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Kay et al.

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(54) **SAMPLE IDENTIFICATION**

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Related U.S. Application Data

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(60) Provisional application No. 63/105,763, filed on Oct. 26, 2020.

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G01J 3/44 (2006.01)
G01N 21/65 (2006.01)

(52) **U.S. Cl.**
CPC **G01N 21/65** (2013.01); **G01N 2021/651** (2013.01); **G01N 2201/022** (2013.01); **G01N 2201/068** (2013.01)

(58) **Field of Classification Search**
CPC G01J 3/44; G01J 3/02; G01J 3/28; G01J 3/00; A61B 5/007; G01N 21/65; G01N 2201/0221; G01N 2021/651
See application file for complete search history.

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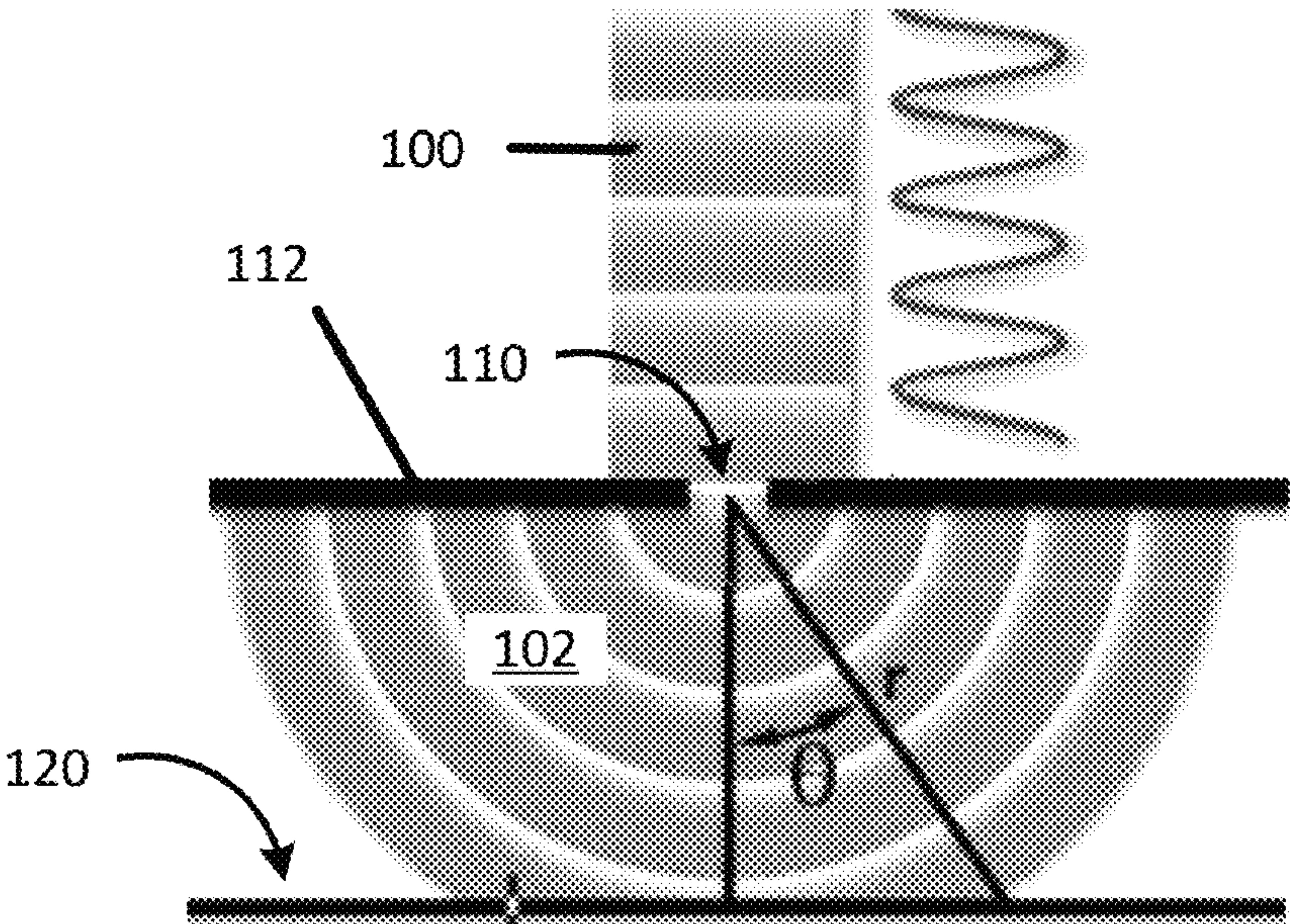
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Primary Examiner — Abdullahi Nur

(57) **ABSTRACT**

A method of analyzing a sample is disclosed. The method includes the steps of measuring a spectral response of the sample, selecting a reference material having a Raman peak with a magnitude at a wave number, measuring a peak value in the spectral response at the wave number, and determining an amount of the reference material in the sample based in part on a ratio of the measured peak value to the magnitude of the Raman peak of the reference material.

20 Claims, 14 Drawing Sheets



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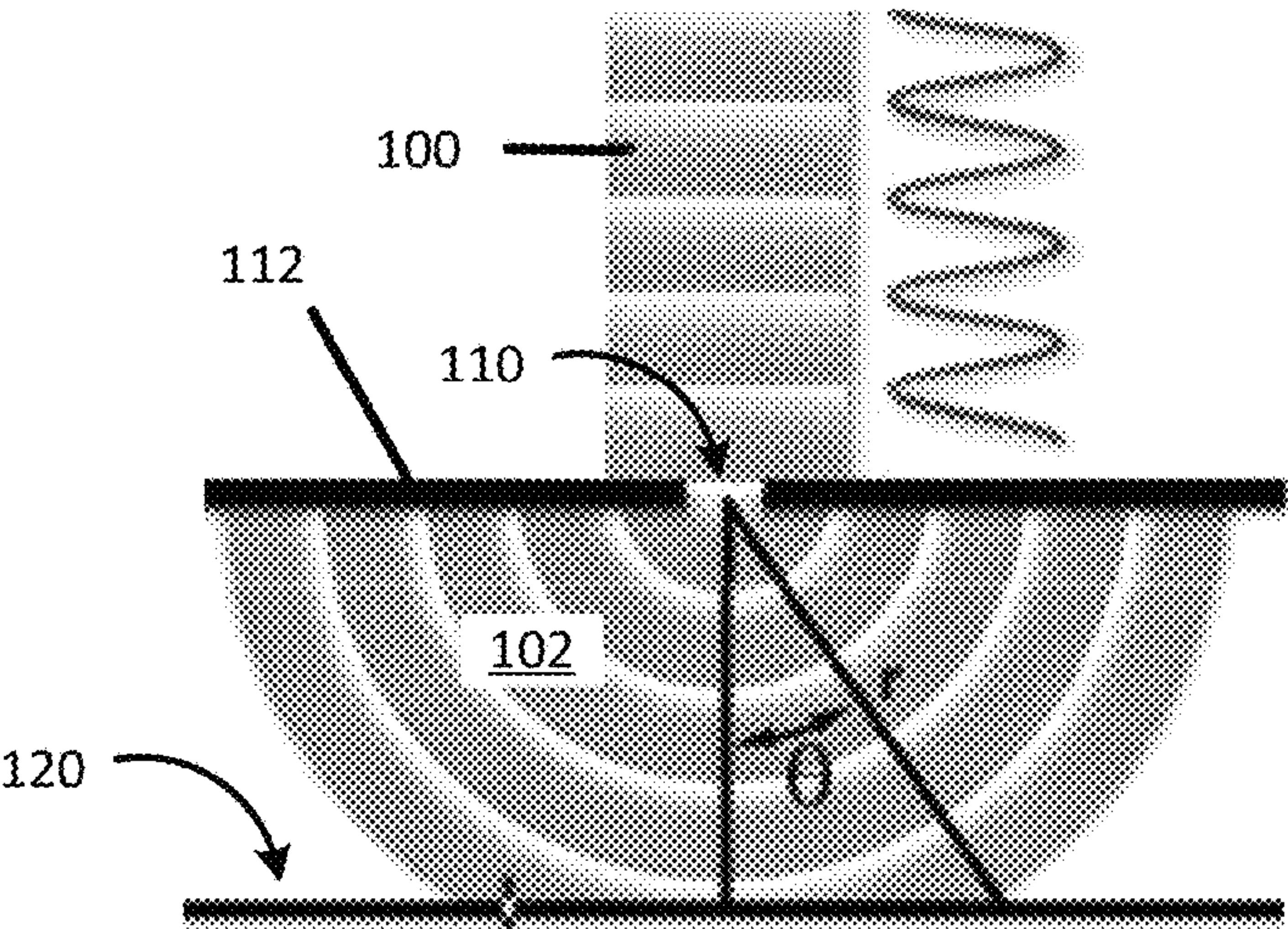


