.

[0045] At block 502, the method 500 includes rotating the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane. An origin of the reciprocal lattice vector is located on the axis.

[0046] At block 504, the method 500 includes tilting the crystal analyzer or translating the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source.

[0047] Figure 6 is a view of the x-z rotation plane. The crystal analyzer 104 may be rotated about the y-axis, via a motor or manually, such that the reciprocal lattice vector 109 is moved from point 602 to point 604. Point 604 is within the y-z instrument plane.

[0048] In practice, the crystal analyzer 104 may be rotated about the y-axis to a plurality

of rotational positions to identify a target rotational position. For each rotational position of the plurality of rotational positions, one may determine an intensity of radiation that is emitted by the radiation source 106 and/or the sample 108, scattered by the crystal analyzer 104, and detected by the detector 110. The determined intensities corresponding respectively to the plurality of rotational positions may be evaluated to determine a target rotational position for the crystal analyzer 104. In this example, the target rotational position may correspond to the reciprocal lattice vector 109 being aligned with point 604. A maximum intensity of the determined intensities may correspond to the position 604 (or a point on the positive end of the z-axis). That is, the signal intensity may be greatest when the reciprocal lattice vector 109 is within the y-z instrument plane and/or on the Rowland circle.

[0049] Figure 7 is a view of the y-z instrument plane. Figure 7 depicts the reciprocal lattice vector 109 after being rotated from point 602 to point 604. Since the reciprocal lattice vector 109 does not bisect a line segment bounded by the detector 110 and the radiation source 106, it may be useful to translate (*e.g.*, move) the detector 110 to account for the misalignment. As such, the detector 110 may be moved, via a motor or manually, to position 115 or position 117 such that the reciprocal lattice vector 109 does bisect a line segment bounded by the detector 110 and the radiation source 106, to satisfy the Rowland Circle condition. This example may reflect an asymmetric configuration.

[0050] Once a suitable rotational position and a suitable detector position is identified for a particular crystal analyzer, this knowledge may be used in the future to perhaps eliminate the need for additional alignment efforts prior to further operation sessions that utilize the particular crystal analyzer. One way of doing this may include marking an edge of the crystal analyzer (*e.g.*, with an ink marker) such that the marking is aligned with a structural feature or any other easily identifiable feature of the stage 102 or the spectrometer 100. This allows the crystal analyzer 104 to be removed from the spectrometer 100 and to be subsequently replaced into the spectrometer 100 and used without further alignment. One can realign the marking on the crystal analyzer 104 with the identified feature of the spectrometer 100. The detector 110 may also be translated or moved to the same position (*e.g.*, position 115 or 117) at which the spectrometer 100 was previously properly aligned for that particular crystal analyzer.

[0051] Figure 8 depicts compensating for misalignment via a one-axis tilt correction of the crystal analyzer 104 instead of translating the detector 110. The crystal analyzer 104 can be tilted about the x-axis such that the reciprocal lattice vector 109 moves from the position depicted in Figure 7 to a position such that the reciprocal lattice vector 109 is aligned with the y-axis as shown in Figure 8. The reciprocal lattice vector 109 now bisects the line segment

bounded by the detector 110 and the radiation source 106, to satisfy the Rowland Circle condition. This example may reflect a symmetric configuration.

[0052] Referring back to Figure 6, in another example the crystal analyzer 104 may be rotated about the y-axis, via a motor or manually, such that the reciprocal lattice vector 109 is moved from point 602 to point 606. At point 606, a projection of the reciprocal lattice vector 109 upon the x-z rotation plane is perpendicular to the y-z instrument plane.

[0053] In practice, the crystal analyzer 104 may be rotated about the y-axis to a plurality of rotational positions to identify a target rotational position. For each rotational position of the plurality of rotational positions, one may determine an intensity of radiation that is emitted by the radiation source 106 and/or the sample 108, scattered by the crystal analyzer 104, and detected by the detector 110. The determined intensities corresponding respectively to the plurality of rotational positions may be evaluated to determine a target rotational position for the crystal analyzer 104. In this example, the target rotational position may correspond to the reciprocal lattice vector 109 being aligned with point 606. A minimum intensity of the determined intensities may correspond to the position 606 (or a point on the negative end of the x-axis). That is, the signal intensity may be minimized when a projection of the reciprocal lattice vector 109 upon the x-z rotation plane is perpendicular to the y-z instrument plane and/or the Rowland circle.

[0054] Figure 9 depicts compensating for misalignment via a one-axis tilt correction of the crystal analyzer 104. The crystal analyzer 104 can be tilted about the z-axis such that the reciprocal lattice vector 109 moves from point 606 to a position such that the reciprocal lattice vector 109 is aligned with the y-axis as shown in Figure 9. The reciprocal lattice vector 109 now bisects the line segment bounded by the detector 110 and the radiation source 106, to satisfy the Rowland Circle condition. This example may reflect a symmetric configuration.

[0055] Prior to rotating the crystal analyzer 104 about the y-axis, one may use an optical source and an optical detector to align the crystal analyzer 104 such that a surface vector of the crystal analyzer 104 bisects a line segment that is bounded by the optical detector and the optical source. This may provide an approach for making “coarse” alignment adjustments prior to making “fine” adjustments as described above.

[0056] While various example aspects and example embodiments have been disclosed herein, other aspects and embodiments will be apparent to those skilled in the art. The various example aspects and example embodiments disclosed herein are for purposes of illustration and are not intended to be limiting, with the true scope and spirit being indicated by the following claims.

CLAIMS

1. A method for aligning a spectrometer, wherein a radiation source, a crystal analyzer, and a detector of the spectrometer are all positioned on an instrument plane, the method comprising:

rotating the crystal analyzer about an axis that is within the instrument plane and perpendicular to a rotation plane such that (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane, wherein an origin of the reciprocal lattice vector is located on the axis; and

tilting the crystal analyzer or translating the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source.

2. The method of claim 1, wherein the radiation source comprises an x-ray source.

3. The method of any of claims 1-2, wherein the crystal analyzer comprises a crystalline material.

4. The method of any of claims 1-3, wherein the crystal analyzer comprises a spherically curved crystal analyzer.

5. The method of any of claims 1-4, wherein the crystal analyzer comprises a doubly-curved crystal analyzer having at least one axis of rotational symmetry.

6. The method of any of claims 1-5, wherein rotating the crystal analyzer comprises rotating the crystal analyzer such that the reciprocal lattice vector is within the instrument plane.

7. The method of claim 6, further comprising:
after rotating the crystal analyzer, determining that the reciprocal lattice vector is within the instrument plane; and
tilting the crystal analyzer such that the reciprocal lattice vector moves parallel to the instrument plane to bisect the line segment.

8. The method of any of claims 6-7, further comprising:
rotating the crystal analyzer to a plurality of rotational positions;
for each rotational position of the plurality of rotational positions, determining an intensity of radiation that is emitted by the radiation source, scattered by the crystal analyzer, and detected by the detector; and
using the determined intensities corresponding respectively to the plurality of rotational positions to determine a target rotational position for the crystal analyzer,

wherein rotating the crystal analyzer such that the reciprocal lattice vector of the crystal analyzer is within the instrument plane comprises rotating the crystal analyzer to the target rotational position.

9. The method of claim 8, wherein using the determined intensities comprises selecting the target rotational position from the plurality of rotational positions such that the target rotational position corresponds to a maximum intensity of the determined intensities.

10. The method of any of claims 1-5, wherein rotating the crystal analyzer comprises rotating the crystal analyzer such that the component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane.

11. The method of claim 10, further comprising:
after rotating the crystal analyzer, determining that the component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane; and
tilting the crystal analyzer such that the reciprocal lattice vector moves perpendicularly to the instrument plane so as to subsequently rest in the instrument plane.

12. The method of any of claims 10-11, further comprising:
rotating the crystal analyzer to a plurality of rotational positions;
for each rotational position of the plurality of rotational positions, determining an intensity of radiation that is emitted by the radiation source, scattered by the crystal analyzer, and detected by the detector; and

using the determined intensities corresponding respectively to the plurality of rotational positions to determine a target rotational position for the crystal analyzer,
wherein rotating the crystal analyzer such that the component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane comprises rotating the crystal analyzer to the target rotational position.

13. The method of claim 12, wherein using the determined intensities comprises selecting the target rotational position from the plurality of rotational positions such that the target rotational position corresponds to a minimum intensity of the determined intensities.

14. The method of claim 6, further comprising:
after rotating the crystal analyzer, determining that the reciprocal lattice vector is within the instrument plane; and
translating the detector within the instrument plane such that the line segment becomes bisected by the reciprocal lattice vector.

15. The method of claim 14, further comprising:
rotating the crystal analyzer to a plurality of rotational positions;

for each rotational position of the plurality of rotational positions, determining an intensity of radiation that is emitted by the radiation source, scattered by the crystal analyzer, and detected by the detector; and

using the determined intensities corresponding respectively to the plurality of rotational positions to determine a target rotational position for the crystal analyzer,

wherein rotating the crystal analyzer such that the reciprocal lattice vector of the crystal analyzer is within the instrument plane comprises rotating the crystal analyzer to the target rotational position.

16. The method of claim 15, wherein using the determined intensities comprises selecting the target rotational position from the plurality of rotational positions such that the target rotational position corresponds to a maximum intensity of the determined intensities.

17. The method of any of claims 1-16, further comprising: prior to rotating the crystal analyzer, using an optical source and an optical detector to align the crystal analyzer such that a surface vector of the crystal analyzer bisects a line segment that is bounded by the optical detector and the optical source.

18. The method of any of claims 1-17, further comprising:

marking the crystal analyzer to indicate a rotational position of the crystal analyzer at which the reciprocal lattice vector bisects the line segment that is bounded by the detector and the radiation source;

removing the crystal analyzer from the spectrometer; and

thereafter mounting the crystal analyzer within the spectrometer in the indicated rotational position.

19. The method of any of claims 1-18, wherein rotating the crystal analyzer comprises rotating the crystal analyzer manually.

20. The method of any of claims 1-18, wherein rotating the crystal analyzer comprises rotating the crystal analyzer via a motor.

21. A spectrometer comprising:

a stage configured to hold a crystal analyzer, wherein the stage is rotatable about a first axis that is within an instrument plane of the spectrometer, wherein the stage is rotatable about a second axis that is within the instrument plane or perpendicular to the instrument plane, and wherein the stage is rotationally fixed about a third axis that is perpendicular to both the first axis and the second axis;

a radiation source that is located on the instrument plane and (i) aligned to emit radiation toward the stage or (ii) aligned to emit radiation toward a sample, thereby causing radiation to be emitted toward the stage; and

a detector that is located on the instrument plane and configured to detect radiation that is scattered by the crystal analyzer.

22. The spectrometer of claim 21, further comprising:

a frame; and

a right-angle bracket attached to the frame, wherein the stage is mounted on the right-angle bracket.

23. The spectrometer of any of claims 21-22, further comprising:

a first rail and a second rail, wherein the radiation source is coupled to the second rail to allow movement of the radiation source along the second rail, and wherein the detector is coupled to the first rail to allow movement of the detector along the first rail;

a first arm that couples the detector to the stage, wherein the first arm is configured to maintain a constant distance between the stage and the detector as the detector is moved along the first rail; and

a second arm that couples the radiation source to the stage, wherein the second arm is configured to maintain a constant distance between the stage and the radiation source as the radiation source is moved along the second rail.

24. The spectrometer of claim 23, wherein the first arm, the second arm, the first rail, and the second rail are further configured to restrict movement of the stage, the detector, and the radiation source such that the stage, the detector, and the radiation source remain positioned on a common circle.

25. The spectrometer of claim 24, further comprising a third hinged arm, wherein the third hinged arm restricts movement of the stage such that the stage remains at a fixed distance from a center of the common circle, and wherein the third hinged arm restricts movement of the radiation source such that the radiation source also remains at the fixed distance from the center of the common circle.

26. The spectrometer of any of claims 21-25, wherein the radiation source comprises an x-ray source.

27. A spectrometer comprising:

a stage configured to hold a crystal analyzer, wherein the stage is rotatable about a first axis that is within an instrument plane of the spectrometer, wherein the stage is rotationally fixed about a second axis that is perpendicular to the first axis, and wherein the

stage is rotationally fixed about a third axis that is perpendicular to both the first axis and the second axis;

a radiation source that is located on the instrument plane and (i) aligned to emit radiation toward the stage or (ii) aligned to emit radiation toward a sample, thereby causing radiation to be emitted toward the stage;

a detector that is located on the instrument plane and configured to detect radiation that is scattered by the crystal analyzer; and

a mechanism configured to translate the detector within the instrument plane such that the detector is positioned to detect radiation scattered by the crystal analyzer.