Figure 1

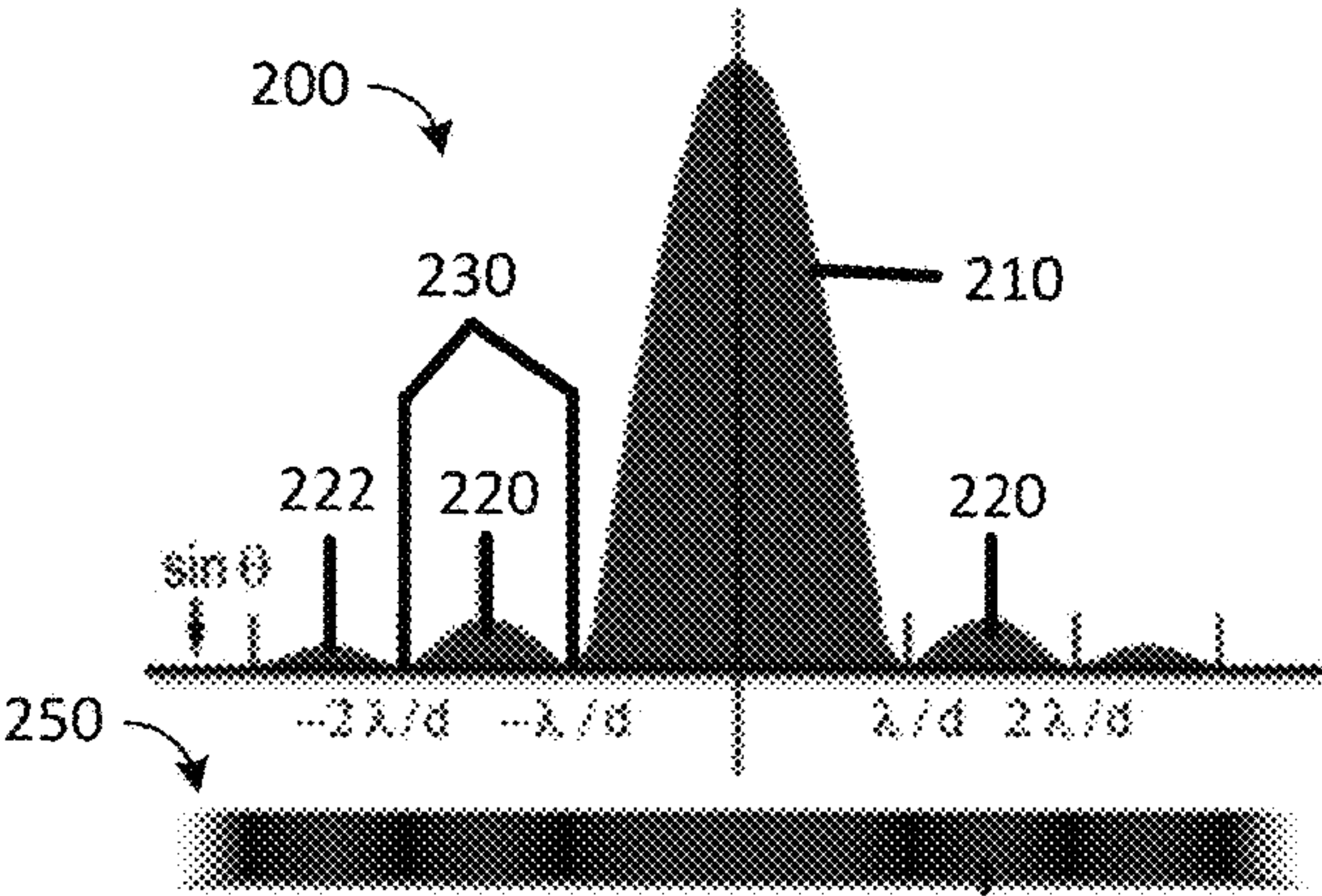


Figure 2

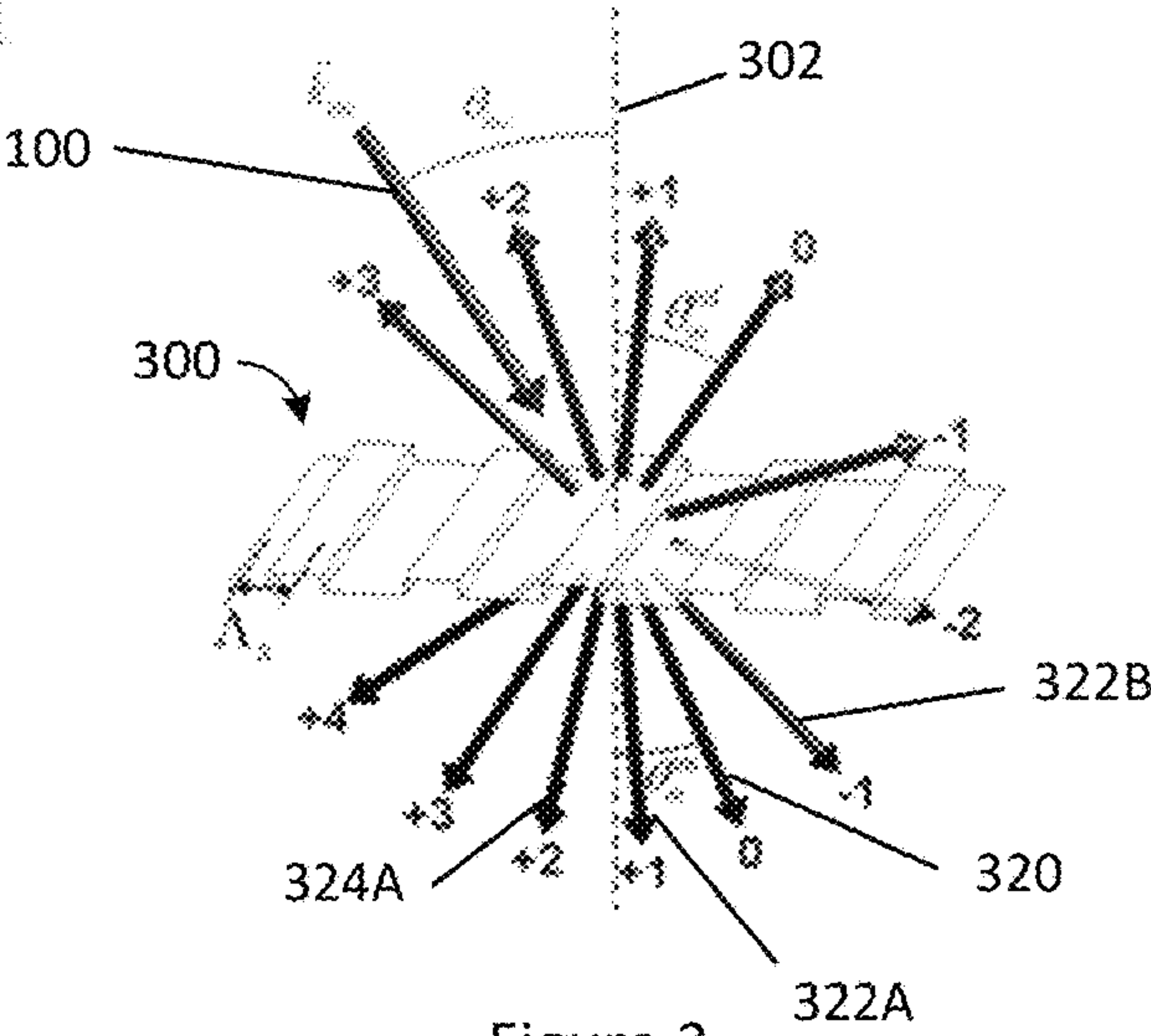


Figure 3

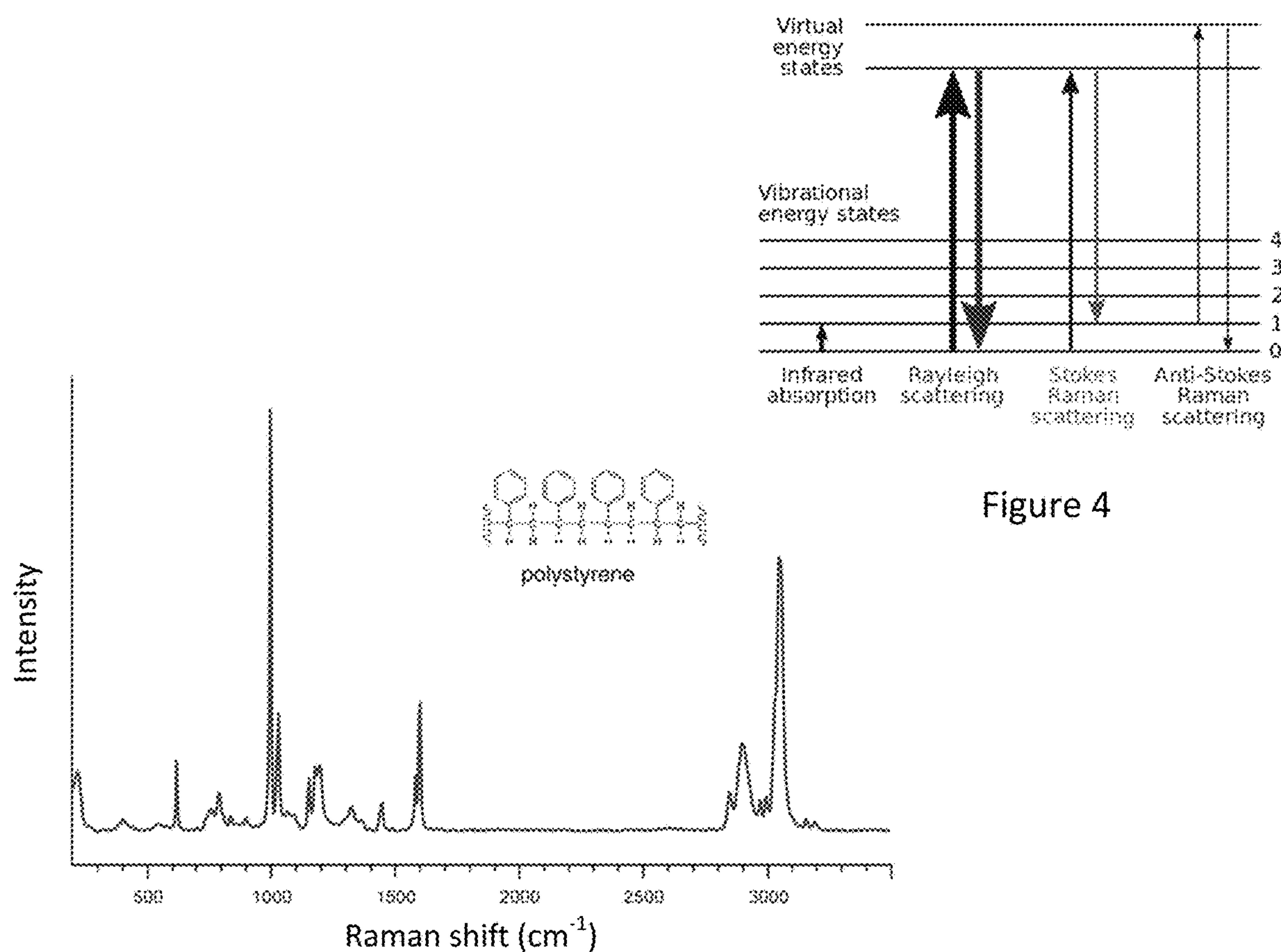


Figure 4

Figure 5

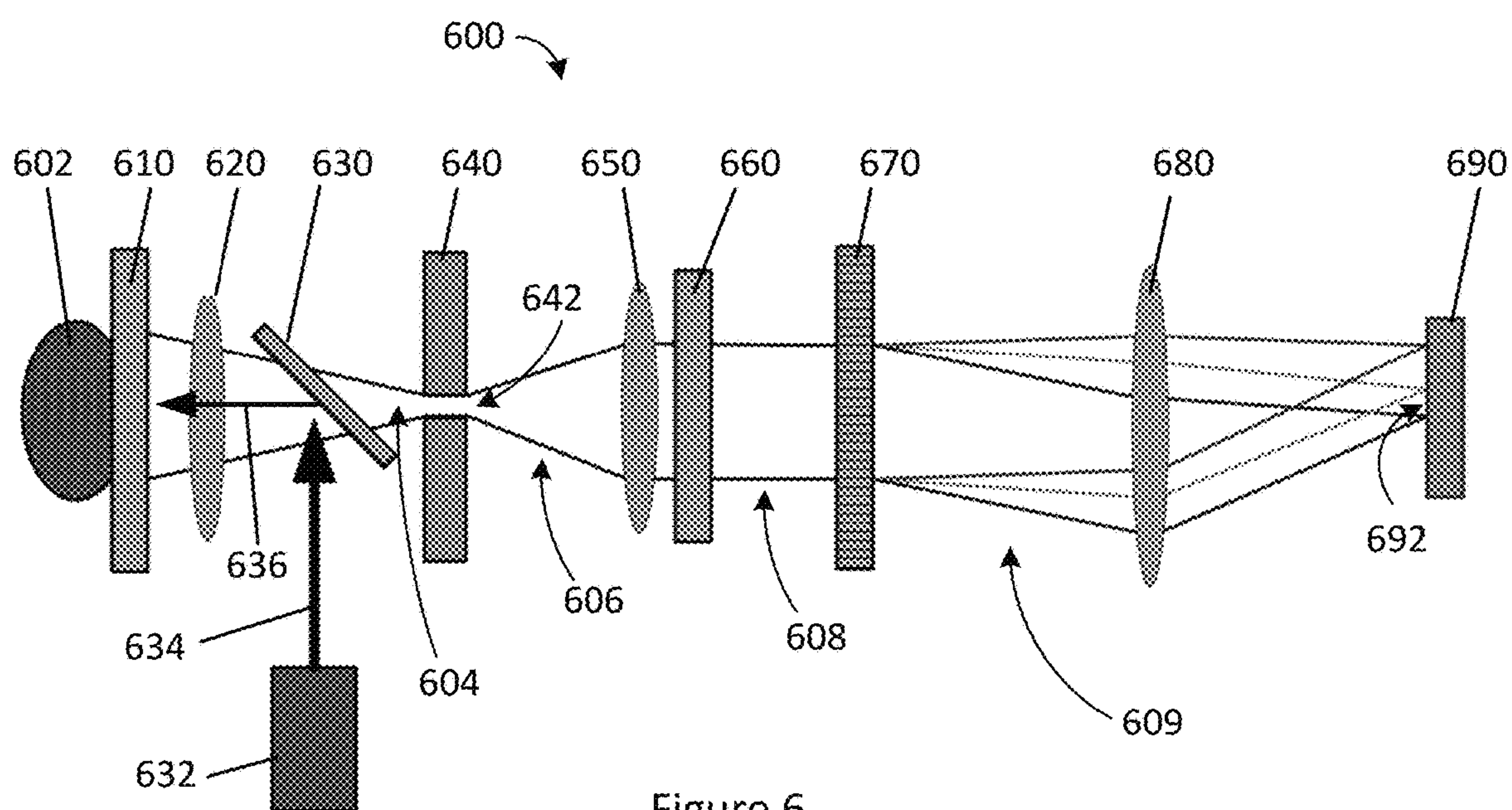


Figure 6

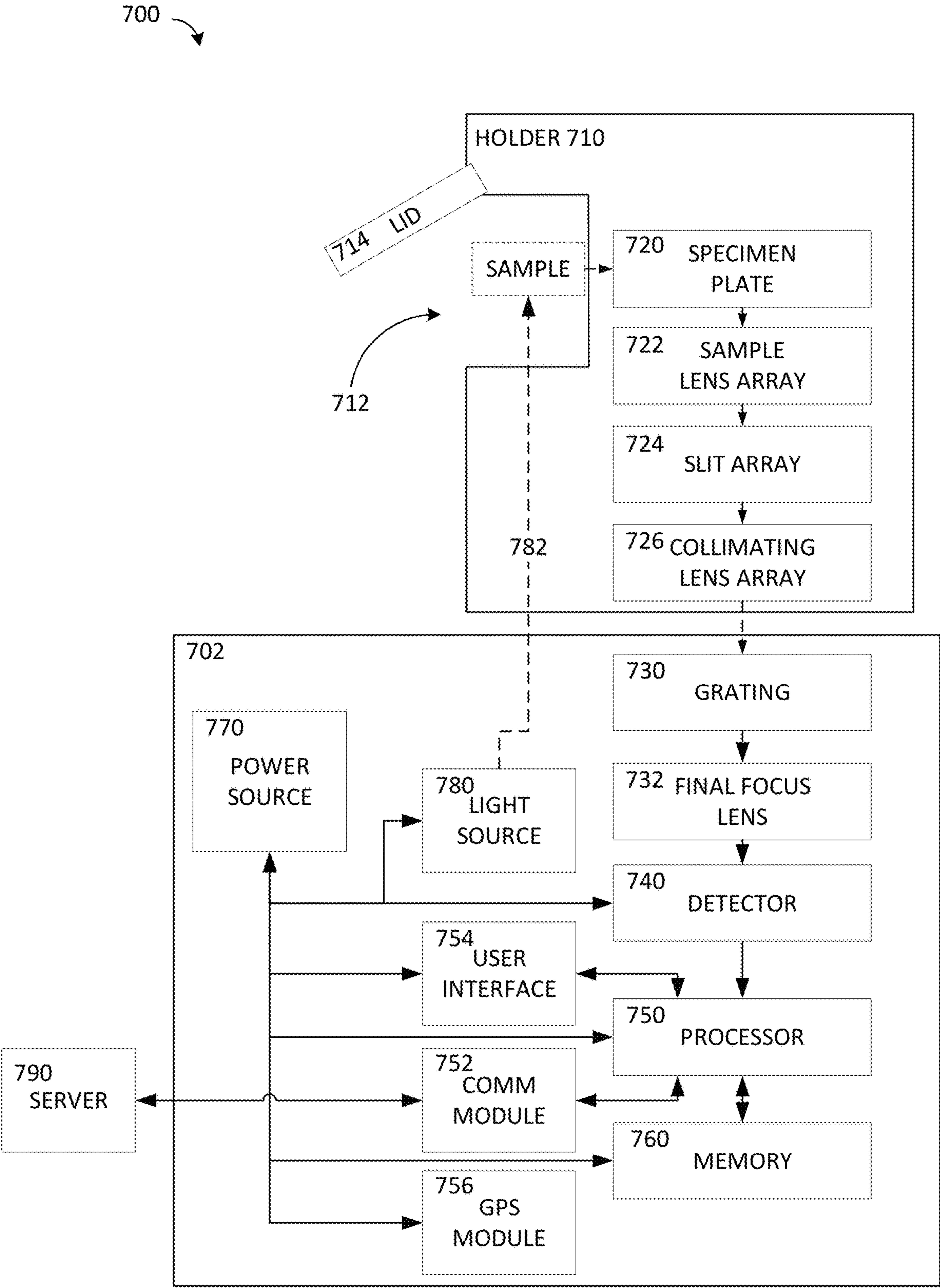


Figure 7

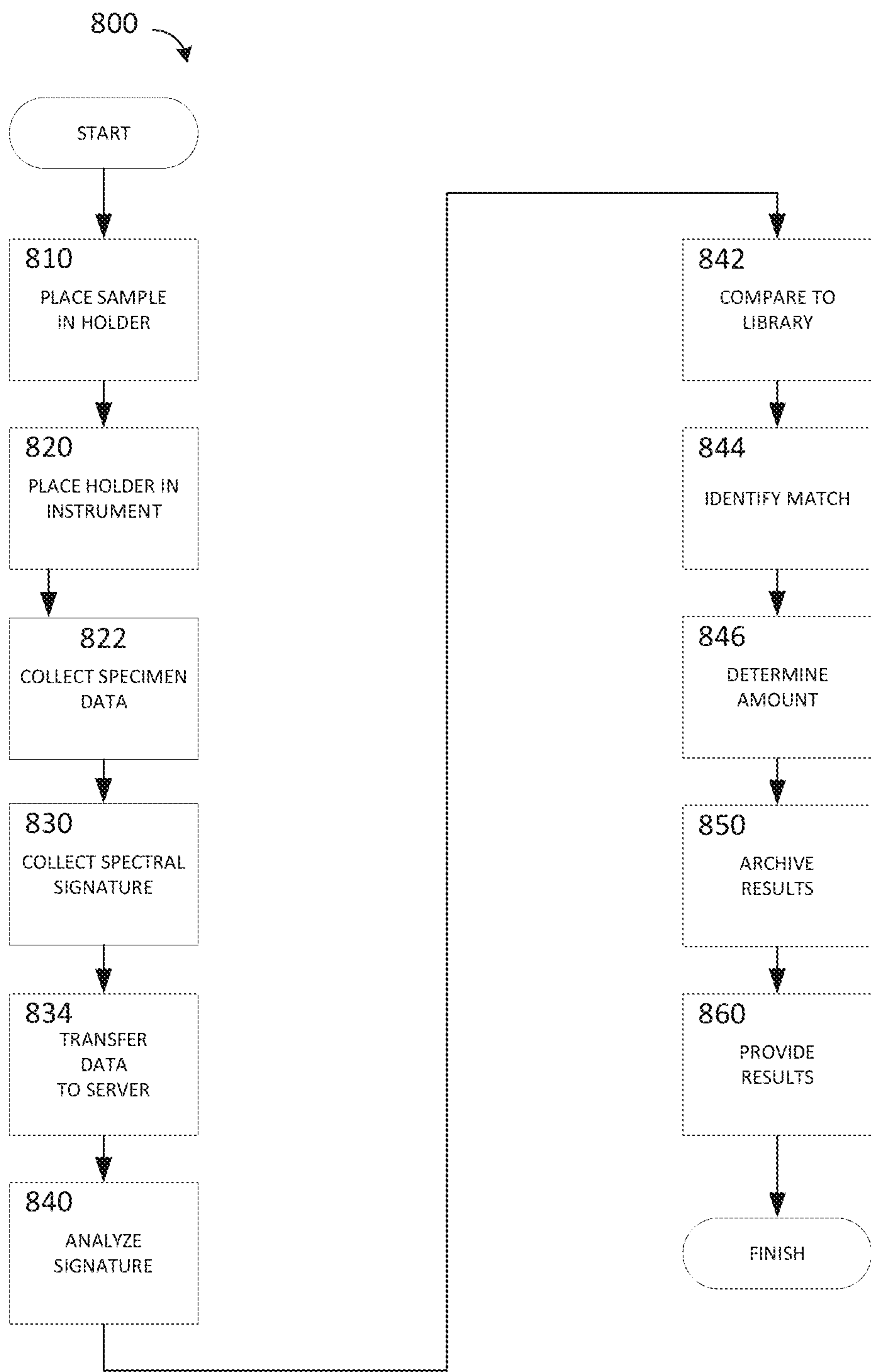


Figure 8

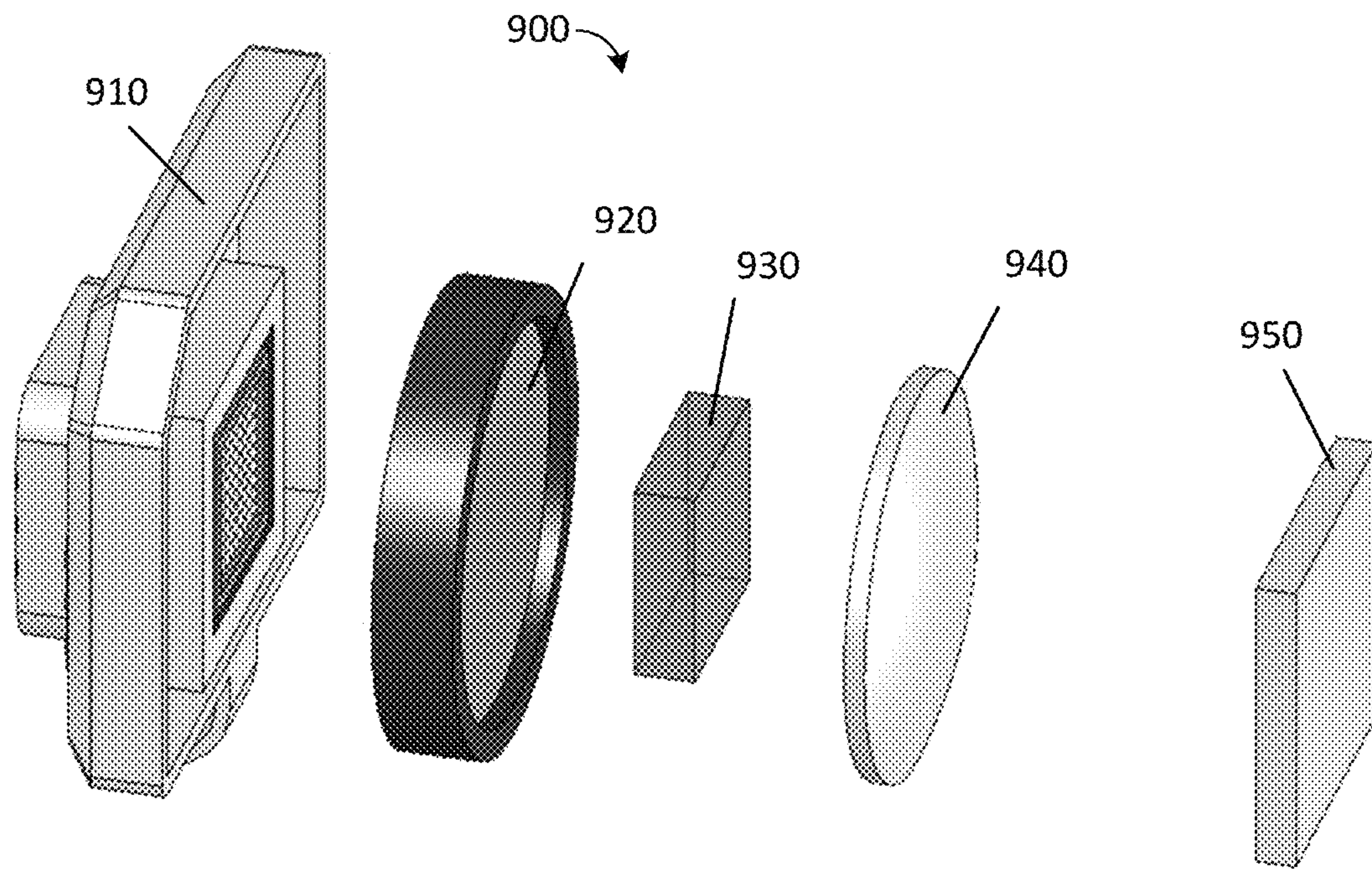