28. The spectrometer of claim 27, further comprising:

a frame; and

a right-angle bracket attached to the frame, wherein the stage is mounted on the right-angle bracket.

29. The spectrometer of any of claims 27-28, further comprising:

a first rail and a second rail, wherein the radiation source is coupled to the second rail to allow movement of the radiation source along the second rail, and wherein the detector is coupled to the first rail to allow movement of the detector along the first rail;

a first arm that couples the detector to the stage, wherein the first arm is configured to maintain a constant distance between the stage and the detector as the detector is moved along the first rail; and

a second arm that couples the radiation source to the stage, wherein the second arm is configured to maintain a constant distance between the stage and the radiation source as the radiation source is moved along the second rail.

30. The spectrometer of claim 29, wherein the first arm, the second arm, the first rail, and the second rail are further configured to restrict movement of the stage, the detector, and the radiation source such that the stage, the detector, and the radiation source remain positioned on a common circle.

31. The spectrometer of claim 30, further comprising a third hinged arm, wherein the third hinged arm restricts movement of the stage such that the stage remains at a fixed distance from a center of the common circle, and wherein the third hinged arm restricts movement of the radiation source such that the radiation source also remains at the fixed distance from the center of the common circle.

32. The spectrometer of any of claims 27-31, wherein the radiation source comprises an x-ray source.

33. A non-transitory computer readable medium storing instructions that, when executed by a computing device, cause the computing device to perform any of the methods of claims 1-20.

34. A computing device comprising:

one or more processors; and

a non-transitory computer readable medium storing instructions that, when executed by the one or more processors, cause the computing device to perform any of the methods of claims 1-20.

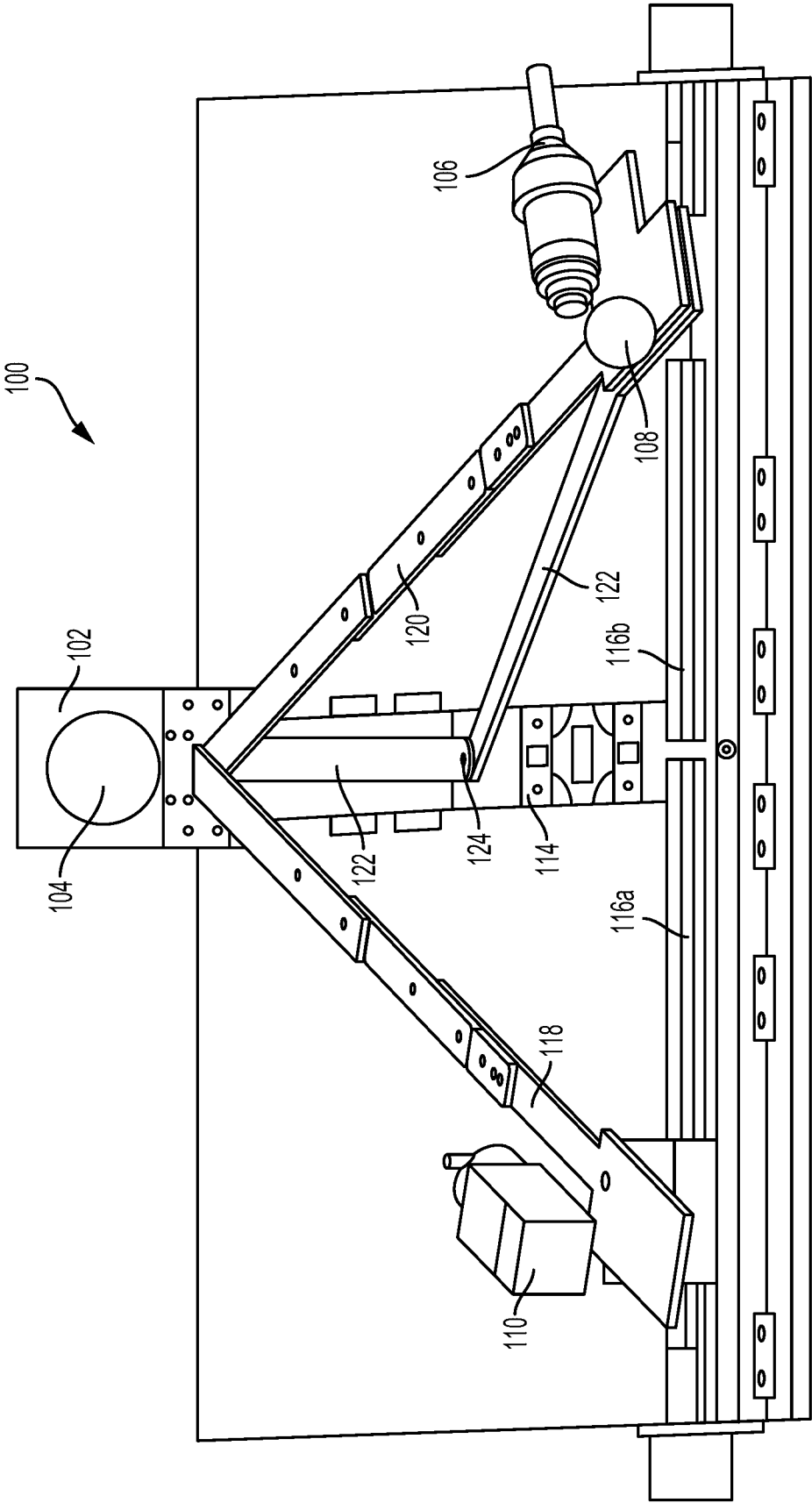


FIG. 1

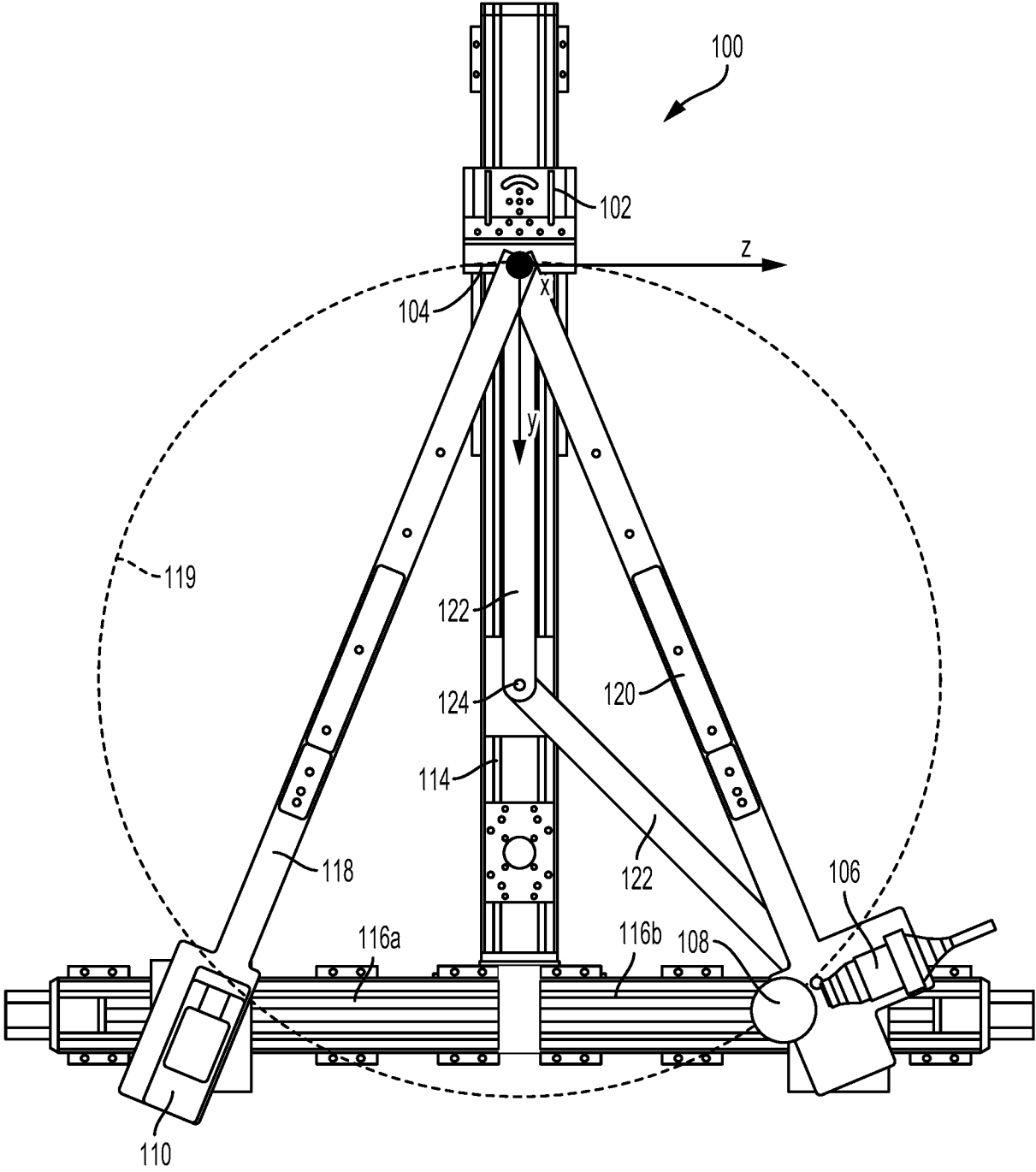


FIG. 2

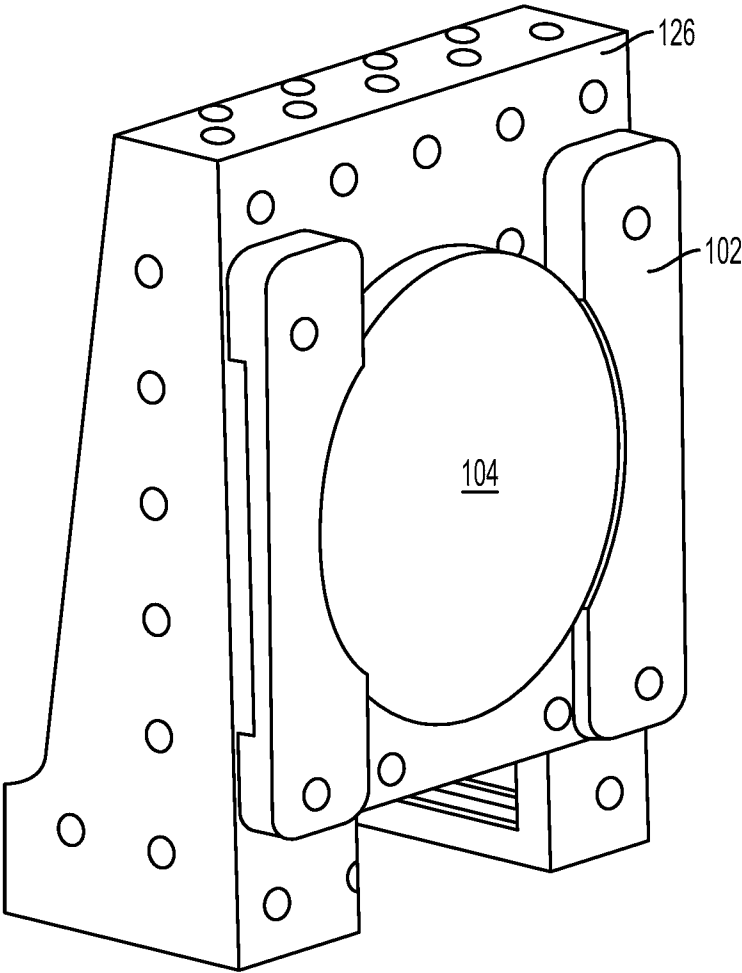


FIG. 3

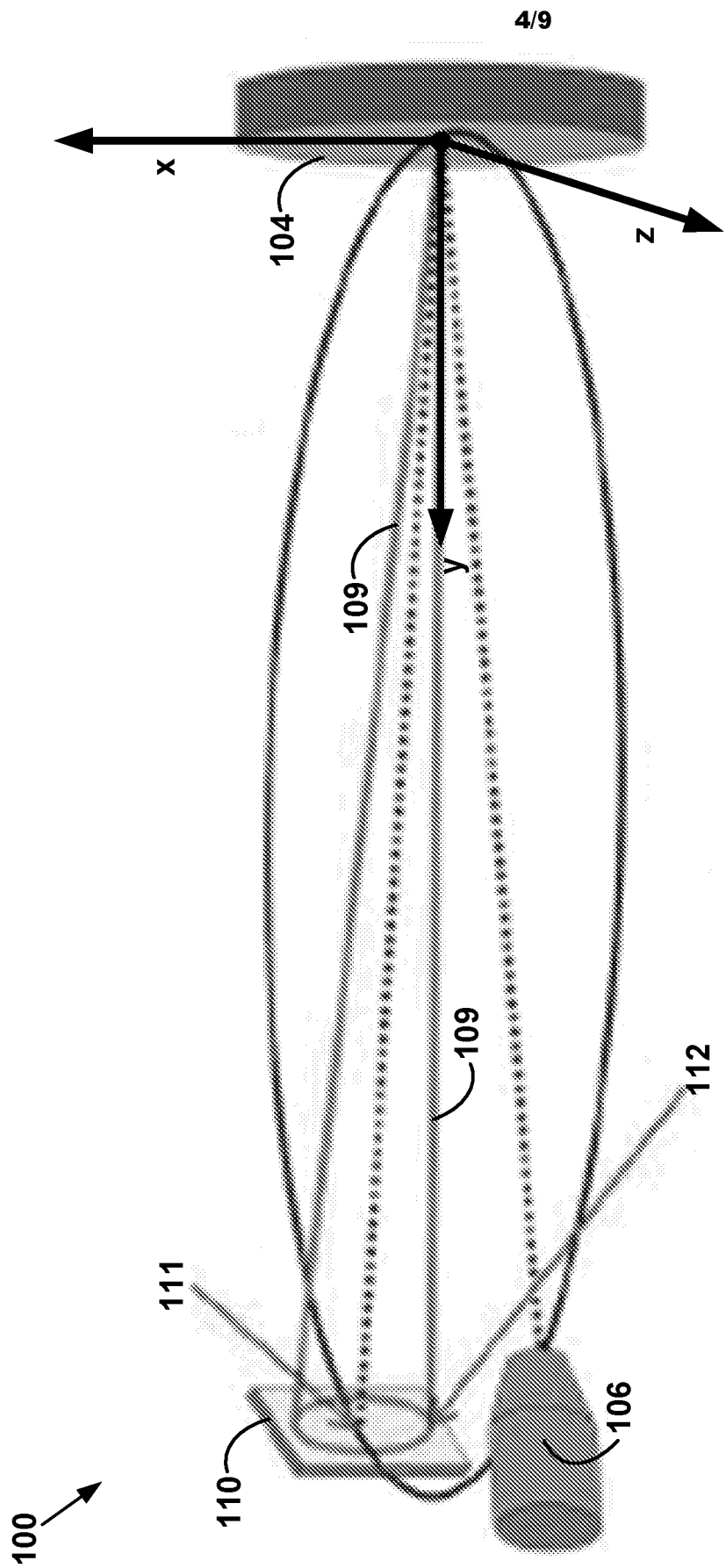


FIG. 4

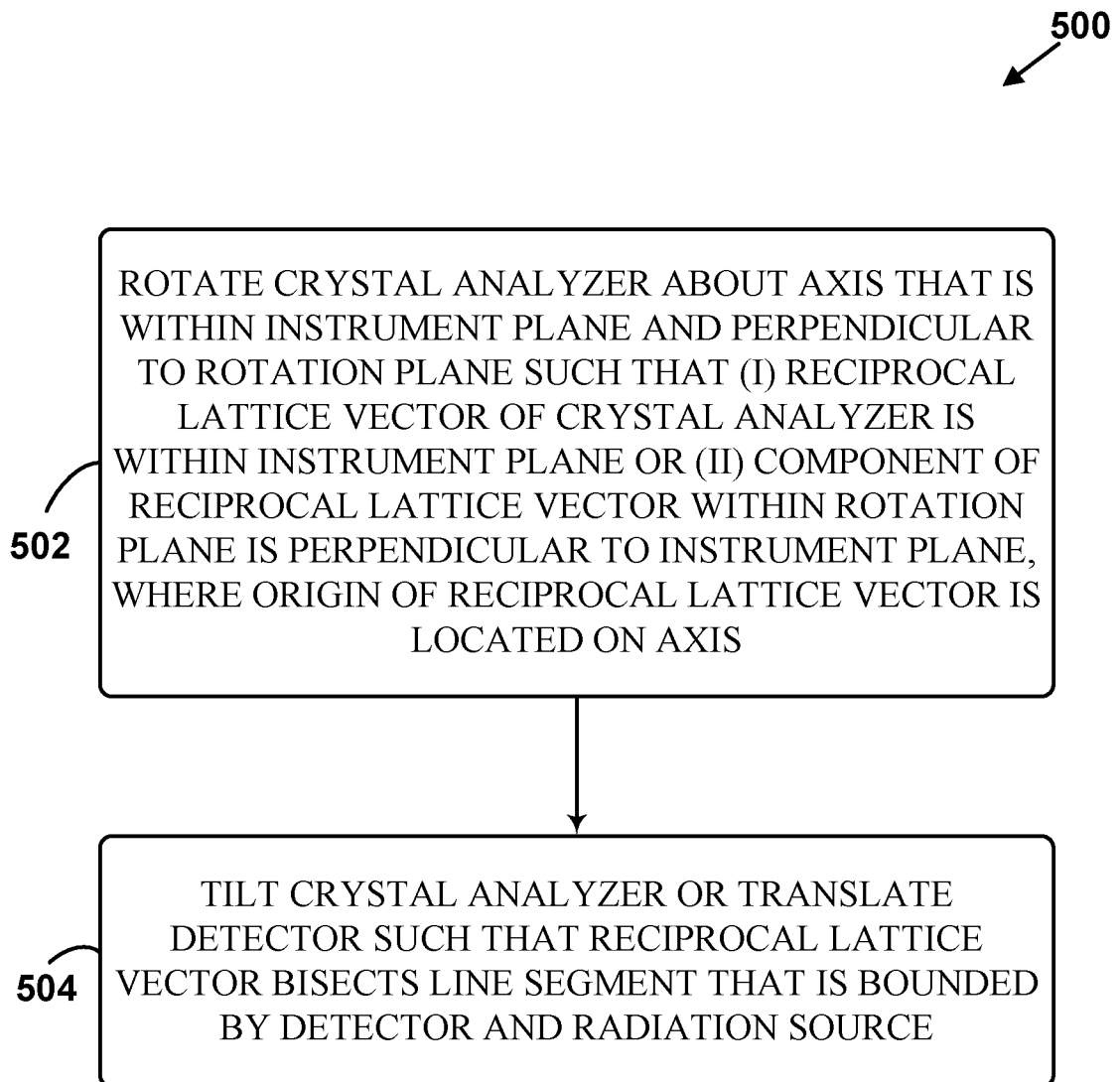


FIG. 5

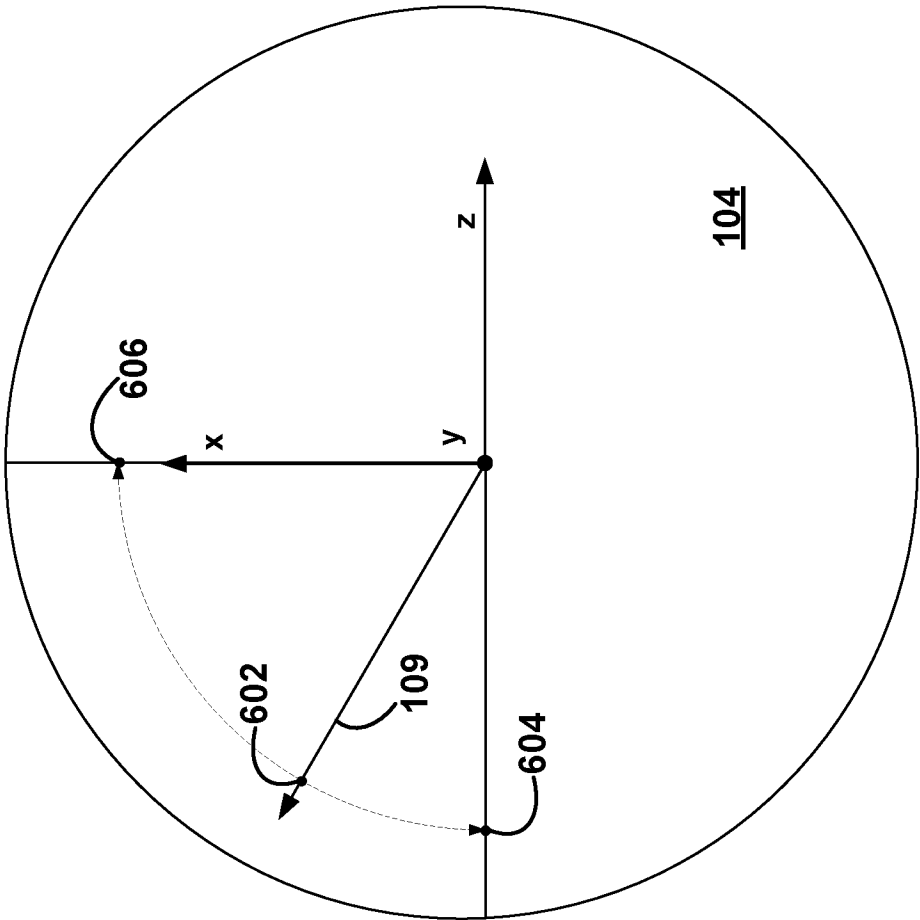


FIG. 6

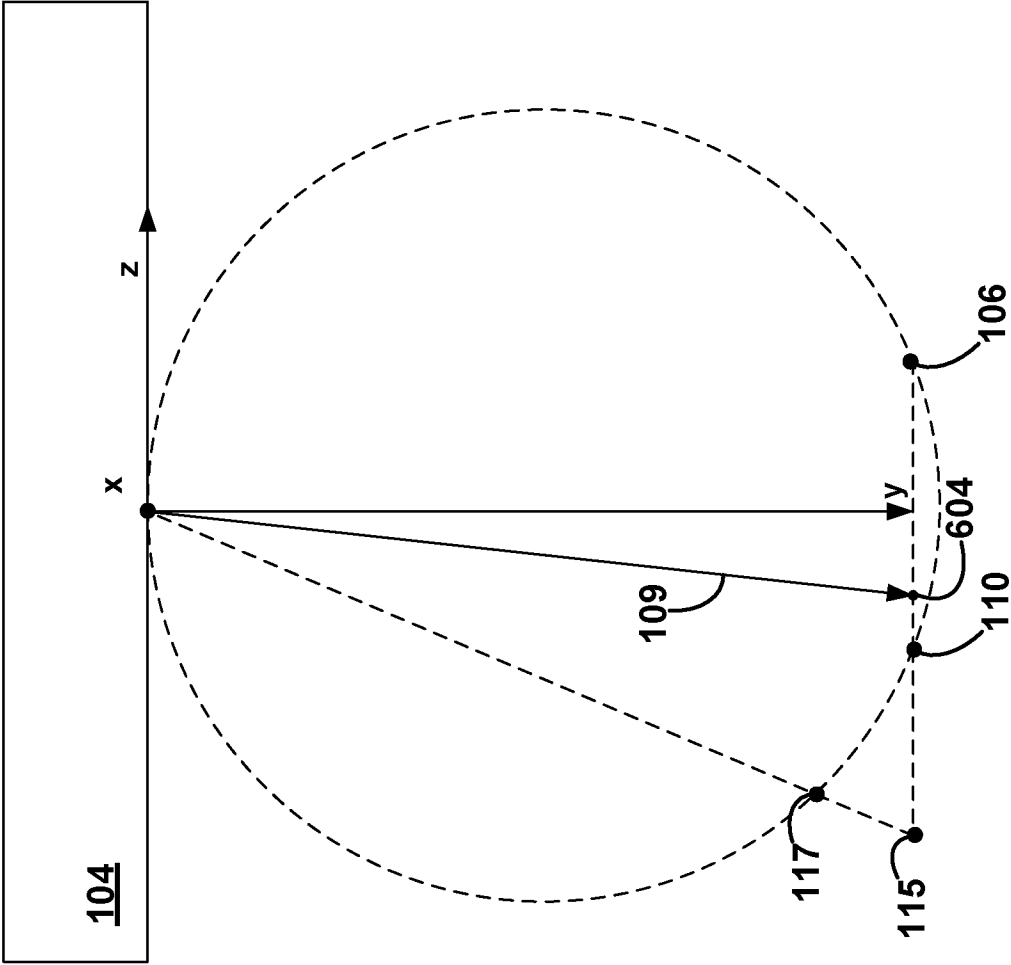


FIG. 7

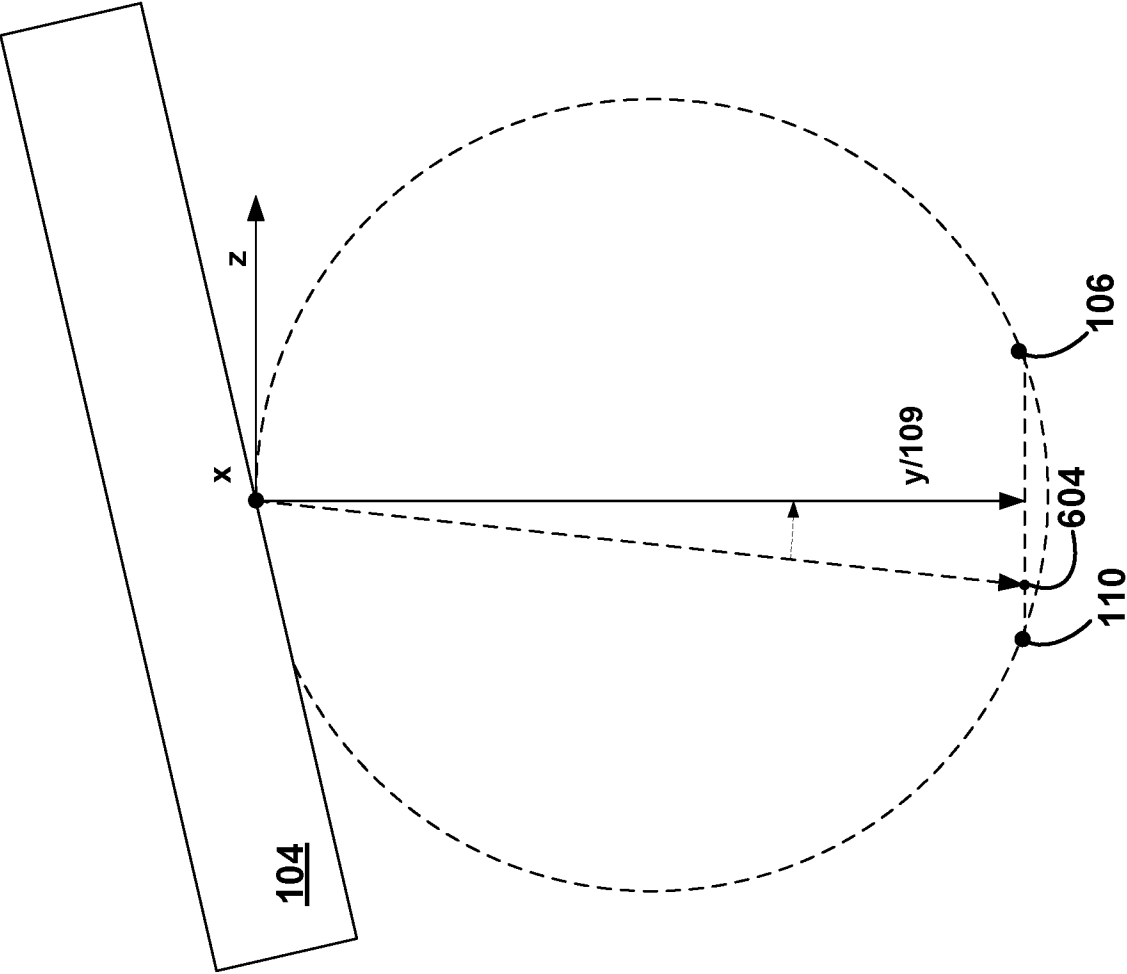


FIG. 8

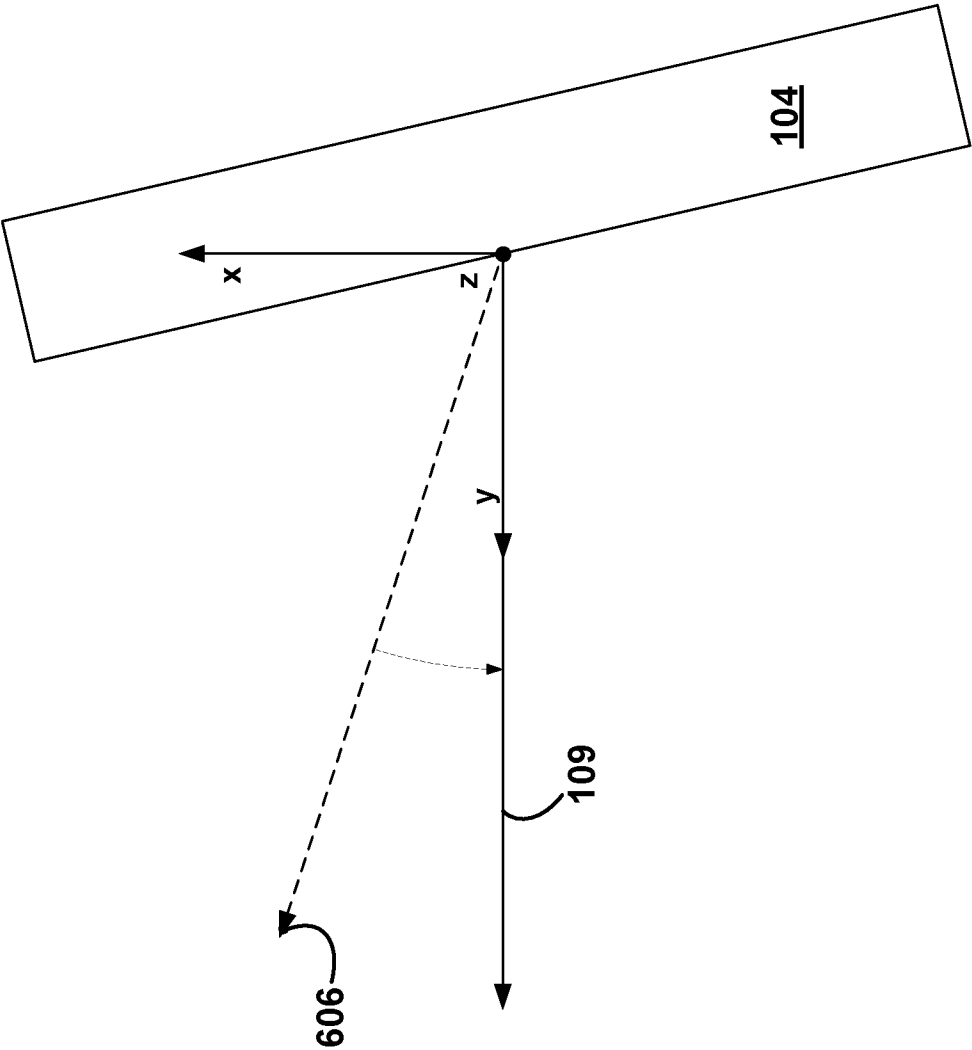


FIG. 9

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US16/68837

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. ☒ Claims Nos.: 4-20, 26, 32-34
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

-Please see extra sheet-

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
1-3

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.
- ☐ The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.
- ☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.:

PCT/US16/68837

A. CLASSIFICATION OF SUBJECT MATTER

IPC - G01J 3/02; G01N 23/20, 23/207, 21/63; G02F 1/355 (2017.01)

CPC - G01J 3/0289, 3/0278, 3/0202; G01N 23/20008, 23/2076, 21/63; G02F 1/3551

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

See Search History document

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