Figure 9A

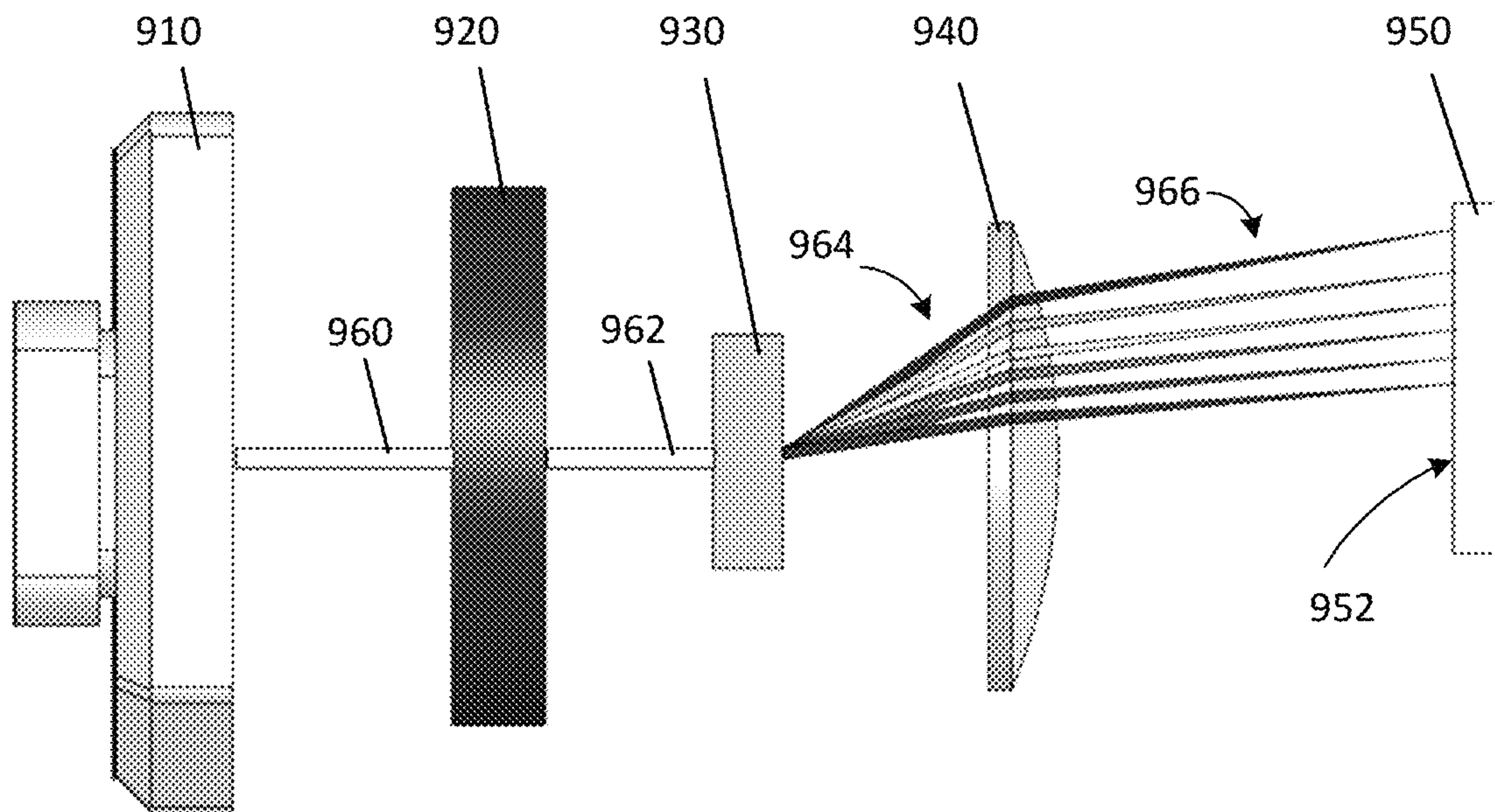


Figure 9B

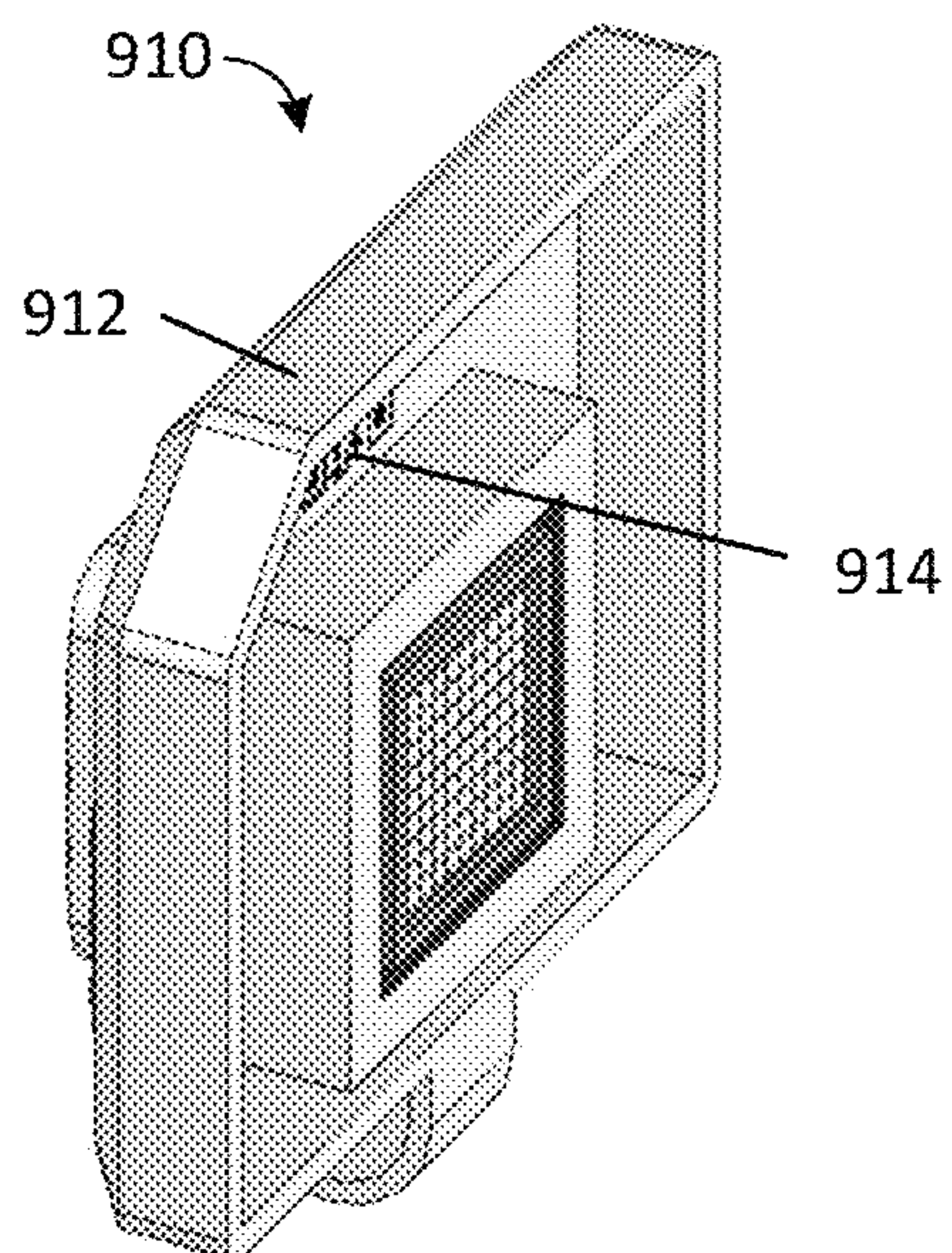


Figure 10A

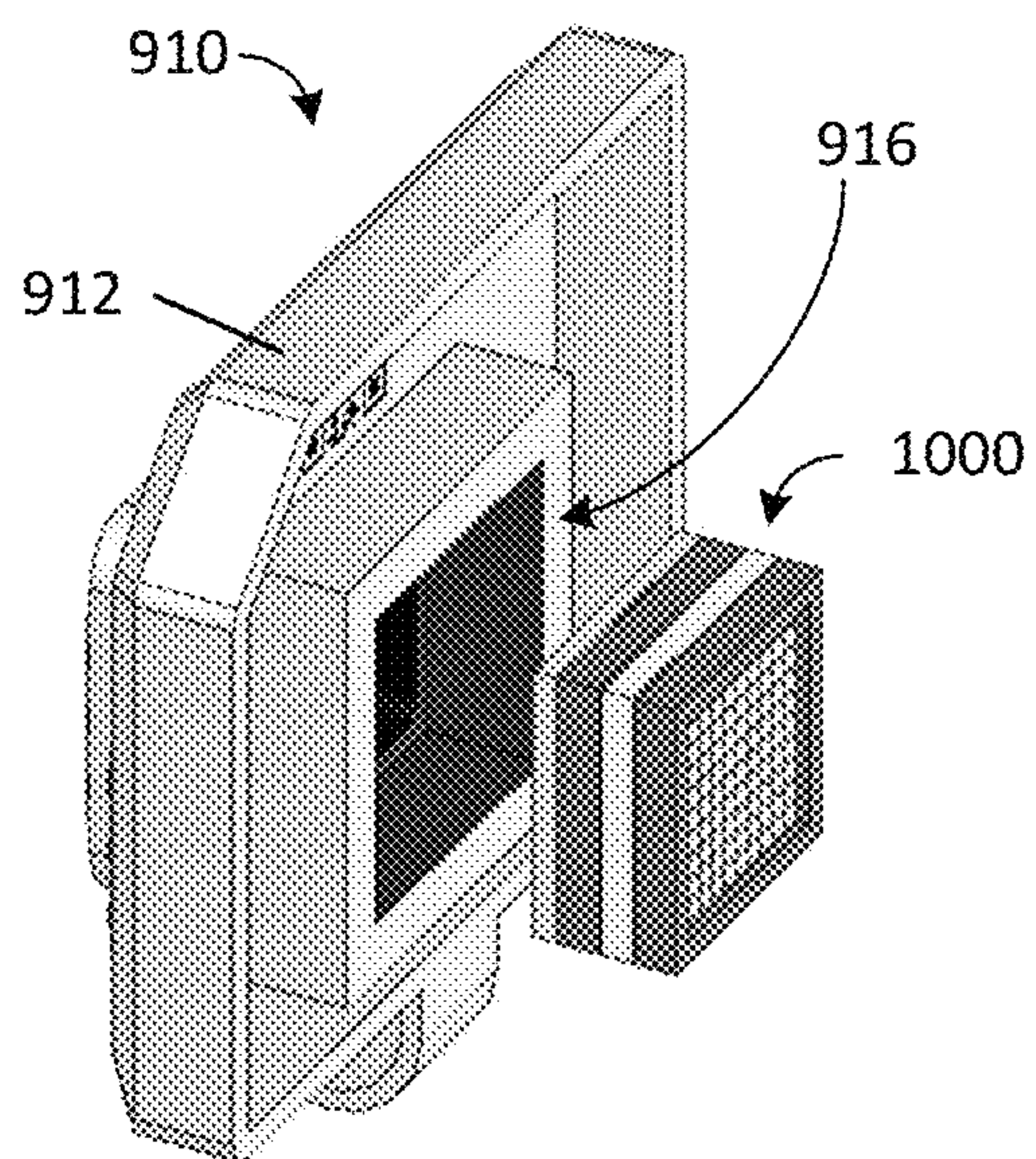


Figure 10B

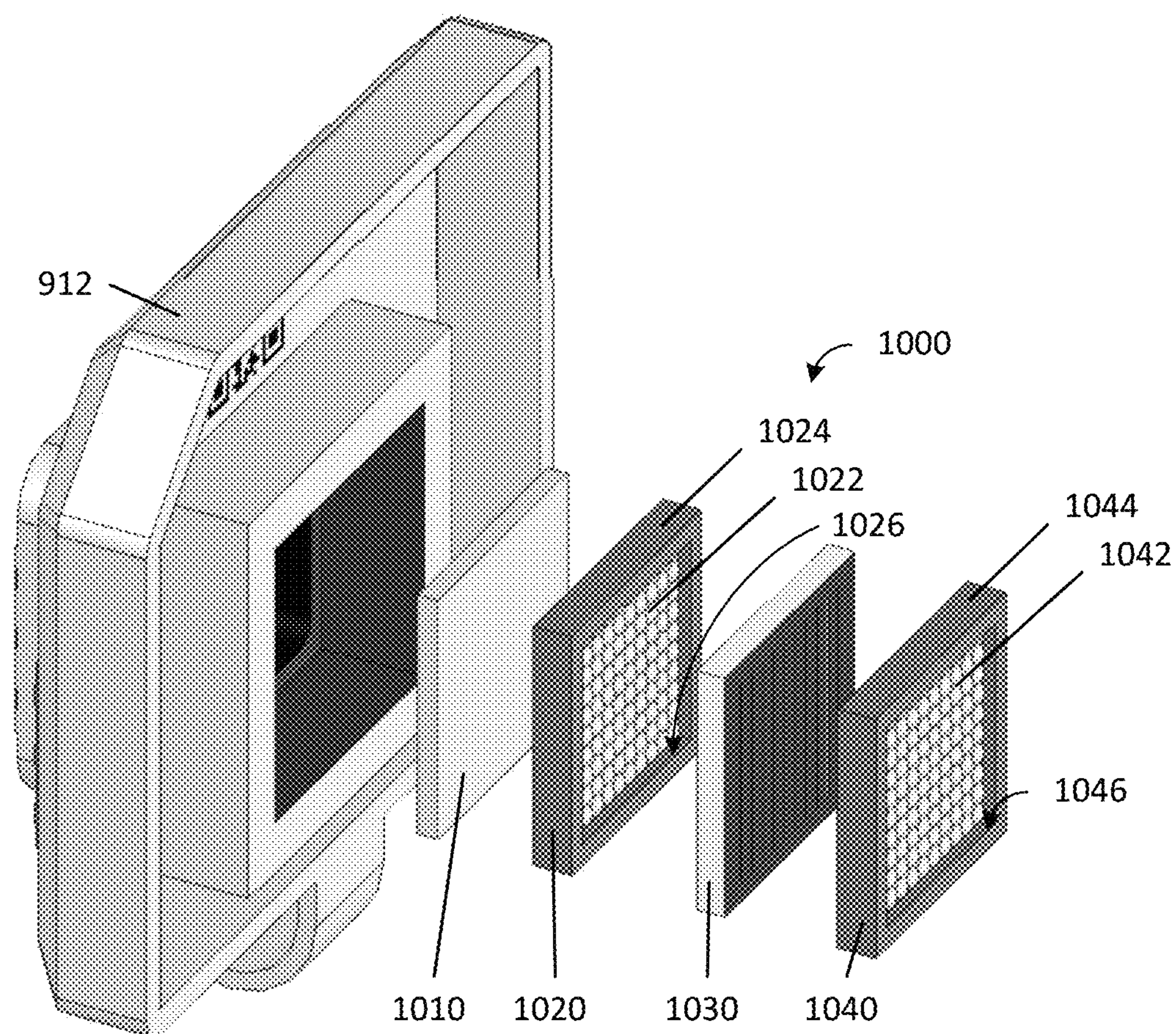


Figure 10C

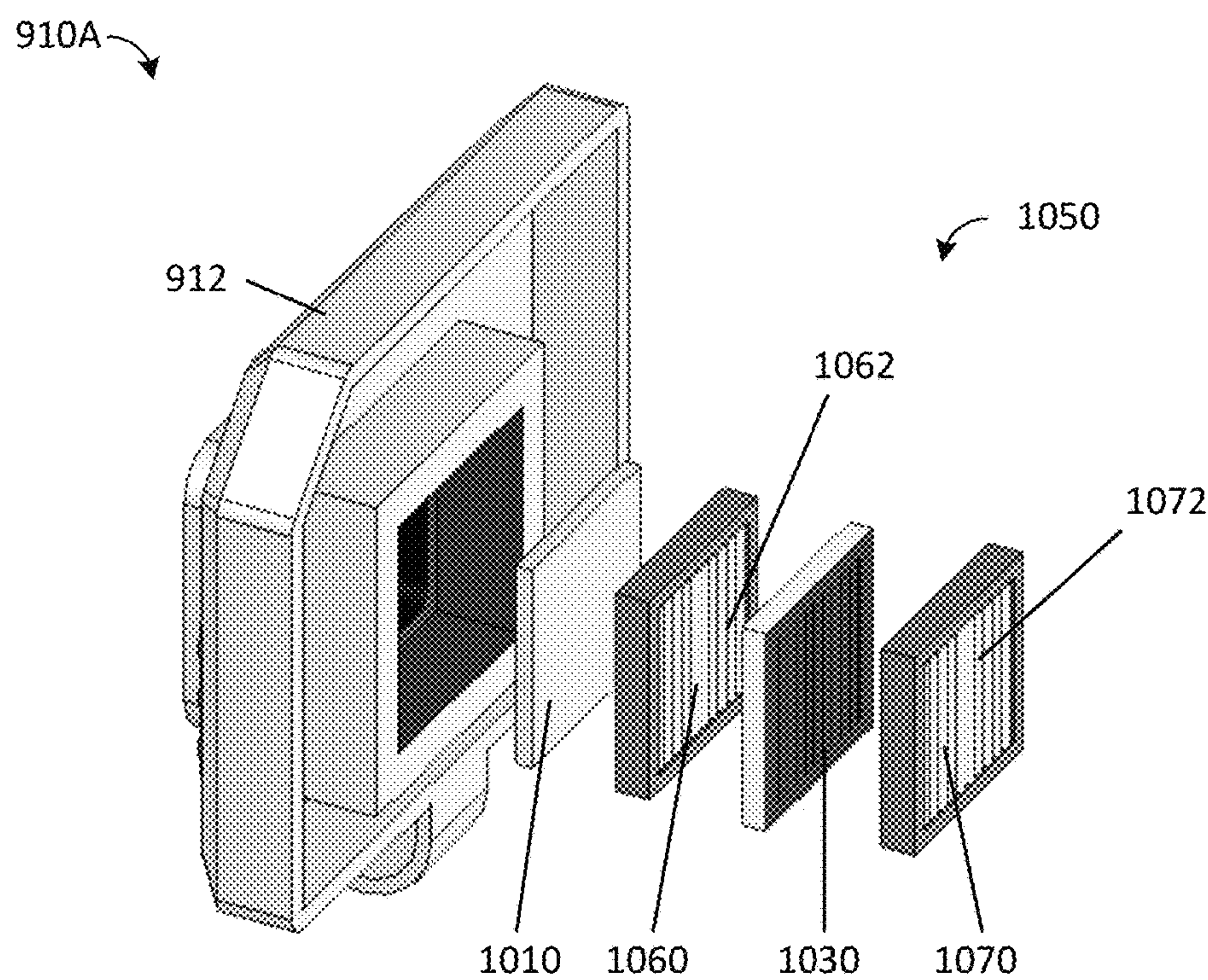


Figure 10D

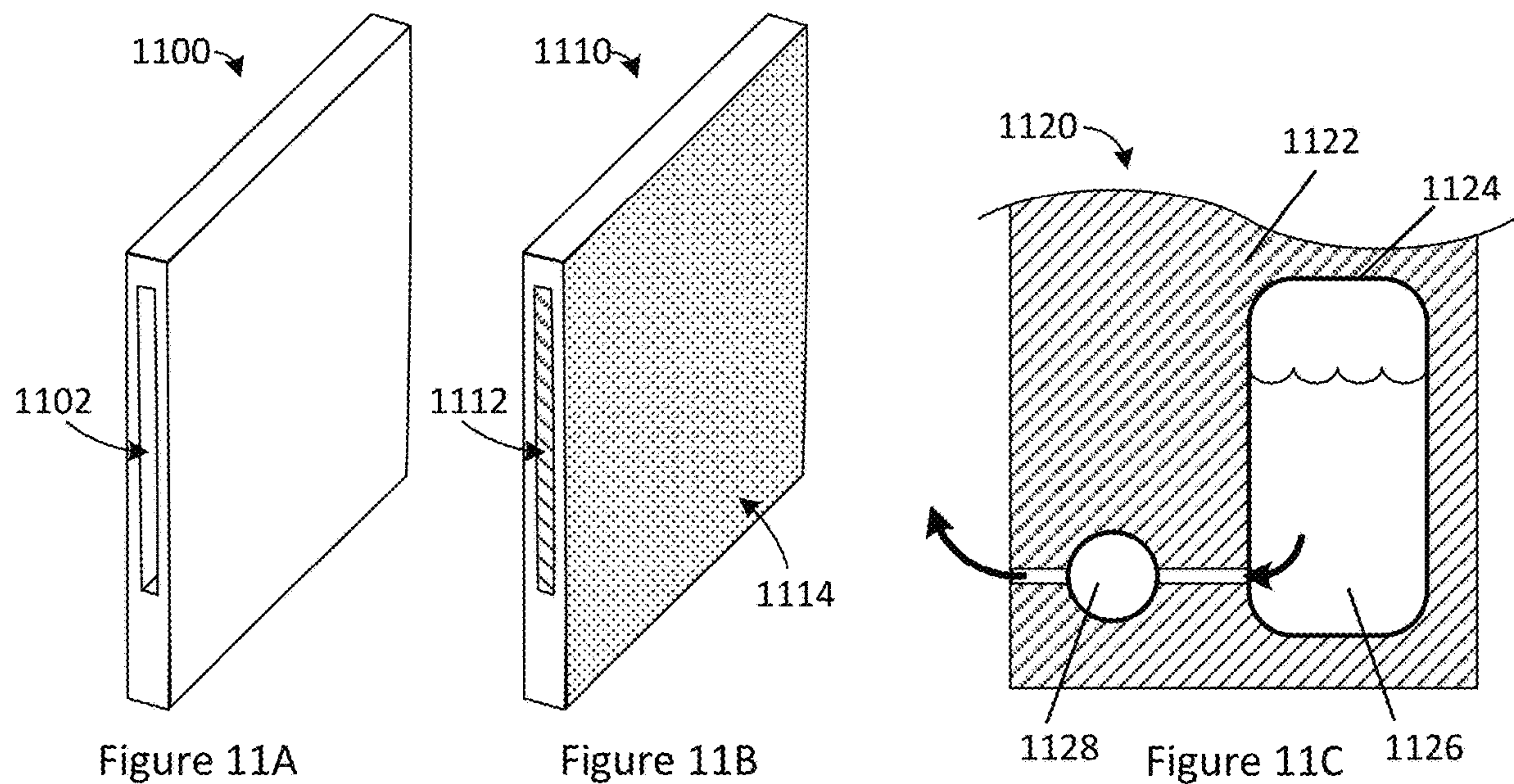


Figure 11A

Figure 11B

Figure 11C

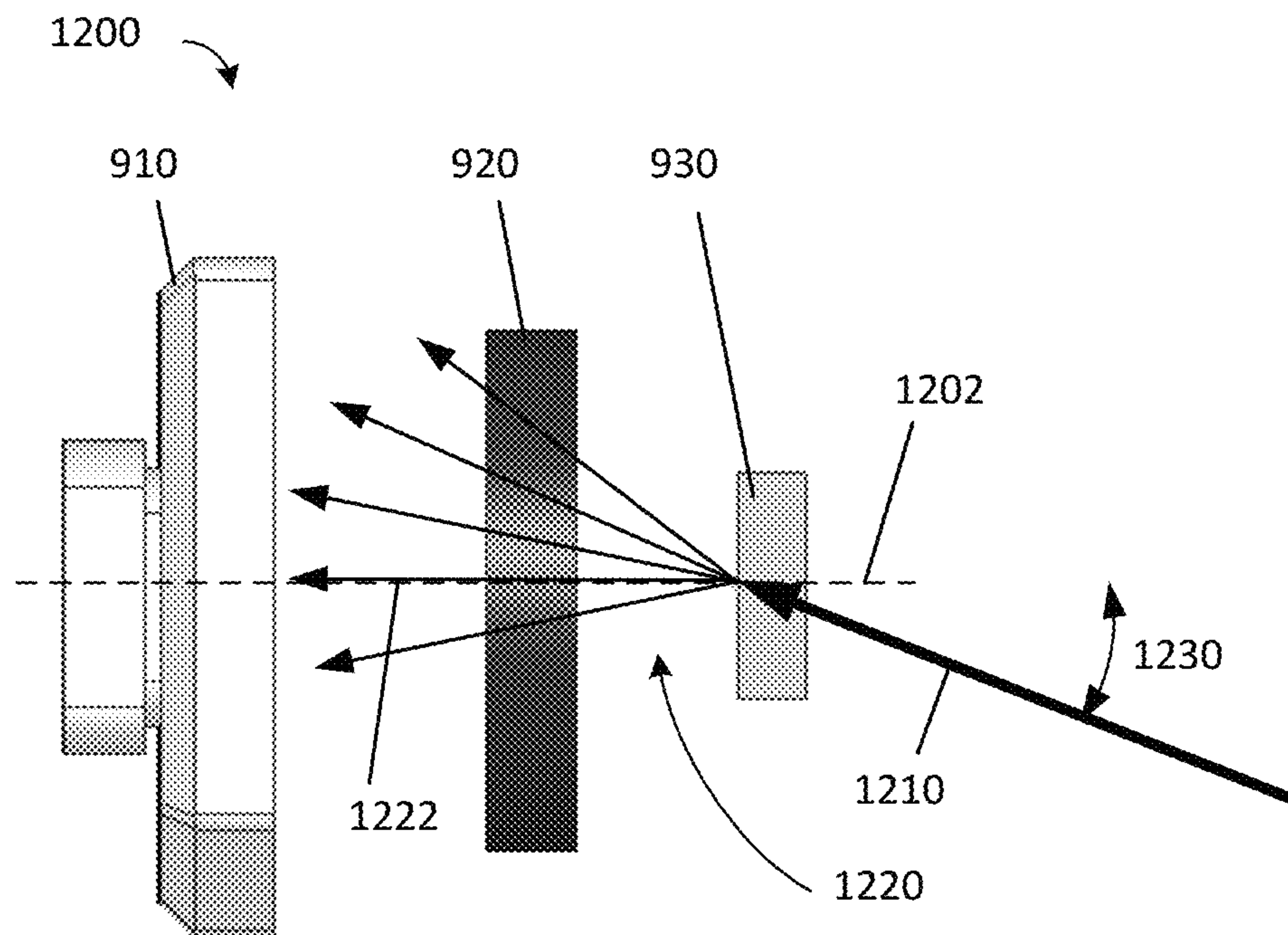


Figure 12A

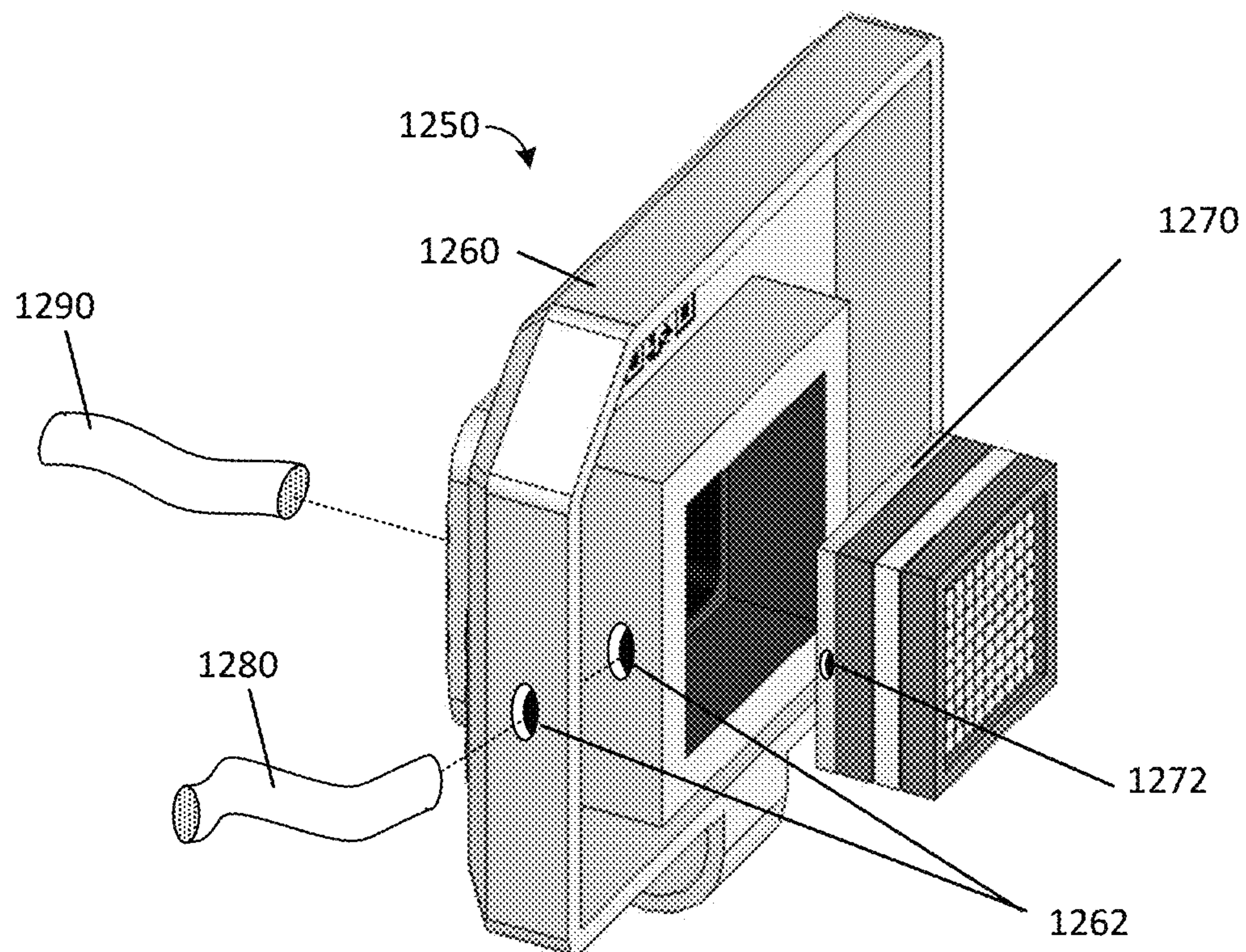


Figure 12B

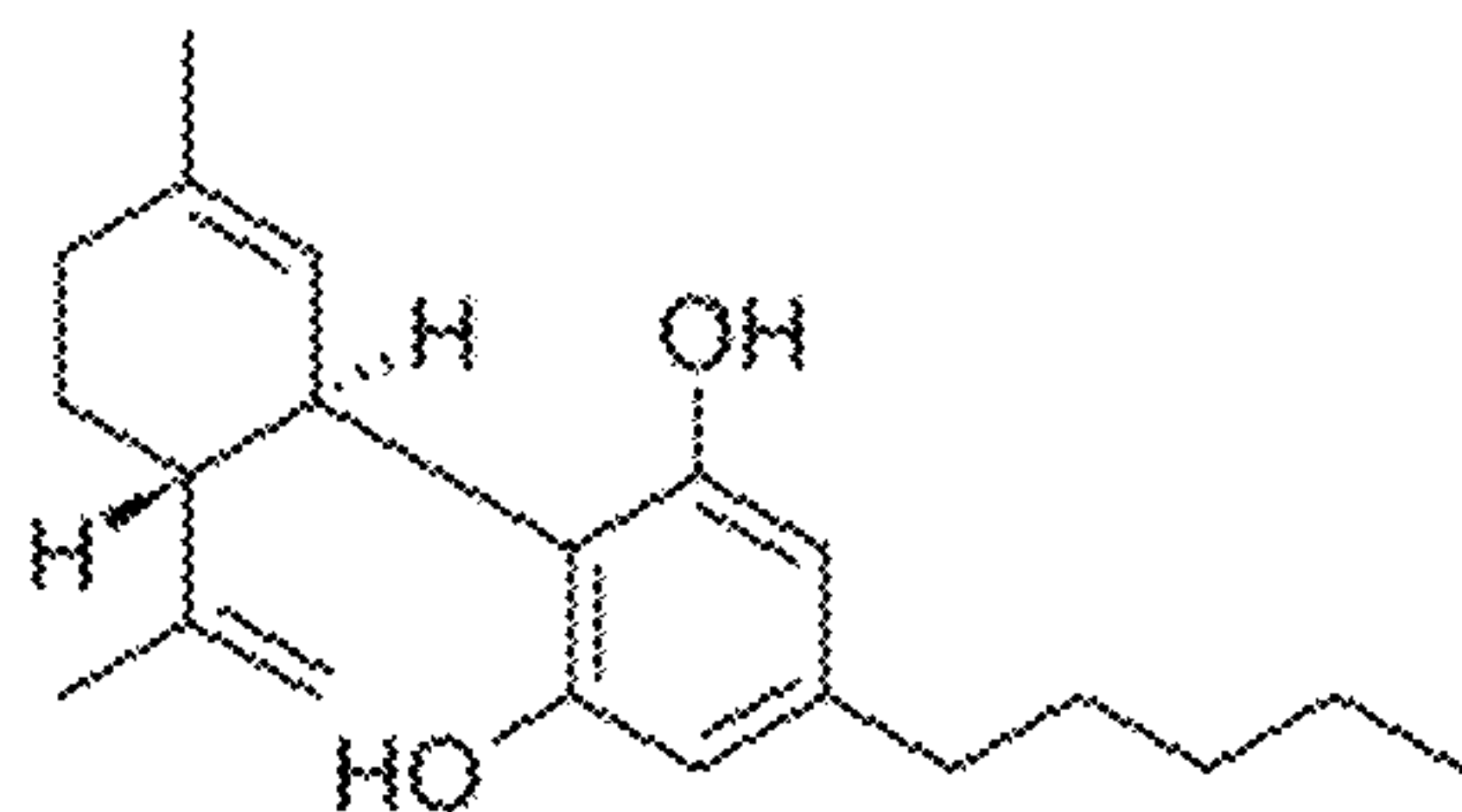


Figure 13A
(CBD)

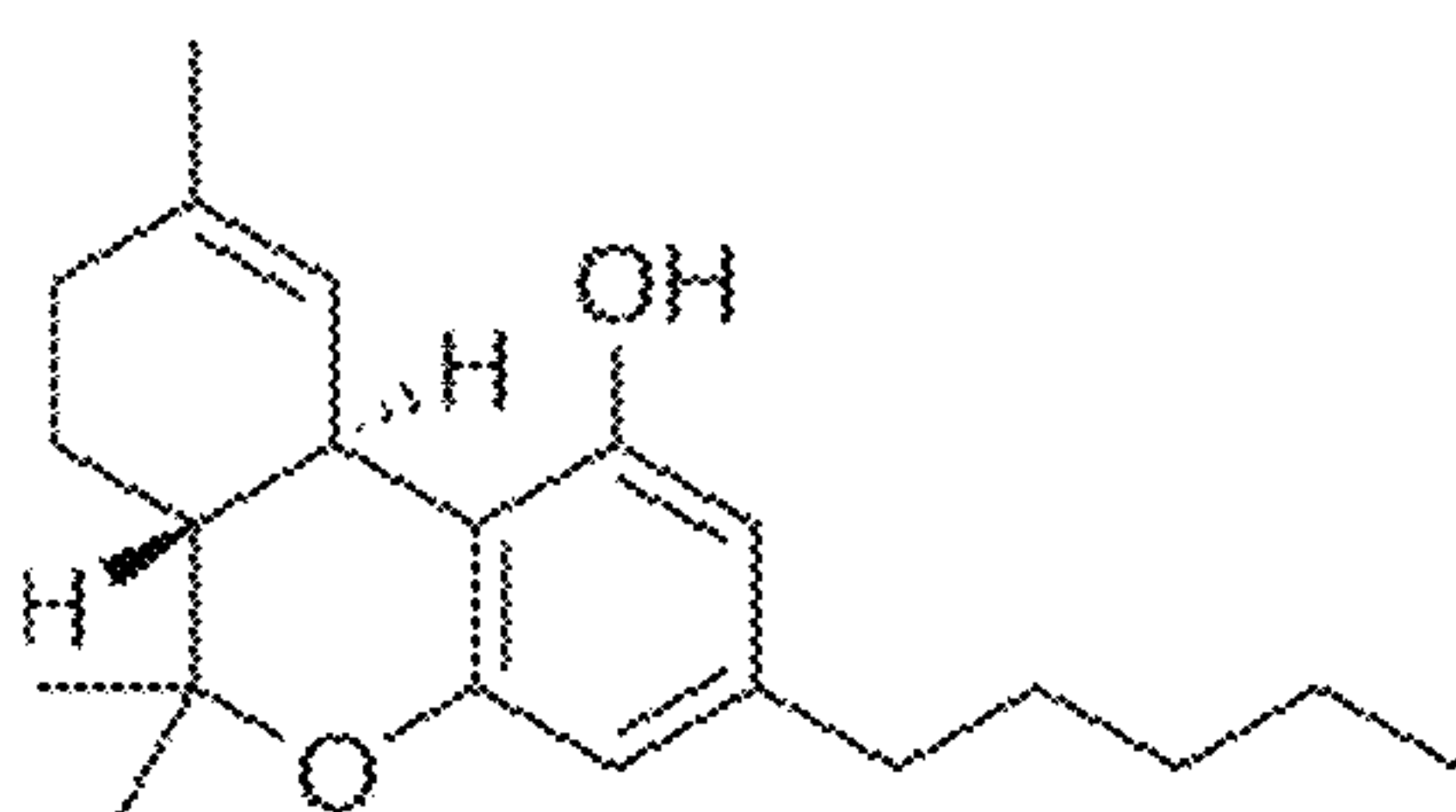
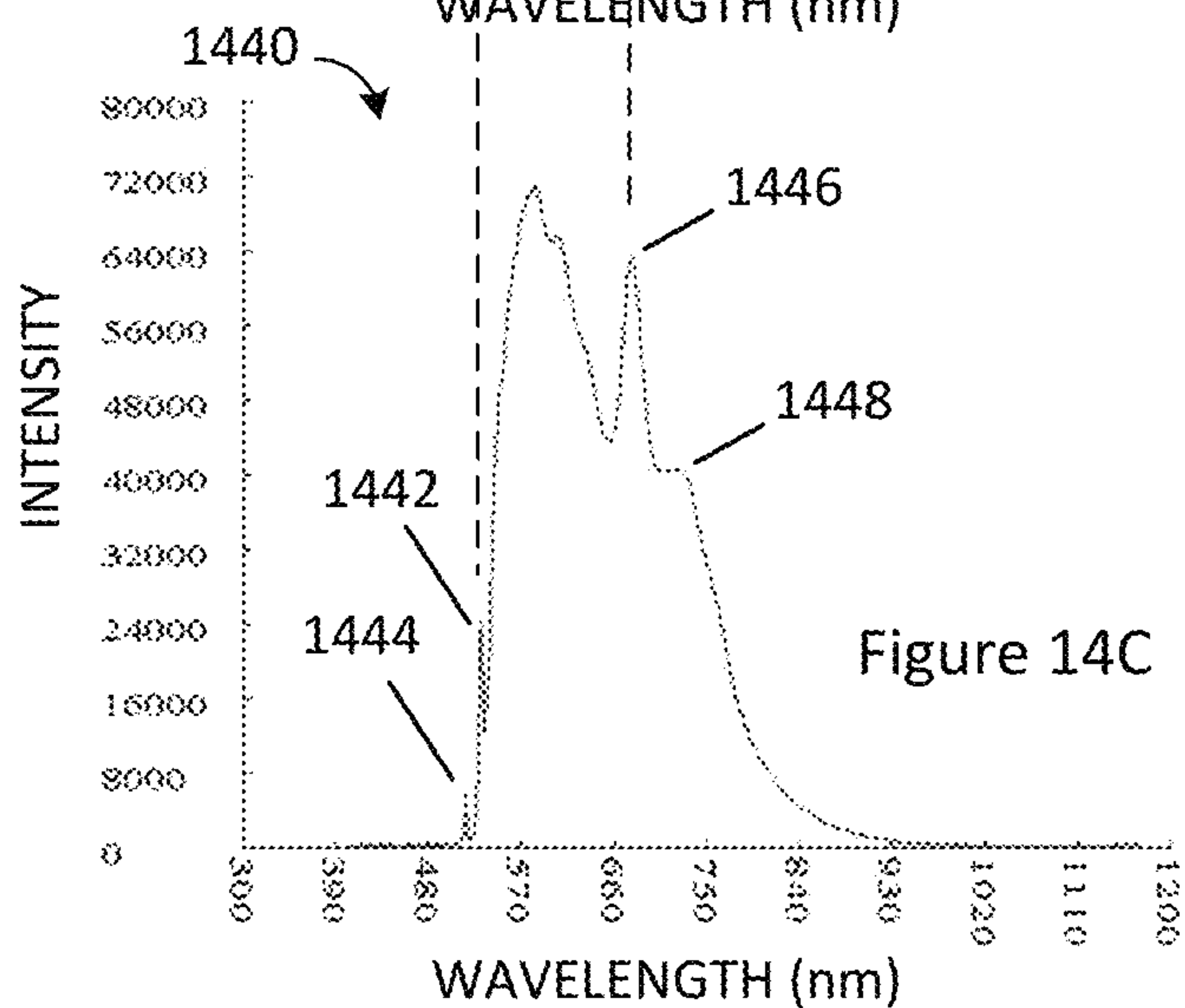
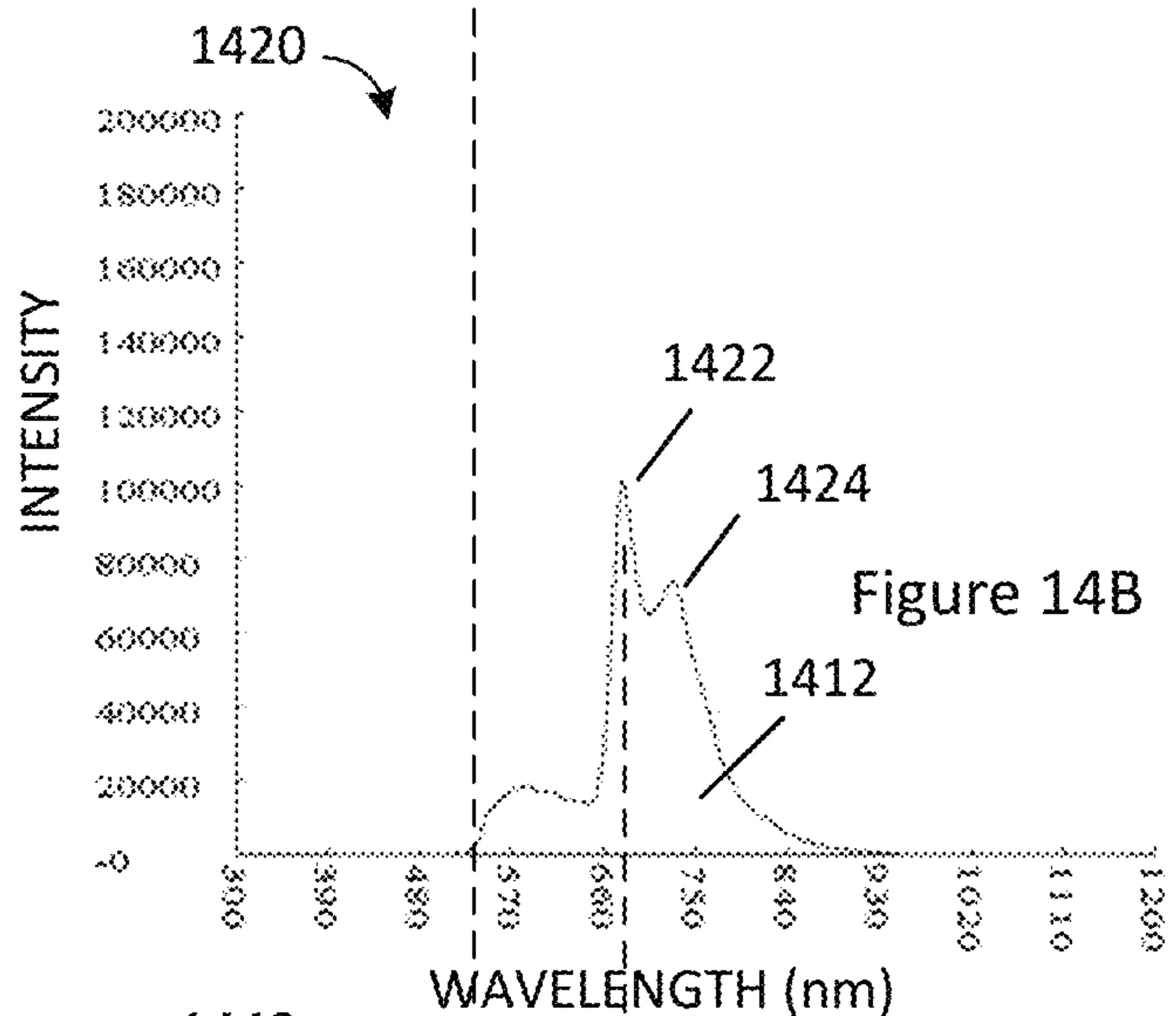
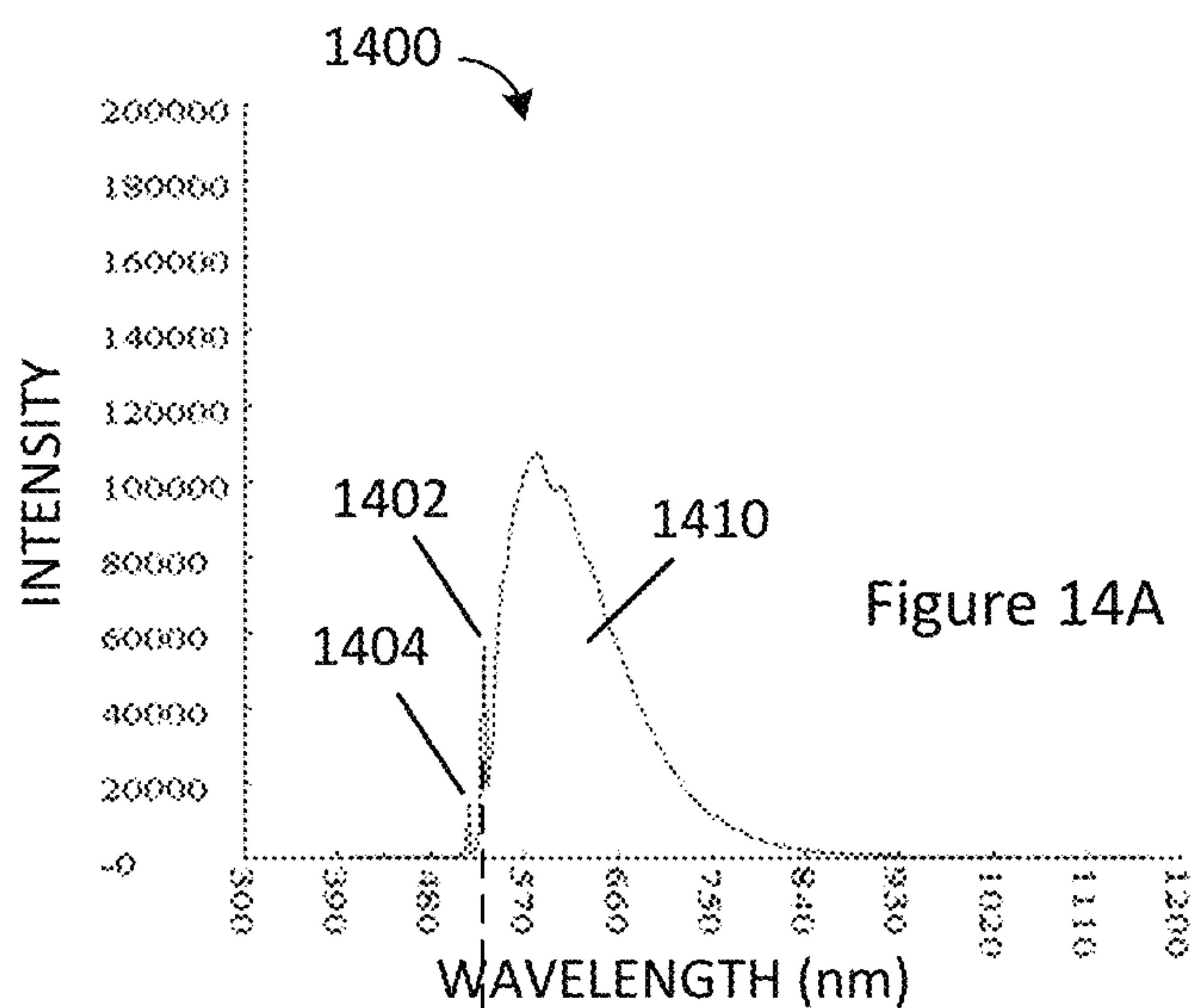


Figure 13B
(THC)