See Search History document

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

See Search History document

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P, X	MORTENSEN, D et al. "Robust optic alignment in a tilt-free implementation of the Rowland circle spectrometer"; Journal of Electron Spectroscopy and Related Phenomena, Vol. 215; Publication [online]. November 18, 2016 [retrieved 03 March 2017]. Retrieved from the Internet: <URL: http://www.sciencedirect.com/science/article/pii/S0368204816301025 >; pp 8-15.	1-3
A	US 2013/0138382 A1 (RIGAKU CORPORATION) May 30, 2013; figures 1, 2, paragraphs [0062], [0071], [0079], [0086], [0087], [0107], [0110]	1-3
A	"Rowland Circle Geometry based X-ray Spectrometer Alignment Guide"; XRS TECH LLC; Article [online]. May 23, 2012 [retrieved 03 March 2017]. Retrieved from the Internet: <URL: http://xrstech.com/wp-content/uploads/2015/05/spectrometer-alignment-b-1.pdf >; figure 1, page 1, paragraph 1, page 2, steps 1a-e	1-3
A	IIS 2015/330918 A1 (KOREA RESEARCH INSTITUTE OF STANDARDS AND SCIENCE) November 19, 2015; figure 2, paragraphs [0040], [0048]-[0050], [0069], [0070]	1-3
A	US 2011/0007869 A1 (GENDREAU, K et al.) January 13, 2011; entire document	1-3