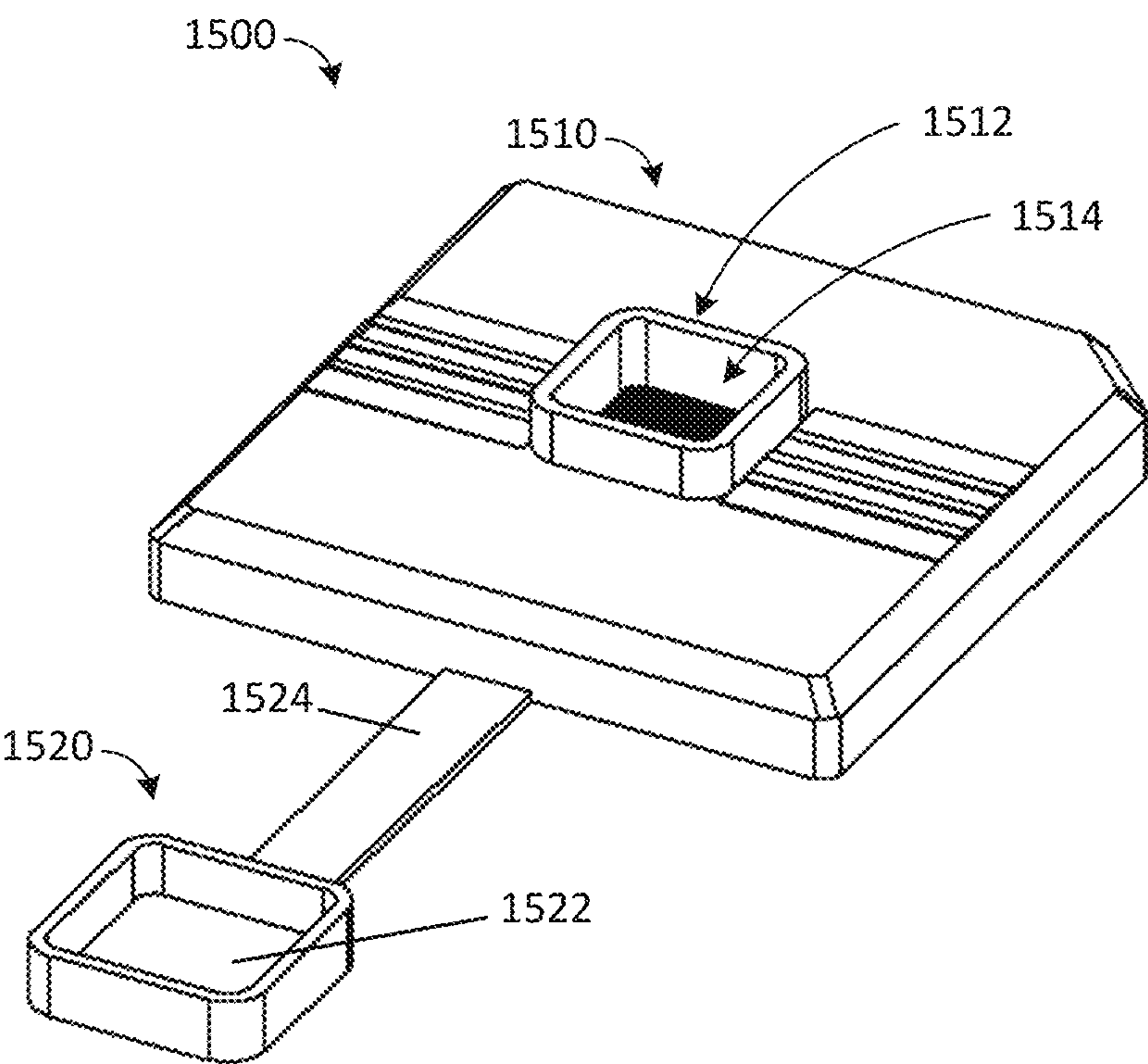


Figure 15A

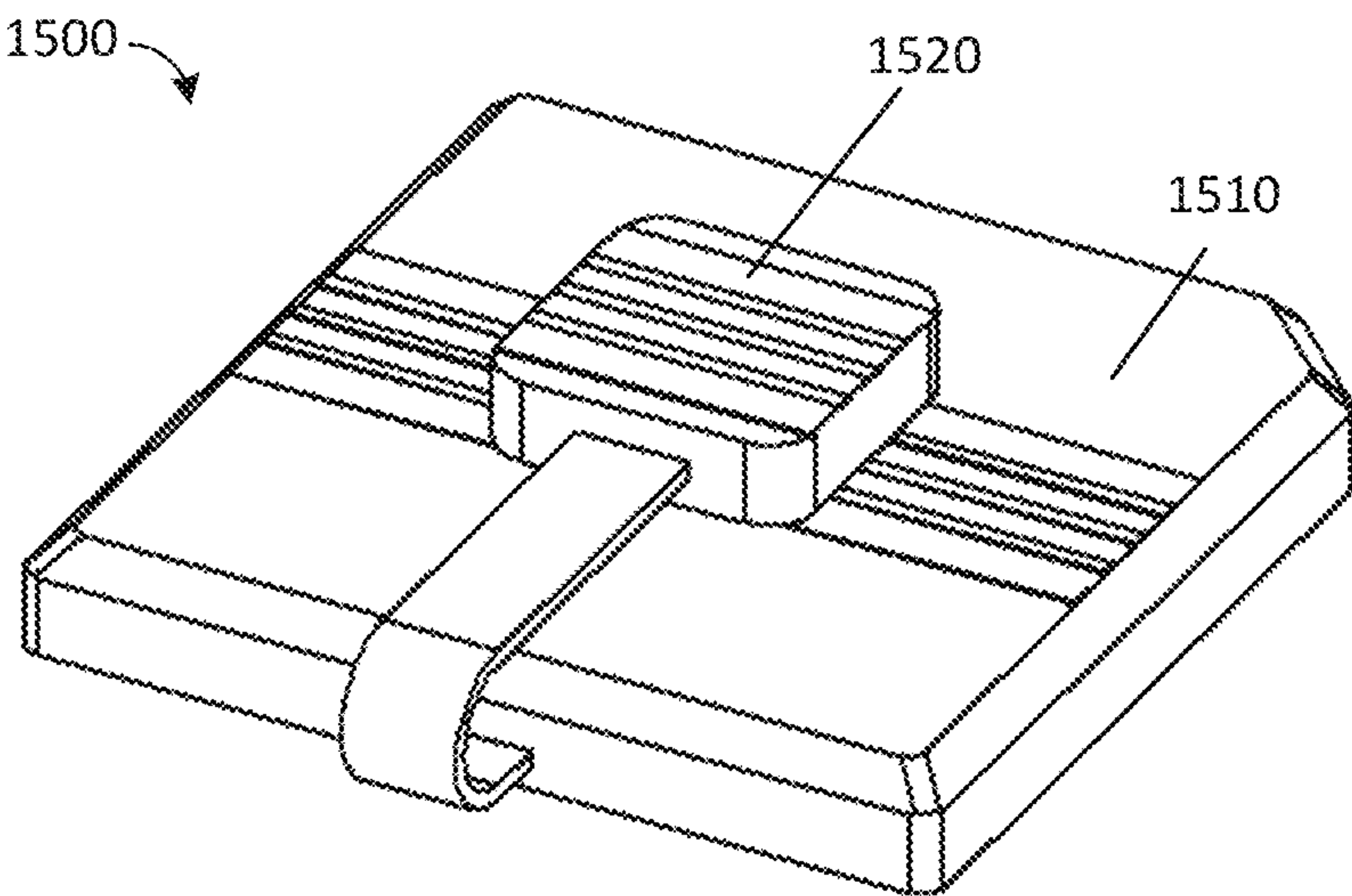
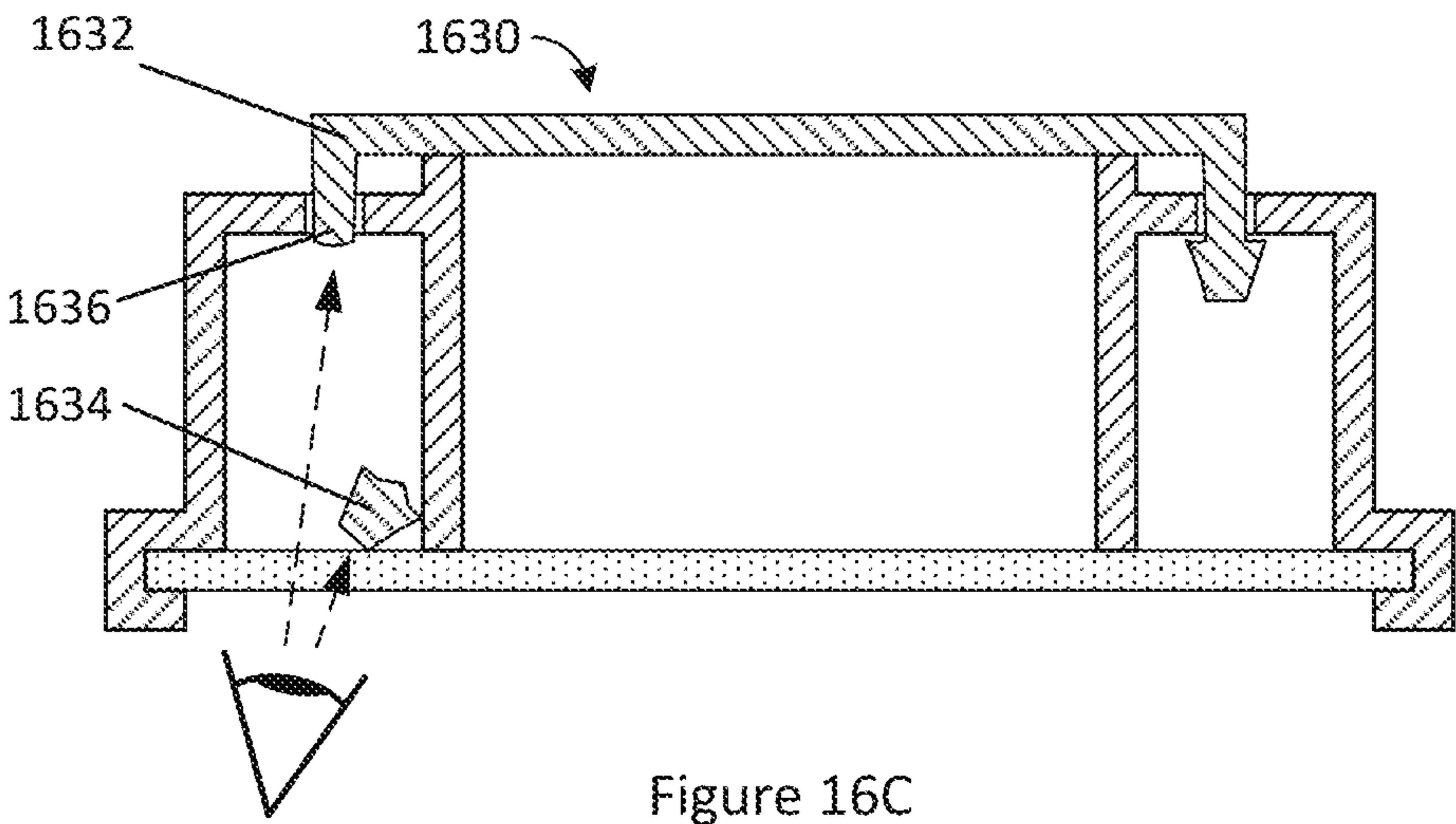
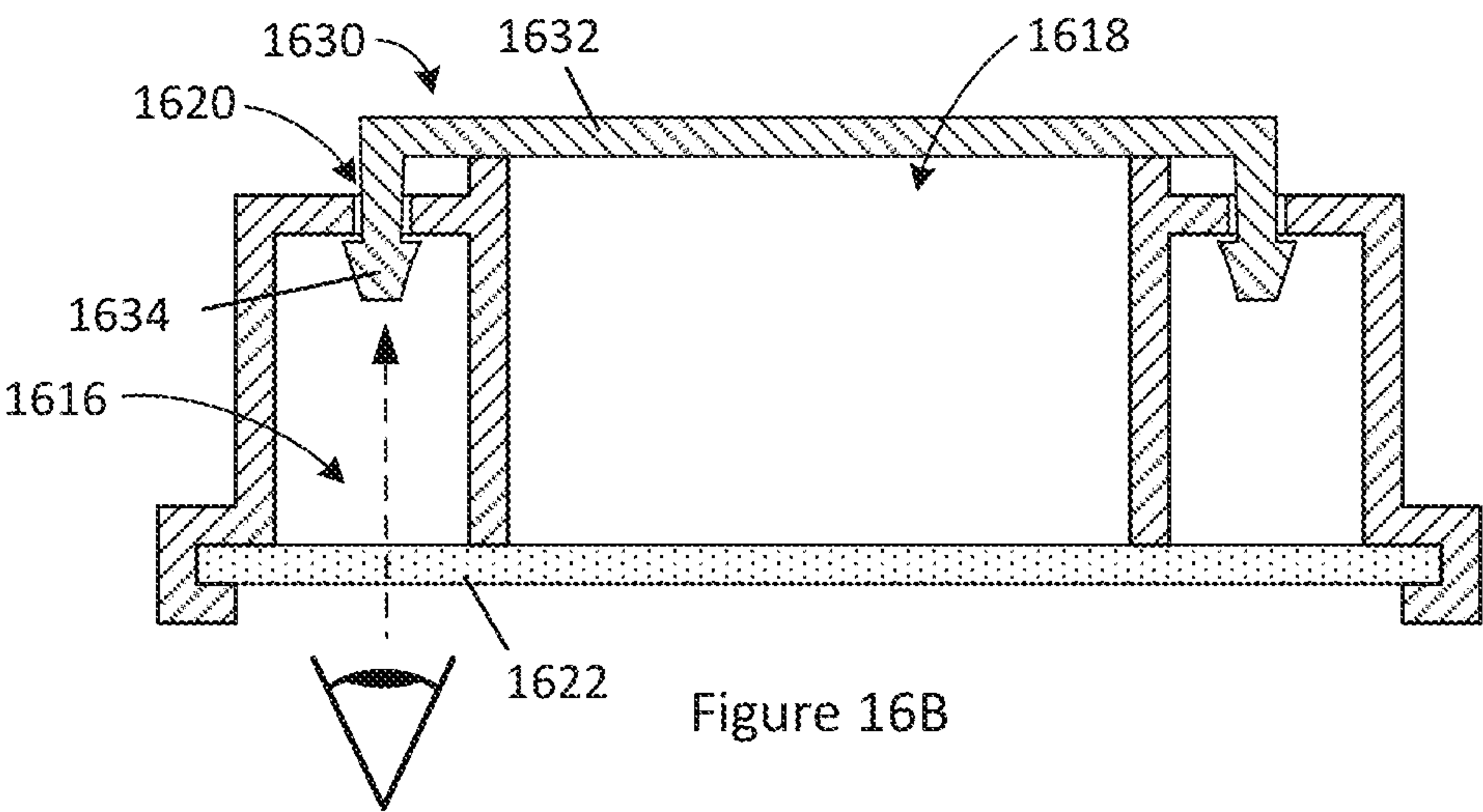
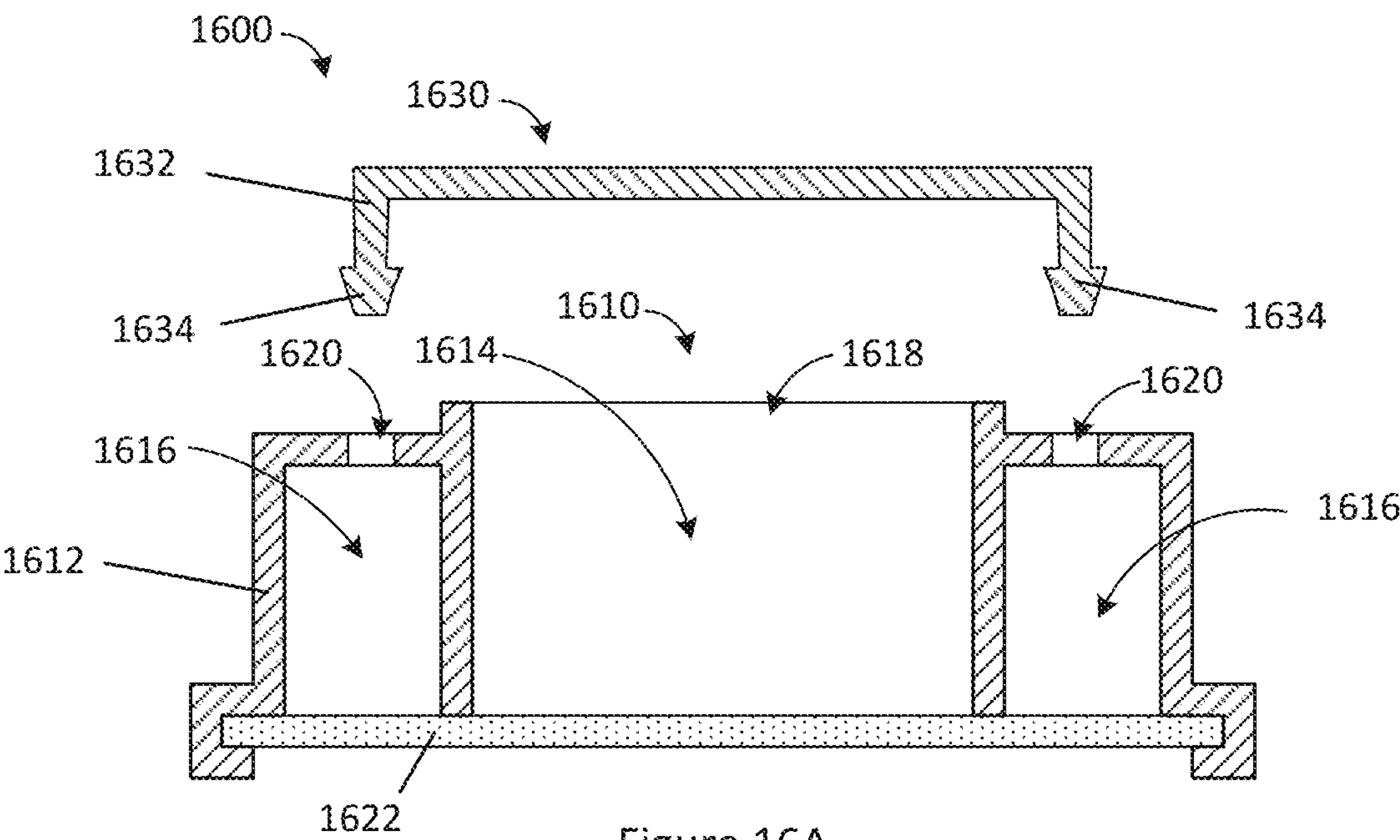


Figure 15B



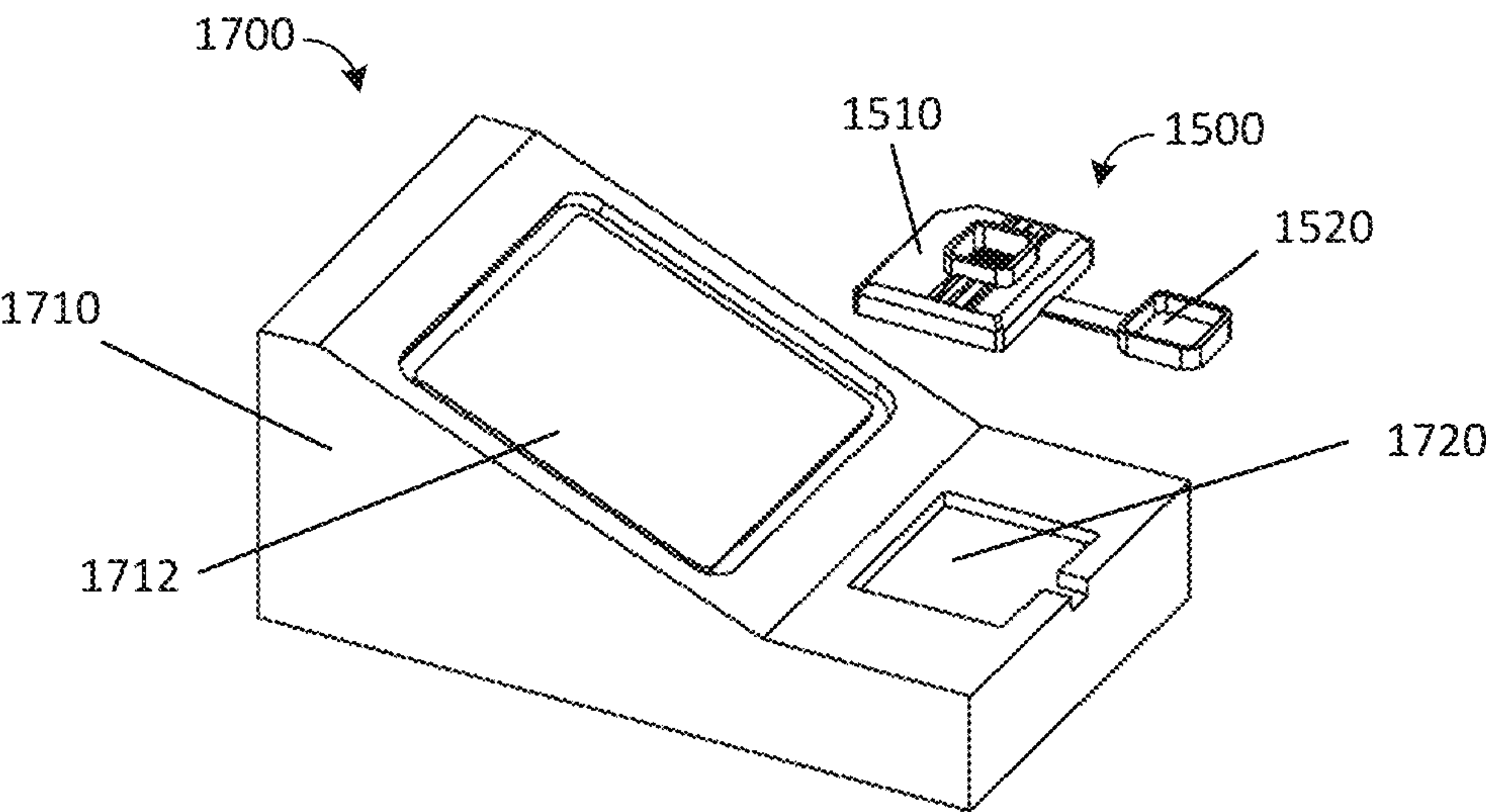


Figure 17A

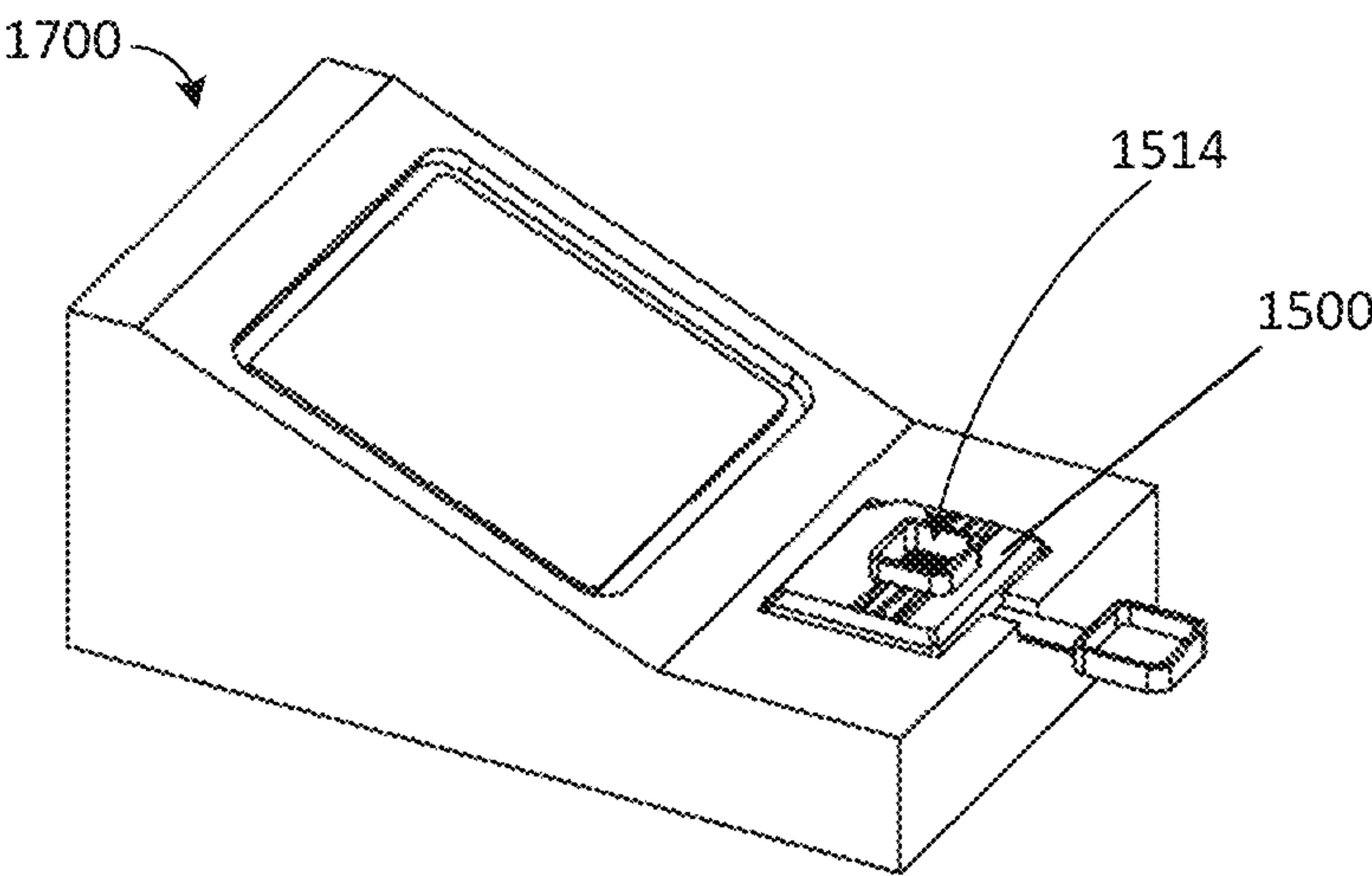


Figure 17B

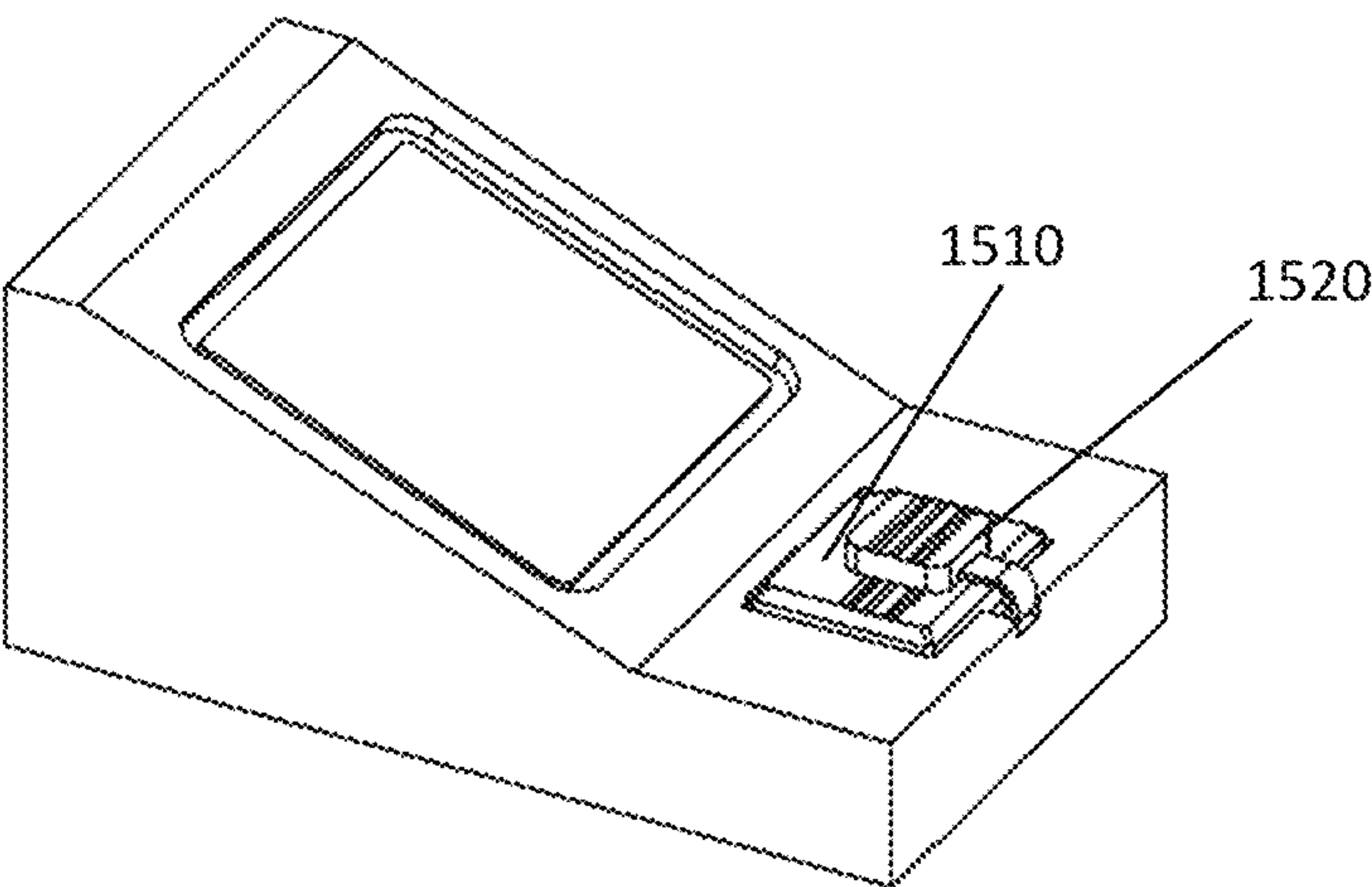


Figure 17C

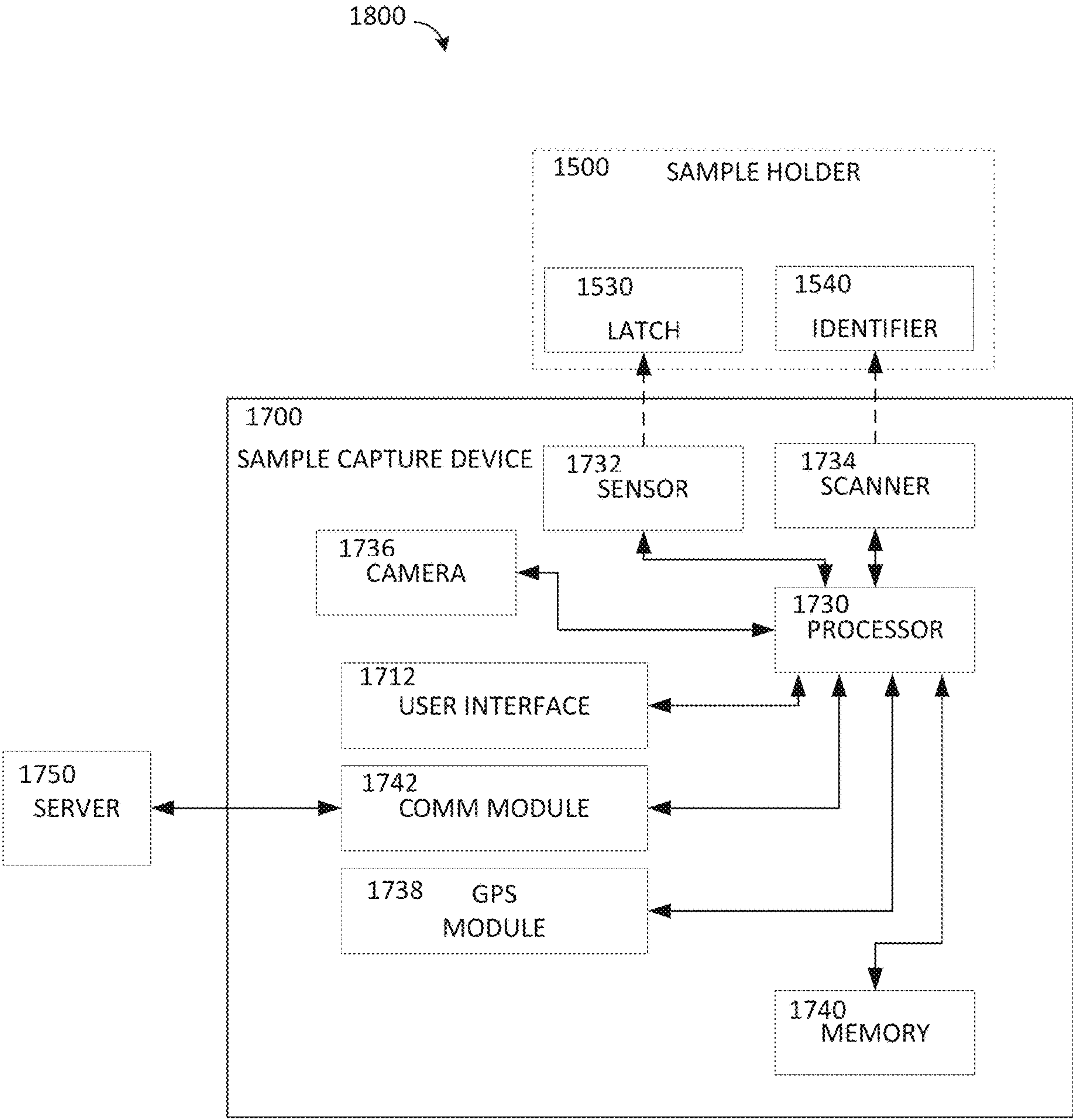


Figure 18

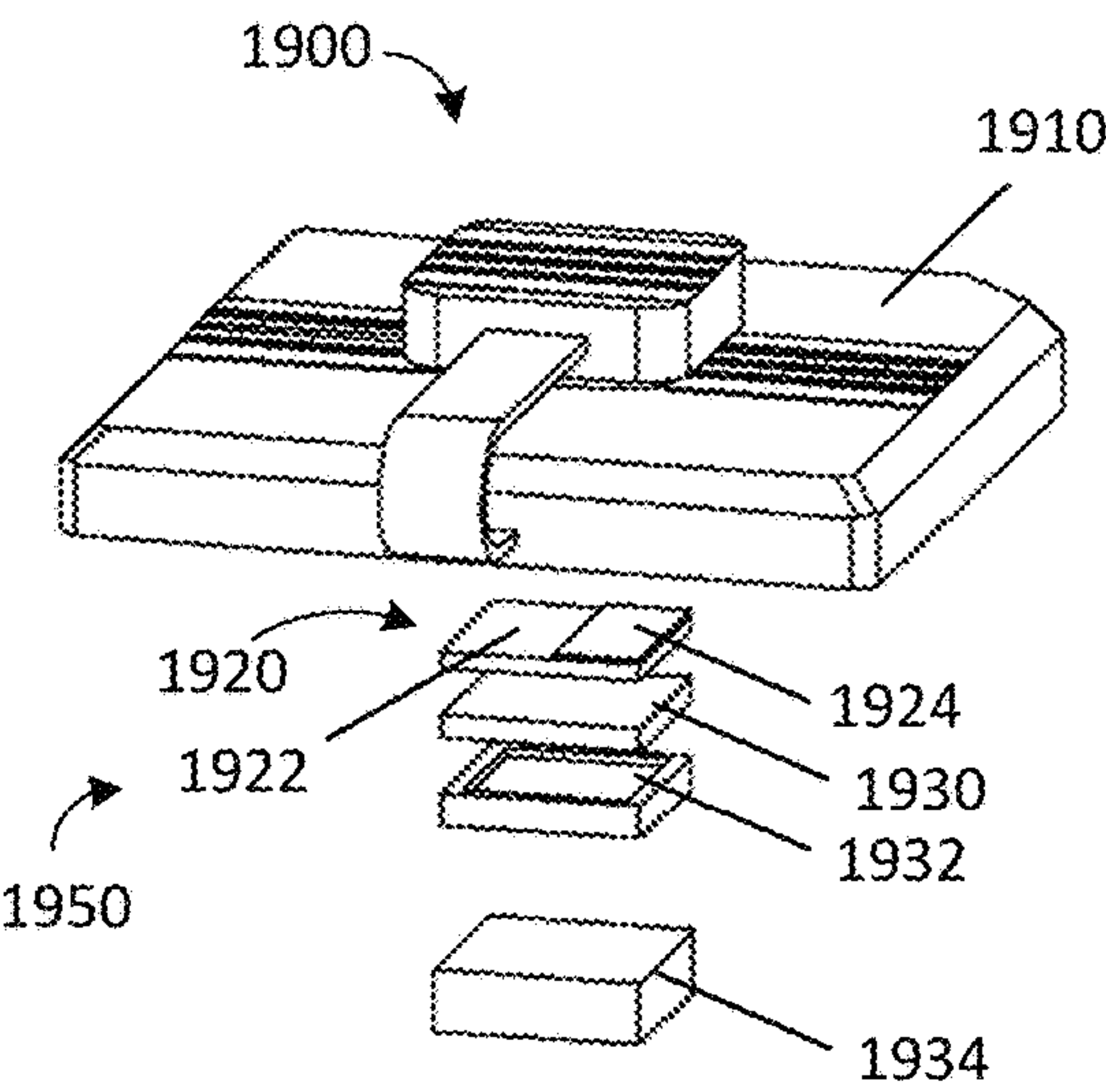


Figure 19A

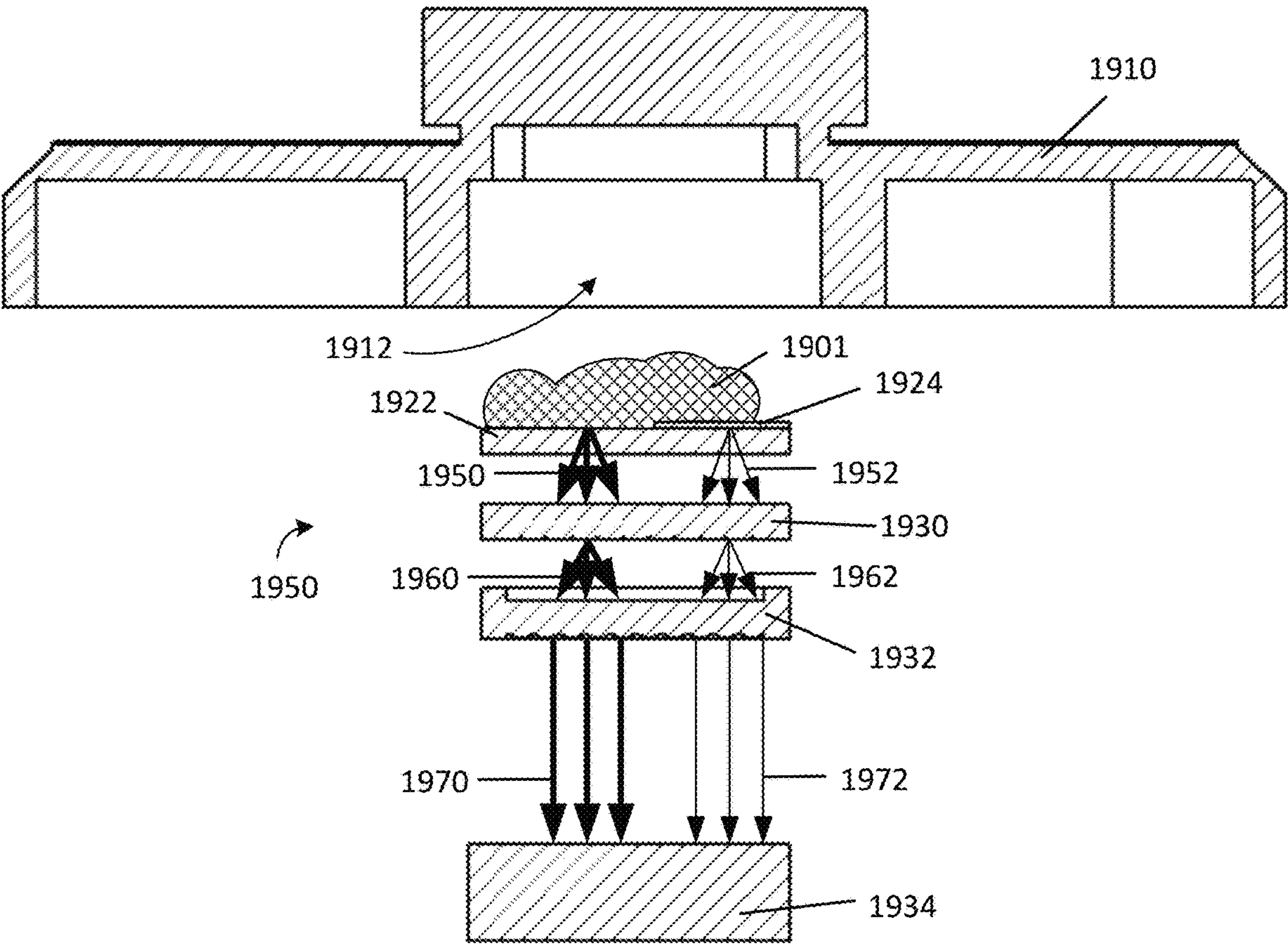


Figure 19B

1**SAMPLE IDENTIFICATION****CROSS-REFERENCE TO RELATED APPLICATIONS**

This application claims priority to U.S. application Ser. No. 17/395,814 filed on Aug. 6, 2021 that claims priority to 63/105,763 filed Oct. 26, 2020, both of which are incorporated herein by reference in their entireties.

STATEMENT REGARDING FEDERALLY SPONSORED RESEARCH OR DEVELOPMENT

Not applicable.

BACKGROUND**Field**

The present invention generally relates to identification and handling of a sample of a material.

Description of the Related Art

Raman spectroscopy, named after Indian physicist C. V. Raman, is a spectroscopic technique used to identify materials. A source of monochromatic light illuminates a sample. The photons of the source light excite the molecules of the sample, which then emit photons that will be at a higher or lower energy level, compared to the incident photons, depending on the vibrational modes of the molecules of the sample. Every molecule has a characteristic “fingerprint” based on its structure. Comparison of the results generated by a sample to a library of material fingerprints enables the determination of the materials in the sample.

Conventional Raman spectrometers suffer from a number of drawbacks including a limited Field of View (FOV), a high numerical aperture (NA) that inherently results in a shallow Depth of Field (DOF), and a significant loss of signal due to the use of a single narrow slit. The limited FOV is the result of using a microscope objective as the primary light gathering component. The optical elements of a conventional Raman spectrometer are designed to observe only a small area of the sample, which then requires a scanning mechanism to gather sample observations from multiple points of samples. The optics commonly implement a high NA to maximize the collection of light from a small sample point. A conventional Raman spectrometer uses a single slit in the optical path and the spectral resolution of the spectrometer is inversely related to the width of the slit; i.e., higher spectral resolution requires a narrower slit that inherently causes a reduction in optical signal strength.

Maintaining the integrity of a sample of material when the sample is handled by multiple people and transferred between locations and organizations is a long-standing challenge. Many organizations have strict chain-of-custody procedures to ensure that samples are handled only by authorized individuals. Conventional tamper-evident containers provide some assurance as to whether the container has been opened and reclosed if, and only if, appropriate records are also maintained. For example, if a serialized tie wrap is used to secure a container in a closed configuration, it is necessary to create a record of the original serial number and manually check the current serial number against the record at each step of handling, otherwise a new serialized tie wrap can be installed after the container is opened and re-closed.

2**SUMMARY**

In certain embodiments, it is desirable to provide a robust, compact Raman spectrometer that utilizes a single-use sample holder to eliminate cross-contamination and replaces the conventional optical elements with arrays of collection lenses, slits, and collimation lenses so as to achieve a larger FOV, greater DOF, and increased light capture and provide a spatially averaged determination of material characteristics across a sample without scanning the sample.

A method of analyzing a sample is disclosed. The method includes the steps of measuring a first spectral response of the sample, selecting a reference material having a first Raman peak having a first magnitude at a first wave number, measuring a first peak value in the first spectral response at the first wave number, and determining an amount of the reference material in the sample based in part on a first ratio of the measured first peak value to the first magnitude of the first Raman peak of the reference material.

A holder for analyzing a sample is disclosed. The holder has a slit array with a plurality of slits and a collimating lens array with a plurality of cylindrical lenses each configured to capture light that emerges from a respective slit of the slit array and collimate the light emerging from the plurality of cylindrical lenses in a common direction. In certain embodiments, the holder also has a sample plate having a surface configured to be in contact with the sample and to be illuminated by a source light. In certain embodiments, the holder also has a sample lens array with a plurality of cylindrical lenses configured to capture light reflected from respective parallel areas of the sample and focuses the captured light onto a respective slit of the slit array.

A tamper-evident holder is disclosed. The holder has a body with an access opening, a closure compartment, a latch opening into the closure compartment, and a window that provides visibility into the closure compartment. The holder also has a cap with a non-return fitment. The cap is configured to seal the access opening when the cap is placed in a closure position. The fitment passes through the latch opening to a latched position when the cap is placed in the closure position. The fitment is visible through the window while in the latched position. The fitment is configured to separate from the cap when the cap is dislodged from the closure position and a separated fitment is retained in the closure compartment.

BRIEF DESCRIPTION OF THE DRAWINGS

The accompanying drawings, which are included to provide further understanding and are incorporated in and constitute a part of this specification, illustrate disclosed embodiments and together with the description serve to explain the principles of the disclosed embodiments. In the drawings:

FIG. 1 illustrates diffraction at a slit, according to certain aspects of the present disclosure.

FIG. 2 depicts the intensity distribution of diffracted light, according to certain aspects of the present disclosure.

FIG. 3 depicts the refractive and reflective scattering of modes of an incident beam of monochromatic light, according to certain aspects of the present disclosure.

FIG. 4 illustrates Rayleigh scattering, according to certain aspects of the present disclosure.

FIG. 5 illustrates an example Raman spectrum, according to certain aspects of the present disclosure.

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FIG. 6 depicts a schematic representative of a conventional Raman spectrometer, according to certain aspects of the present disclosure.

FIG. 7 depicts a block diagram of an exemplary apparatus, according to certain aspects of the present disclosure.

FIG. 8 depicts a flow chart of an exemplary method of use, according to certain aspects of the present disclosure.

FIGS. 9A-9B depicts exemplary embodiments of an optical system of the apparatus, according to certain aspects of the present disclosure.

FIGS. 10A-10C depict an exemplary embodiment of a disposable holder, according to certain aspects of the present disclosure.

FIG. 10D depicts another embodiment of a disposable holder, according to certain aspects of the present disclosure.