☐ Further documents are listed in the continuation of Box C.☐ See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search

04 March 2017 (04.03.2017)

Date of mailing of the international search report

25 APR 2017

Name and mailing address of the ISA/

Mail Stop PCT, Attn: ISA/US, Commissioner for Patents

P.O. Box 1450, Alexandria, Virginia 22313-1450

Facsimile No. 571-273-8300

Authorized officer

Shane Thomas

PCT Helpdesk: 571-272-4300

PCT OSP: 571-272-7774

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US16/68837

.-***-Continued from Box No. III - Observations where unity of invention is lacking-***-

This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be examined, the appropriate additional examination fee must be paid.

Group I: Claims 1-3 appears to be directed towards tilting a crystal analyzer or translating a detector such that a reciprocal lattice vector bisects a line segment that is bounded by the detector and a radiation source.

Group II: Claims 21-25 & 27-31 appear to be directed towards a first, second, and third axis of rotation and scattering radiation.

The inventions listed as Groups I & II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features.

The special technical features of Group I are at least (i) a reciprocal lattice vector of the crystal analyzer is within the instrument plane or (ii) a component of the reciprocal lattice vector within the rotation plane is perpendicular to the instrument plane, wherein an origin of the reciprocal lattice vector is located on the axis; and tilting the crystal analyzer or translating the detector such that the reciprocal lattice vector bisects a line segment that is bounded by the detector and the radiation source, which are not present in Group II.

The special technical features of Group II are at least wherein the stage is rotatable about a second axis that is within the instrument plane or perpendicular to the instrument plane, and wherein the stage is rotationally fixed about a third axis that is perpendicular to both the first axis and the second axis: a radiation source that is located on the instrument plane and (i) aligned to emit radiation toward the stage or (ii) aligned to emit radiation toward a sample, thereby causing radiation to be emitted toward the stage; and a detector that is located on the instrument plane and configured to detect radiation that is scattered by the crystal analyzer, which are not present in Group I.

The common technical features of Groups I & II are at least a spectrometer, wherein a radiation source, a crystal analyzer, and a detector of the spectrometer are all positioned on an instrument plane, a stage configured to hold a crystal analyzer, wherein the stage is rotatable about a first axis that is within an instrument plane of the spectrometer, which are previously disclosed by US 2011/0007869 A1 GENDREAU, K et al. (GENDREAU).

GENDREAU discloses a spectrometer (XRD/XRF apparatus 100; paragraph [0043]), wherein a radiation source (x-ray source 100; paragraph [0043]), a crystal analyzer (a processor analyzes received radiation from the sample crystal; paragraphs [0019] & [0090]), and a detector of the spectrometer are all positioned on an instrument plane (CCD 12 positioned in the same plane as XRD/XRF apparatus 100 inherently; paragraph [0044]), a stage configured to hold a crystal analyzer (a stage x, y, z; paragraph [0044]), wherein the stage is rotatable about a first axis that is within an instrument plane of the spectrometer (rotation of the sample about a first axis normal the stage (within an instrument plane); paragraph [0090]).

Since these common features are previously disclosed by GENDREAU, they are not special and Groups I & II lack unity.