FIGS. 11A-11C depicts exemplary embodiments of a sample plate, according to certain aspects of the present disclosure.

FIG. 12A-12B depicts exemplary means of providing illumination of the sample, according to certain aspects of the present disclosure.

FIGS. 13A-13B are 2D representations of the chemical structures of CBD and THC.

FIGS. 14A-14C depict illustrative experimental results of the output of the analyzer, according to certain aspects of the present disclosure.

FIGS. 15A-15B depict an exemplary sample container, according to certain aspects of the present disclosure.

FIGS. 16A-16C depict an exemplary tamper-evident sample container, according to certain aspects of the present disclosure.

FIGS. 17A-17C depict an exemplary sample capture device, according to certain aspects of the present disclosure.

FIG. 18 depict an exemplary block diagram of the sample capture device, according to certain aspects of the present disclosure.

FIGS. 19A-19B depict an exemplary sample holder configured for analysis based on absorbance of light, according to certain aspects of the present disclosure.

DETAILED DESCRIPTION

The following description discloses embodiments of a Raman spectrometer that is particularly suited to be carried into the field for use.

The detailed description set forth below is intended as a description of various configurations of the subject technology and is not intended to represent the only configurations in which the subject technology may be practiced. The appended drawings are incorporated herein and constitute a part of the detailed description. The detailed description includes specific details for the purpose of providing a thorough understanding of the subject technology. However, it will be apparent to those skilled in the art that the subject technology may be practiced without these specific details. In some instances, well-known structures and components are shown in block diagram form to avoid obscuring the concepts of the subject technology. Like, or substantially similar, components are labeled with identical element numbers for ease of understanding.

As used within this disclosure, the term “light” means electromagnetic energy having a wavelength within the range of 10 nanometers (nm) to 1 millimeter (mm). In certain embodiments, this range is preferably 300-1100 nm. In certain embodiments, this range is preferably 700-1100 nm. In certain embodiments, this range is preferably 10-400

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nm (ultraviolet). In certain embodiments, this range is preferably 400-700 nm (visible). In certain embodiments, this range is preferably 700 nm to 1 mm (infrared).

As used within this disclosure, the terms “frequency” (f) and “wavelength” (λ) should be considered interchangeable in characterizing a beam of light unless explicitly stated otherwise, as they are related by the equation $\lambda=c/f$, wherein “c” is the speed of light, and a value of either parameter is uniquely associated with a respective value of the other parameter. Furthermore, the terms “wavelength” and “wave number” should be considered interchangeable in characterizing a spectral response unless explicitly stated otherwise, as they are inversely related to each other and a value of either parameter is uniquely associated with a respective value of the other parameter.

FIG. 1 illustrates diffraction of a coherent monochromatic light beam **100** at a slit **110** in a plate **112**, according to certain aspects of the present disclosure. The white lines in the incident beam **100** represent the “valleys” of the sinusoidal wave of the light, shown to the right for reference. The light that passes through the slit **110** is diffracted, also referred to as “scattered,” with the diffracted light **102** propagating as a spherical wave toward a surface **120** as seen in FIG. 1.

FIG. 2 depicts the intensity distribution **200** of diffracted light **102** on surface **120**, according to certain aspects of the present disclosure. The central peak **210** is centered under the incident beam **100** and flanked on both sides by secondary lobes (maxima) **220** and dark lines (minima) **230**, with the intensity of each succeeding lobe **222** decreasing as the lateral distance from the center increases. The pattern **250** formed on the surface **120** is governed by equation 1:

$$\sin(\theta_1)=1.22(\lambda/d) \quad \text{Equation 1:}$$

wherein:

θ_1 is the angular position of the first order diffraction minima (the first dark ring)

λ is the wavelength of the incident light

d is the width of the slit

FIG. 3 depicts the refractive and reflective scattering of modes of an incident beam of monochromatic light, according to certain aspects of the present disclosure. A beam **100** of coherent light strikes the grating **300** at an angle θ_{inc} relative to an axis **302** that is perpendicular to the plane of the grating **300**. A portion of the incident beam **100** is transmissively diffracted into various modes at various angles θ_m^{trm} relative to the incident beam **100**, wherein “M” is the mode number. For example, beam **320** is the 0th-order mode (primary) transmitted mode, beams **322A**, **322B** are the 1st-order transmitted modes, and beams **324A**, **324B** are the 2nd-order transmitted modes. The 0th-order mode is at an angle θ_0^{trm} while the 1st-order modes **322A**, **322B** are at $\pm\theta_1^{trm}$ relative to beam **100**.

The angles θ_m^{trm} are dependent upon the frequency of the incident light, the mode order, the geometry, and the index of refraction of the material of the grating **300** as shown in Equation 2. This equation presumes air on both sides of the grating **300**.

$$\sin\theta_m = \sin\theta_{inc} - m \frac{\lambda}{\Lambda} \quad \text{Equation 2}$$

wherein:

λ is the wavelength of the incident light

Λ is the spacing of the lines of the grating

m is the order of the refracted ray

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θ is the angle from perpendicular to the grating, the subscript “inc” indicates the incident ray and the subscript “m” indicates the m^{th} refracted ray

A portion of the incident beam 100 may be reflectively diffracted into various modes at various angles θ_m^{ref} relative to axis 302.

FIG. 4 illustrates Rayleigh scattering, according to certain aspects of the present disclosure. Raman spectroscopy relies upon inelastic scattering of photons. An incident beam of monochromatic light introduces energy into the molecules of a sample material and excites the system. The material emits the absorbed energy at frequencies associated with the various energy states of its molecules. The shift in energy gives information about the vibrational modes in the system.

FIG. 5 illustrates an example Raman spectrum, according to certain aspects of the present disclosure. The light emitted by a material is plotted as intensity vs. frequency shift relative to the frequency of the source light, referred to as the “Raman shift,” traditionally measured in a unit called the wavenumber, which is the number of waves per cm (cm^{-1}). The spikes of the plot are associated with vibrational modes of chemical bonds in one of the component materials. These spikes are referred to as “Raman bands” and the frequency and relative intensities of the bands allow us to identify the material by comparison of their spectral “signature” with a library of reference signatures of known materials. Heavy atoms and weak bonds have low Raman shifts. Light atoms and strong bonds have high Raman shifts.

The plot of FIG. 5 is the Raman spectrum of polystyrene. The high frequency carbon-hydrogen (C—H) bonds have a resonant frequency that creates the Raman band at about 3000 cm^{-1} . The carbon-carbon (C—C) bonds create the small Raman band at around 800 cm^{-1} . The C—H vibrations have a higher frequency than the C—C vibrations because hydrogen is lighter than carbon. The vibrations of a complex molecule partly consist of many simple diatomic vibrations while also showing the vibrational modes of larger groups of atoms, such as the expanding/contracting “breathing mode” of the aromatic carbon rings in polystyrene that appears at 1000 cm^{-1} .

FIG. 6 depicts a schematic representative of a conventional Raman spectrometer 600, according to certain aspects of the present disclosure. A sample 602 to be characterized is placed against a surface of a sample holder 610. A partially reflective mirror 630 deflects a portion of beam of source light 634 emitted by a light source 632 to travel toward the sample 602 as illumination beam 636. The scattered light emitted by the sample 602 passes through the sample holder 610 and the sample lens 620 to the mirror 630, where a portion 604 of the scattered light continues through a spatial filter, e.g., a slit, 642. The sample lens 310 focuses the light 604 on the spatial filter 642. The light 606 that has passed through the spatial filter 642 is formed into a unidirectional beam 608 by the collimating lens 650. An excitation filter 660 blocks the transmission of the light from source 632. The beam of filtered light 608 strikes the transmissive diffraction grating 670. The diffracted light 609 coming out of the grating 670 is focused by the final focus lens 680 onto surface 692 of a detector 690, which may be a charge-coupled device (CCD) sensor or camera.

FIG. 7 depicts a block diagram 700 of an exemplary Raman spectrometer, according to certain aspects of the present disclosure. An instrument body 702 is configured to accept a holder 710 that has a compartment 712 configured to accept a sample of a material. In certain embodiments, the holder 710 includes a specimen plate 720, a sample lens

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array 722, a slit array 724, and a collimating lens array 726. In certain embodiments, the specimen plate forms a portion of the compartment 712.

In certain embodiments, the holder 710 comprises a lid 714 configured to selectably close over the accepted sample and permanently prevent removal of the sample from the holder compartment 712. In certain embodiments, closure of the lid 714 is a non-reversible event wherein the lid 714 cannot be opened again without damage to the lid 714 or holder 710, i.e., evidence of tampering. This feature makes the holder 710 into a tamper-resistant sample container that can be archived for later retrieval and re-examination. In certain embodiments, the lid 714 is hingedly attached to the body of the holder 710.

The instrument body 702 is coupled to a transmissive grating 730, a focusing lens 732, and a detector 740. The detector 740 is communicatively coupled to a processor 750 and configured to provide information about the Raman spectrum of this sample, i.e., the sample signature, to the processor 750. The processor 750 can store the sample signature and associated data, e.g., a date, a sample ID, a location such as where the sample was collected, a field designator, a user name, etc., in the memory 760. The processor 750 is coupled to a comm module 752 that is communicatively coupled to a server 790 that may be at a remote location or implemented as a virtual device on a “cloud” server. In certain embodiments, the server 790 is implemented as a software service. The body 702 is also coupled to a user interface 754, for example a color graphics display with an overlaid touchscreen. The body 702 is also coupled to a power supply 770 that provides power to all of the electronic components of the apparatus and, in certain embodiments, received information from one of more of the components. In certain embodiments, the body 702 is also coupled to a GPS module 756 that provides location information to the processor 750.

Light 782 from the light source 780 is guided to the sample, which is shown as contained in compartment 712 having a lid 714 in this example. The sample is stimulated by the light 782 to emit light, a portion of which passes through the sample plate 720, the sample lens array 722, the slit array 724, and the collimating lens array 726 to the grating 730. The light is refracted by the grating 726 and a portion of the refracted light passes through the final focus lens 732 to the detector 740.

Detector 740 creates data that is provided to the processor 750. The processor 850 is communicatively coupled a memory 760 via a bidirectional path. In certain embodiments, the memory 760 contains instructions that, when transferred to the processor 750 and executed by the processor 750, cause the processor 750 to receive the data from the detector 740, compare the received data with a portion of one or more reference files, and determine an attribute of the sample.

In certain embodiments, memory 760 also contains the one or more reference files that are respectively associated with one or more materials and the instructions comprise instructions to transfer a portion of the files to the processor 750. In certain embodiments, the one of more reference files are stored on the server 790 that is communicatively connected to the processor 750 through the comm module 752, for example over a wired and/or wireless network.

In certain embodiments, the light source 780 emitting light at a determined frequency. In certain embodiments, the frequency is in the infrared band. In certain embodiments, the frequency is in the visible band. In certain embodiments, the frequency is in the ultraviolet band. In certain embodi-

ments, the light source **780** comprises an optical filter (not shown in FIG. 7) that passes light only in a selected band having a frequency bandwidth. In certain embodiments, the source **780** emits light in a band having a bandwidth that is less than or equal to 5 nm. In certain embodiments, the source **780** emits light in a band having a bandwidth that is less than or equal to 2 nm. In certain embodiments, the light source **780** comprises a plurality of sources each emitting light at a different frequency.

FIG. 8 depicts a flow chart **800** of an exemplary method of use, according to certain aspects of the present disclosure. In the first step **810**, a user places a sample of a material in the holder. This step may include closing a lid over the sample and, in certain embodiments, closing of the lid may be a one-time action, i.e., a non-reversible event. In step **820**, the user places the holder in the instrument body. In step **822**, the user performs set-up and data entry operations. In certain embodiments, one of steps **820** and **822** includes the instrument retrieving a unique identifier (ID) from the holder that was placed in the body and storing this ID. In certain embodiments, one of steps **820** and **822** includes determination of the current physical location of the instrument using a locating system, e.g., an internal global position system (GPB) module and storage of the location.

Once the instrument is fully configured for this sample, the user initiates the analysis of the sample in step **830**. In certain embodiments, step **830** comprises one of more of collection of multiple spectral signatures using different frequencies of source light and collection of multiple spectral signatures using different optical filters to modify the light emitted by the sample. In certain embodiments, step **830** comprises stimulation of the sample, for example by exposure of the sample to one or more of a magnetic field, an electrostatic field, and a radio frequency (RF) field. In certain embodiments, step **830** comprises introduction of a fluid into the sample.

After the spectral signatures are collected, the instrument transfers a portion of the data, which includes one or more of the spectral signatures and information entered by the user and determined by the instrument, to a server that may be remote.

Software on the server analyzes the data in step **840**, compares the results of the analysis to a library of signatures in step **842**, and identifies a match between the sample and the materials of the library in step **844**.

In step **846**, the software on the server analyzes the spectral signatures and determines an amount of the matched material in the sample. In certain embodiments, the analysis determines an amount present only for a pre-determined material. In certain embodiments, the analysis may calculate a ratio of the amount of one material to the amount of another material.

Step **850** stores the results of the analysis and the data in a memory on the server. In certain embodiments, the memory is located separate from the server. In certain embodiments, the results are sent to the instrument and stored in a memory in the instrument or a removable drive, e.g., a thumb drive, attached to the instrument. The results are sent to the instrument in step **860** and provided to the user on the user interface. In certain embodiments, step **860** includes providing the information on one of a personal computer, a laptop, a tablet, a smart phone, or other display.

FIG. 9A depicts an exemplary embodiment of an optical system **900** of the apparatus, according to certain aspects of the present disclosure. In this embodiment, the system **900** comprises a holder **910**, an optical filter **920**, a grating **930**, a focusing lens **940**, and a detector **950**. The optical filter **920**

is configured to block the wavelength of the excitation light. The grating **930** separates the light emitted by the sample into its various wavelengths. The focusing lens **940** focuses each separated wavelength onto the detector **950** in a spatially separated position.

FIG. 9B depicts the passage of light emitted by the sample (not visible as it is located within the holder **910**) through the optical system **900**, according to certain aspects of the present disclosure. A single beam **960** of collimated light being emitted from the holder **910** is shown for clarity, although there are a plurality of adjacent beams of light coming from the holder **910** that are collimated and parallel to each other. After passing through the filter **920**, the filtered light **962** strikes the grating **930** and a portion is transmissively refracted into a refracted beam **964**. Each of the matching-wavelength spectral sub-component beams **964** of the plurality of adjacent beams of light that are exiting the grating **930** are still collimated and parallel to each other, i.e., all sub-components at the same wavelength will enter the focusing lens **940** at the same angle. For example, the green portions from the multiple beams are all collimated and parallel to each other as they enter the focusing lens **940**. The focusing lens **940** focuses the spectral sub-component beams **964** into converging sub-component beams **966** that have foci on a plurality of spatially separate locations on the detector **950**.

In certain embodiments, the focusing lens **940** comprises multiple elements for focusing and beam shaping. In certain embodiments, the focusing lens **940** comprises one or more of a curved mirror and a flat mirror. In certain embodiments, the detector **950** comprises one or more of a linear 1D array of sensing elements, e.g., pixels, and a 2D array of sensing elements.

FIG. 10A depicts an exemplary embodiment of a single-use holder **910**, according to certain aspects of the present disclosure. The holder **910** has a frame **912** on which is printed a unique identifier **914**, e.g., a matrix code. In certain embodiments, the identifier **914** comprises a human-readable code. In certain embodiments, the identifier **914** comprises an electronic device, e.g., a ROM chip or an RFD chip, that stores the identifier.

FIG. 10B depicts an optical assembly **1000** removed from the cavity **916** of the holder. The cavity **916** is adjacent to a compartment (not visible in FIG. 10B) of the frame **912** that is configured to accept a sample of a material such that the sample is pressed against the optical assembly **1000**.

FIG. 10C depicts an exploded view of an exemplary optical assembly **1000**, according to certain aspects of the present disclosure. In this example, optical assembly **1000** comprises one or more of a sample plate **1010**, a sample lens array **1020**, a slit array **1030**, and a collimating lens array **1040**, each coupled to at least one of the adjacent component and to the frame **912**. In this embodiment, the sample plate **1010** is an optically clear planar sheet that is disposed, when the optical assembly **1000** is mounted in the frame **912**, proximate to the sample compartment such that the sample is in contact with a surface of the sample plate **1010**. In certain embodiments, optical assembly **1000** comprises a sample plate **1010**, a slit array **1030**, and a collimating lens array **1040**. Other embodiments of the sample plate are discussed with respect to FIGS. 12A and 12B.

The sample lens array **1020** comprises a plurality of focusing elements **1022** that are mounted in a frame **1024** with a set-back **1026** that provides clearance for the height of the focusing elements **1022** as well as a portion of a separation of the focusing elements **1022** from the next component. In certain embodiments, the focusing elements

1022 comprise one or more of spherical, aspherical, and diffractive optical components. In certain embodiments, the plurality of focusing elements **1022** are configured to collect light from a respective plurality of regions of the surface of the sample and produce a respective plurality of beams of light.

The slit array **1030** comprises one or more slits each having a width. In certain embodiments, a portion of the plurality of focusing elements **1022** is arranged in a straight row that is parallel to a slit of the slit array **1030** and the focusing elements of the row are configured to focus the respective beams of light on the slit. In certain embodiments, the plurality of focusing elements and the plurality of slits are arranged in a non-rectilinear pattern, e.g., concentric circles.

The collimating lens array **1040** comprises a plurality of collimating lenses **1042** mounted in a frame **1044** with a set-back **1046** that provides clearance for the height of the collimating lenses **1042** as well as a portion of a separation of the collimating lenses **1042** from the next component. In certain embodiments, a portion of the plurality of collimating lenses **1042** is arranged in a straight row that is parallel to a slit of the slit array **1030**. Each collimating lens **1042** is configured to accept the refracted light emanating from one of the slits and modify the light to form a collimated beam of light. All of the modified plurality of beams of light are collimated in a common direction.

In certain embodiments, the diameter of the individual focusing elements **1022** and/or the collimating lenses **1042** is less than 125 μm . In certain embodiments, the focusing elements **1022** and/or the collimating lenses **1042** are holographic lenses. In certain embodiments, the use of holographic lenses in place of conventional lenses provides a 10 $\times$ improvement in light capture. In certain embodiments, the use of holographic lenses in place of conventional lenses provides a 50 $\times$ improvement in light capture. In certain embodiments, the use of holographic lenses in place of conventional lenses provides a 100 $\times$ improvement in light capture.

In certain embodiments, the separation of the sample plate **1010** from the sample lens array **1020** is less than 5 mm. In certain embodiments, the separation of the sample plate **1010** from the sample lens array **1020** is less than 2 mm. In certain embodiments, the separation of the sample lens array **1020** and the slit array **1030** is less than 5 mm. In certain embodiments, the separation of the sample lens array **1020** and the slit array **1030** is less than 2 mm. In certain embodiments, the separation of the slit array **1030** and the collimating lens array is less than 5 mm. In certain embodiments, the separation of the slit array **1030** and the collimating lens array is less than 2 mm.

FIG. 10D depicts another embodiment of a disposable holder, according to certain aspects of the present disclosure. The optical assembly **1000** of FIG. 10C is replaced by optical assembly **1050** that replaces sample lens array **1020** with a sample lens array **1060** and the collimating lens array **1040** with a collimating lens array **1070**. Each column of individual lenses **1022** and **1042** is replaced by a cylindrical lens **1062** and **1072**. Each cylindrical lens **1062** focuses light on one of the slits of slit array **1030** and the light emerging from each slit is collimated by one of the cylindrical lenses **1072**.

With the cylindrical lens arrays of optical assembly **1050**, the sample lens array **1060** captures light reflected from respective parallel areas of the sample and focuses the light onto a respective slit of slit array **1030**. Compared to a conventional spectrometer, this arrangement captures light

from a much larger area of the sample, in certain embodiments 2 $\times$, 5 $\times$, 10 $\times$, 20 $\times$, 50 $\times$, and 100 $\times$ the amount of light, and consequently the intensity of the light from the sample is increased by approximately the same amount. An increase in intensity creates a stronger signal from the detector, thereby improving the measurement of small signals, e.g., values of Raman peaks.

The collimating lens array **1070** captures light that emerges from a respective slit of slit array **1030** and collimates the light in a direction common to all the cylindrical lenses **1072**. With reference to FIG. 9B, the grating **930** will disperse the light from all collimating lenses **1072** at common angles, e.g., light of a common frequency is collimated in a single direction. The focusing lens **940** will focus light of a common frequency to a common location on the sensor **950**. By gathering light from a large area of the sample, the intensity of the light at the sensor is proportional to a total area of the parallel areas of the sample from which reflected light is captured by the sample lens array **1060**. This increase in intensity is effectively optical amplification increases the sensitivity of the analyzer in the same way that a larger diameter telescope is able to detect dimmer stars by collecting more light from the sky. In certain embodiments, the intensity of the light at the sensor is 10 $\times$ that of a conventional spectrometer having a single slit. In certain embodiments, the intensity of the light at the sensor is 20 $\times$ that of a conventional spectrometer having a single slit. In certain embodiments, the intensity of the light at the sensor is 50 $\times$ that of a conventional spectrometer having a single slit. In certain embodiments, the intensity of the light at the sensor is 100 $\times$ that of a conventional spectrometer having a single slit.

In certain embodiments, the holder **910**, or **910A**, is separable from the main spectrometer, which contains one or more of the optical filter **920**, the grating **930**, the focusing lens **940**, and the detector **950** as well as one or more of a light source, a power supply, a user interface, a processor, a memory, and other components (not shown in FIG. 9A) necessary to measure aspects of the light provided by the holder **910**. In certain embodiments, one or more of the optical filter **920**, the grating **930**, the focusing lens **940** are provided as part of the holder **910** and therefore not part of the main spectrometer. In certain aspects, the body **912** comprises an interface configured to detachably mate with a spectrometer. In this manner, a plurality of holders **910**, or **910A**, may be used to capture a respective plurality of samples, wherein each holder **910** is sequentially mated to the spectrometer and the sample of that holder analyzed.

FIG. 11A depicts an exemplary embodiment of a sample plate **1100**, according to certain aspects of the present disclosure. The sample plate **1100** comprises a channel **1102** that is configured to accept a liquid sample (not shown in FIG. 11A). In certain embodiments, the channel **1102** passes through the width of the sample plate **1100** so as to form a passage through which a liquid sample can flow, thus enabling continuous monitoring of a stream to be periodically tested. In certain embodiments, the channel **1102** is a sealed compartment with entrance and exit ports (not shown in FIG. 11A) so as to facilitate introduction of a liquid sample into the channel **1102** and removal of air.

FIG. 11B depicts an exemplary embodiment of a sample plate **1110**, according to certain aspects of the present disclosure. In certain embodiments, the sample plate **1110** comprises an actuator **1112** at least partially embedded in the sample plate **1110**. In certain embodiments, the actuator **1112** is selected from the group of a temperature-control element, a filtering element, and a stimulation element. In

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certain embodiments, the temperature-control element can perform at least one of heating or cooling the sample. In certain embodiments, the filtering element can selectively allow or block selected frequencies of light. In certain embodiments, the stimulation element generates one of a magnetic field, an electrostatic field, and a dynamically oscillating electric field, e.g., a radiofrequency (RF) field. In certain embodiments, the sample plate 1110 comprises a coating 1114 on one or more surfaces. In certain embodiments, the coating 1114 functions as one or more of an optical filter, an electric shield, an antenna, and an electric conductor that may be patterned.

FIG. 11C depicts an exemplary embodiment of a sample plate 1120, according to certain aspects of the present disclosure. In certain embodiments, the sample plate 1120 comprises a reservoir 1124 embedded within the body 1122 of the sample plate 1120 and configured to contain a fluid 1126 and a pump 1128 fluidically coupled between the reservoir 1124 and a surface of the sample plate 1120 and configured to selectably expel a portion of the fluid 1126 from the sample plate.

FIG. 12A-12B depicts exemplary means of providing illumination to the sample, according to certain aspects of the present disclosure.

FIG. 12A depicts a schematic of certain aspects of a novel Raman spectrometer 1200, according to certain aspects of the present disclosure. In this exemplary embodiment, an incident ray 1210 of coherent, monochromatic, unidirectional illuminating light strikes a transmissive diffraction grating 930 at an angle 1230. In certain embodiments, angle 1230 is selected such that one of the mode rays 1220 is directed along the optical axis 1202 of the spectrometer 1200. In certain embodiments, the angle 1230 is selected to direct a higher-order mode ray, for example a 1st-order ray 1222, along the optical axis 1202. In certain embodiments, the angle 1230 is selected to direct the primary ray along the optical axis 1202.

One advantage of the novel arrangement of the light source (not shown in FIG. 12A) is the elimination of the partially reflective mirror 630 shown in FIG. 6. As the light in a conventional spectrometer must be first reflected and then transmitted by the mirror 630, there is a loss of energy, normally about 50%, of the scattered light coming from the sample. Although the selected mode will have only a portion of the energy of the incident beam 1210, there is no energy loss in the optical path from the sample to the grating 930.

A second advantage of the spectrometer 1200 is the more compact arrangement of components, as the light source is now generally aligned with the long dimension of the device, while a conventional spectrometer 600 has a laser light source 632, which may be large and heavy, positioned on one side. Repositioning the source 632 in a conventional design requires additional optical elements, for example folding mirrors and rigid supporting structure, that add weight and cost.

Light passing through grating 920 from a first surface to a second surface on the opposite side of the grating 920 from the first surface is described as passing through the grating 920 in a first direction, regardless of the angle of the path of the light to a perpendicular reference axis, such as axis 1202. Similarly, light passing through grating 920 from the second surface to the first surface is described as passing through the grating 830 in a second direction regardless of whether the path of the light traveling in the second direction is parallel to the path of the light traveling in the first direction. The use

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of “first direction” and “second direction” are meant only to convey the general direction of transmission from one surface to another.

FIG. 12B depicts another exemplary embodiment of means of providing illumination of the sample, according to the certain aspects of the present disclosure. In certain embodiments, a beam of illuminating light is provided via a fiber optic cable 1280, or functional equivalent, that passes through openings 1262 in the frame 1260 of holder 1250 and then into a receiving port 1272 of the sample plate 1270. This type of side illumination is known in optics and provides light output across the planar surface of the sample plate 1272.

In certain embodiments, the beam of illuminating light is provided via a fiber optic cable 1290, or functional equivalent, that passes through the holder 1250 from a backside and mates with a diffuser (not visible in FIG. 12B) within the frame 1260 and disperses the light across the planar surface of the sample plate 1270.

In certain embodiments, the illumination light is modulated, for example by driving the light source with a square wave, thereby producing periods of illumination of the sample, i.e., when the source is on, separated by intervals of dark, i.e., when the source is off. Sensing of the output of the detector is synchronized with the square wave, for example by recording the output only while the source is off and adding the recordings of multiple dark intervals. In certain embodiments, sensing of the output of the detector occurs during portions of both the illuminated periods and the dark periods and the respective sets of measurements are compared during analysis.

Certain embodiments of the disclosed Raman spectrometer incorporate a novel arrangement of a light source that introduces the light into the optical path of the apparatus by passing the light through the transmissive diffraction grating in direction opposite the direction of the light passing from the sample to the detector. This novel arrangement beneficially reduces the size and complexity of the optical path by eliminating components that are critical in conventional spectrometers.

Certain embodiments of the disclosed Raman spectrometer consolidate critical elements of the optical path into a single-use holder. Miniaturization of the optical elements and the use of arrays of lenses in place of single lenses enables precise alignment without requiring complex alignment techniques during manufacturing.

Material Analysis

Cannabidiol (CBD) is a phytocannabinoid discovered in 1940. It is one of 113 identified cannabinoids in cannabis plants, along with tetrahydrocannabinol (THC), and accounts for up to 40% of the plant's extract. CBD has been found to have beneficial medical effects, including relief from pain and stiffness. CBD may be supplied as an oil, a powder, or as a liquid suspension. The mechanism of action for its biological effects has not been determined. CBD does not have the psychoactivity of THC and is not listed as a proscribed substance.

Hemp is a subspecies of cannabis that contains significant levels of CBD and low levels of THC. The 2018 United States Farm Bill removed hemp and hemp extracts (including CBD) from the Controlled Substances Act. THC, on the other hand, is still listed under Schedule I under the Controlled Substances Act. Federal law classifies a plant as hemp and therefore exempt from the Controlled Substances Act if the THC content, specifically delta-9 tetrahydrocan-

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nabinol, is $\leq 0.3\%$ by weight. This is echoed in the California Code of Regulations that require that hemp crops be tested for THC content prior to harvest and that a hemp crop found to contain more than this amount of THC must be destroyed.

FIGS. 13A-13B are the 2D representations of the chemical structures of CBD and THC, respectively. It can be seen that while there is a great deal of structure in common, there are small differences in the composition and bond structure between CBD and THC that produce different Raman responses.

FIGS. 14A-14C present experimental results provided by the Raman analyzer disclosed herein.

Graph 1400 depicts the spectral response of a sample of CBD powder having $\leq 0.3\%$ THC when illuminated with a source light having a wavelength of 515 nm. The x-axis is the frequency of the response in nanometers while the y-axis is an intensity. The response curve includes a large generally smooth portion 1410 that is the photoluminescence of the sample combined with narrow spikes 1402, 1404 that are Raman peaks associated with the chemical structure of CBD. In this experiment, peak 1402 has an intensity of approximately 60,000 and peak 1404 has an intensity of approximately 18000.

Graph 1420 depicts the spectral response of a sample of plant material containing approximately 47% by weight of THC when illuminated with a source beam of light having a wavelength of 515 nm. The curve includes the photoluminescence 1412, which has a markedly different shape than the photoluminescence 1410 of the CBD sample, and Raman spikes 1422 and 1424. In this experiment, peak 1422 has an intensity of approximately 100,000 and peak 1424 has an intensity of approximately 75000.

Graph 1440 depicts the spectral response of a sample consisting of a mixture of 40% of the powder of graph 1400 and 60% of the plant material of graph 1420 when illuminated with a source beam of light having a wavelength of 515 nm. Peaks 1442, 1444 correspond to peaks 1402, 1404 and peak 1446 corresponds to peak 1422. Peak 1442 has an intensity of approximately 24000, peak 1444 has an intensity of approximately 7000, and peak 1446 has an intensity of approximately 64000. The shoulder 1448 corresponds to the peak 1424 but does not provide a distinct peak.

In certain embodiments, the ratios of the intensities of corresponding peaks provides a measure of the amount of the associated material in the sample. In this case, the values of corresponding peaks and their respective ratios are shown in Table 1.

TABLE 1

PEAK-A	INTENSITY	PEAK-B	INTENSITY	RATIO
1442	24000	1402	60000	0.4
1446	64000	1422	105000	0.6

The ratio of peaks 1442/1402 represents the relative amount of the CBD powder in the mixture of graph 1440 and the ratio of peaks 1446/1422 represents the relative amount of the THC-containing plant material powder in the mixture. The respective ratios of 0.4, 0.6 are complementary and together support an assessment that the mixture is approximately 40% CBD powder and 60% plant material.

This data demonstrates the principle of establishing “fingerprints” of two reference materials and then being able to determine the proportions of a mixture of the two materials using this analyzer disclosed herein. In certain embodiments, the determination compares the magnitudes of one or

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more Raman peaks of a measurement of a sample of the mixture to the fingerprints. In certain embodiments, the determination compares attributes of the overall response curve to the fingerprints. In certain embodiments, the attribute is a curve value at a specific wavelength or wave number. In certain embodiments, the fingerprint is a computational prediction of a wavelength or wave number of a Raman peak based on one or more aspects of the chemical structure of a reference material.

It must be noted that the measurement made by the disclosed apparatus is based on the surface area of the sample illuminated by the light source and examined by the sensor of the disclosed apparatus while the limit of THC content is provided as a weight percentage. Conversion of the sensed results to a weight percentage is accomplished by use of reference samples that have been characterized by an accepted standard process, for example liquid chromatography coupled with mass spectrometry. In the example of FIGS. 14A-14C, the THC content of the plant material was determined by a third party using an accepted laboratory process and the THC content of the mixture of graph 1440 is therefore 60% of 47%=0.28% by weight.

The wavelengths of the various attributes of the spectral response of a sample are related to the wavelength of the source light. In addition, the shape and overall intensity of the photoluminescence may be different depending on the wavelength of the source beam. The graphs of FIG. 14A-14C, for example, are produced by a source beam of 515 nm. In certain embodiments, the frequency of the source beam is selected to maximize the visibility of a Raman peak, i.e., to provide the greatest difference between the intensity of a Raman peak and the intensity of the photoluminescence at and around the frequency of that Raman peak. In certain embodiments, the frequency of the source beam is selected to maximize the visibility of a particular Raman peak that is characteristic of a target molecule.

In certain embodiments, measurements are made with a plurality of light sources having a respective plurality of wavelengths. In certain embodiments, the plurality of wavelengths are selected to each maximize the visibility of one of a plurality of Raman peaks characteristic of a target molecule. In certain embodiments, the intensity of a Raman peak is determined only when the source light is the wavelengths selected to maximize the visibility of that Raman peak. In certain embodiments, the intensity of a Raman peak of a reference sample is determined at the same wavelengths as selected to maximize the sample. In certain embodiments, the ratios of a plurality of Raman peaks to their corresponding peak of a reference standard made with the same wavelengths of source light are combined to produce a composite value of the amount of a target material present in a sample.

In certain embodiments, the intent of the analysis of the spectral response is not to identify a material within a sample and is simply to determine the amount of a pre-determined molecule is present. For example, a sample of a hemp plant is analyzed to determine the amount of THC present in the sample. In another example, a sample of a food product is analyzed to determine the amount of a pre-determined pesticide in the sample. In another example, a sample of a wine is analyzed to determine the amounts of pre-determined molecules in the sample, wherein the pre-determined molecules are associated with the one or more of the taste, smell, and texture of wine.

Sample Holder

FIG. 15A depicts an exemplary sample holder 1500 in an open configuration, according to certain aspects of the

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present disclosure. The holder **1500** has a body **1510** with an access opening **1512** into a sample compartment **1514**. The cap **1520** has an interior surface **1522** and is connected to the body **1510** by a strap **1524**. In certain embodiments, the cap **1520** is separate from the body **1510**.

FIG. **15B** depicts sample holder **1500** in a closed configuration, wherein the surface **1522** of cap **1520** seals the opening **1512**. In certain embodiments, the materials of one or more of the body **1510**, the contact surface of opening **1512**, cap **1520**, and surface **1522** are selected to maintain a controlled environment in the compartment **1514**. In certain embodiments, one or more of the body **1510**, the contact surface of opening **1512**, cap **1520**, and surface **1522** comprise a coating. In certain embodiments, the contact surface of opening **1512** and surface **1522** comprise a sealing material, for example a gasket, to enhance the sealing of the opening **1512**.

Tamper-Evident Sample Holder

FIG. **16A** depicts an exemplary tamper-evident sample holder **1600**, according to certain aspects of the present disclosure. In certain embodiments, the holder **1600** comprises a body **1610** having a sample compartment **1614**, a closure compartment **1616**, and a window **1622** providing visibility into one or more of the sample compartment **1614** and the closure compartment **1616**. There is an access opening **1618** to the sample compartment **1614** and a latch opening **1620** to the closure compartment **1616**. There is a cap **1630** with a body **1632** coupled to a non-return fitment **1634**. In certain embodiments, the sample compartment **1614** is separated from the closure compartment **1616** such that a sample placed in the sample compartment **1614** does not obscure the visibility of the latch opening **1620** through the window **1622**. In certain embodiments, there is no access into the closure compartment **1616** regardless of whether the cap **1630** is installed on the body **1612**. In certain embodiments, window **1622** is replaced by separate windows (not shown) respectively covering the sample compartment **1614** and closure compartment **1616**. In certain embodiments, the window **1622** is implemented as an opening (not shown) from the exterior into the latching compartment **1616** that provides visibility of the inside of latching opening **1620** while preventing access to the interior of the latching compartment as well as preventing a broken-off fitment **1634** (see FIG. **16C**) from coming out of the latching compartment **1616**. In certain embodiments, a portion of window **1622** comprises a transparent material and is sealed to the body **1612** such that a sample in compartment **1614** is protected from contamination.

FIG. **16B** depicts the holder **1600** with the cap **1632** disposed in the closure position relative to the body **1610**, wherein the body **1632** is configured to seal the access opening **1618**. The fitment **1634** has passed through the latching opening **1620** to a latched position within the closure compartment. The fitment **1634** is visible through the window **1622** while in the latched position such that a user can verify that the fitment **1634** is intact and in the intact location so as to verify that the cap **1630** has not been removed, indicating that a sample contained in the sample compartment **1614** is undisturbed.

FIG. **16C** depicts the holder **1600** after the cap **1630** has been removed and replaced. The cap **1630** is configured such that fitment **1634** separates from the body **1632** when the cap **1630** is dislodged from its closure position. The fitment **1634** is retained in the closure compartment **1616** when separated from body **1632** such that a user can see the broken-off

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fitment **1634** and verify that the fitment is not in the intact position of FIG. **16B**. Further, the fitment **1634** is not accessible without further damage to the window **1622** or body **1612**, thus preventing returning the broken-off fitment **1634** to the intact position, for example by gluing it to the stub **1636** of cap **1630**.

If a user attempts to remove the cap **1630** and replace it with a new undamaged cap (not shown), the new cap will present a fitment in the latched position but the broken off fitment **1634** of FIG. **16C** will still be present, thus indicating that the sample has possibly been tampered with.

Determination of Sample Location

FIGS. **17A-17C** depict an exemplary sample capture device **1700**, according to certain aspects of the present disclosure.

FIG. **17A** depicts the sample capture device **1700** as having a body **1710** with a user interface **1712**. In certain embodiments, the user interface **1712** is a graphic user interface with a touchscreen overlay. In certain embodiments, the user interface **1712** comprises a keypad having one or more of numeric and alpha keys, wherein the keypad can be virtual or hardware. The body **1710** further comprises a recess **1720** configured to accept a material sample holder, for example the sample holder **1500** shown in FIGS. **15A-15B** wherein the body **1510** fits into the recess **1720**. In certain embodiments, the device **1700** is coupled to a secondary device, for example a mobile phone or a laptop (not shown) and the secondary device provides the user interface.

FIG. **17B** depicts the sample capture device **1700** with a sample holder **1500** disposed in the recess **1720**. A user is now able to place a sample of a material in the compartment **1514**. The user then closes the cap **1520** and secures it to the body **1510**, thus sealing the sample in the compartment **1514**.

FIG. **18** depict an exemplary block diagram **1800** of the sample capture device **1700**, according to certain aspects of the present disclosure. In certain embodiments, the device **1700** comprises a scanner **1734** that scans an identifier **1540** on the sample holder **1500** and a sensor **1732** that detects whether the cap **1520** has been secured to the body **1510** of sample holder **1500**. In certain embodiments, the device **1700** also includes a camera **1736** and a GPS module **1738** and a communication module **1742** configured to communicate with external devices, for example a server **1750**, over conventional wired and/or wireless networks and communication systems. The device **1700** comprises a memory **1740** is disposed within the body **1710**. In certain embodiments, the memory is remote. In certain embodiments, memory **1740** contains instructions that, when loaded into the processor **1730** and executed, will cause the processor **1730** to perform one or more of the following actions:

- receive information associated with latch **1530** from the sensor **1732**
- receive information associated with identifier **1540** from scanner **1734**
- receive the current location of the device **1700** from the GPS module **1738**
- receive information associated with the user and/or sample from the user interface **1712**
- receive an image from the camera **1736**
- store a portion of the received information in a memory, for example memory **1740**

provide a portion of the received information to an external system, for example server **1750**, over a known communication system such as Wi-Fi or a cellular network

An exemplary use of the sample capture device **1700** is to take the device **1700** into a field planted with a plant and collect one or more samples of the plants for later evaluation. The user enters information associated with this field through the user interface **1712**, for example the user, the field identification, a company farming the field, and the plant. In certain embodiments, the device **1700** captures the identification of the user through an alternate method, for example facial recognition through a camera, scanning a barcode, or detection of an RFD-enabled badge. The user places an empty sample holder **1500** in the sample capture device **1700**. The user takes a picture with the camera **1736** of a plant from which a sample will be collected. The user collects a portion of a plant and places the portion in the compartment **1514** of the sample holder **1500**, then closes the cap **1520** and secures it in place. The device **1700** detects the closure of the cap **1520**, which triggers the processor **1730** to receive the identifier **1540** from the scanner **1734** and the physical location from the GPS module **1738**. The processor **1730** stores the entered and received information in the memory **1740** along with the date and time to create a data record associated with this sample. In certain embodiments, a portion of the data record is copied to the server **1750**. The user then removes the sample holder **1500** from the sample capture device **1700** and places the sample holder **1500** in a transfer container. The user need not mark the sample holder or provide special handling to maintain a record of where the sample was collected or protect the sample. In certain embodiments, the sealed sample holder **1700** provides a traceable and tamper-evident container that can be transferred to an analysis device or a testing service. In certain embodiments, the sample holder is configured to provide a stable environment in order to reduce changes in the sample over time. In certain embodiments, the sample holder **1500** is archived as a long-term record of the sample and measurement.

In certain embodiments, the instructions in memory **1740**, or software running on the server **1750** or another device such as a tablet or personal computer, uses the data record to provide a map showing the location of the sample collection.

Absorbance Spectrometry

In absorbance spectrometry, a material sample is illuminated with a beam of incident light. The material absorbs the light and re-emits a portion of the absorbed energy as light of a frequency determined by the molecular structure of the material. The spectral response of the emitted light will have peaks at resonant frequencies associated with specific types of bonds and structures. These peaks can be measured and compared to reference spectral responses of known reference materials to determine the content of a reference material in a sample, much as discussed with respect to FIG. 14A-14C.

FIG. 19A depicts an exploded view of an exemplary sample holder **1900** configured for analysis of a sample based on absorbance of light, according to certain aspects of the present disclosure. The holder **1900** has a body **1910** that is similar to the body **912** of FIG. 10D. The optical assembly **1050** of FIG. 10D is replaced by an optical assembly **1950** comprising a cover slip **1920**, a slit array **1930**, an array of collimating lenses **1932**, and optionally a grating **1934**. In

certain embodiments, the cover slip **1920** has a transparent body **1922** with a reflective layer **1924** covering a portion of the body **1922**.

FIG. 19B depicts an exemplary illustration of how light emitted by the sample **1901** passes through the elements of optical assembly **1950**. A sample of material **1901** is placed into compartment **1912** that is covered by the optical assembly **1950**. In the exploded view of FIG. 19B, the sample **1901** is shown as located such that the underside of the sample **1901** is in contact with the upper surface of the cover slip **1922**, as it would be in actual use. Although the incident light is omitted from FIG. 19 for clarity, a beam of excitation light is directed upward (in the orientation of FIG. 19A) to illuminate the underside of cover slip **1920** over both reflective layer **1924** and the remaining unobstructed portion of cover slip **1920**. In certain embodiments, the excitation light has a specific wavelength, for example having passed through a selectable filter or generated by a light source that emits light having a narrow bandwidth of light about that wavelength. An example source light is light from a laser that emits light with a nominal wavelength of 532 nm that is passed through a 527-537 nm bandpass filter to produce a narrow-band beam of excitation light that is directed to the sample. In certain embodiments, the sample is serially observed using a plurality of wavelengths of excitation light, for example using a filter wheel comprising a plurality of optical filters.

The light **1950** that is emitted by the sample **1901** is radiated (shown as thick arrows) through the coverslip over a solid angle. A portion of the incident light is reflected by the reflective layer **1924** to produce reference light **1952** (thin arrows). The light **1950** and **1952** both pass through the slit array **1930**, whereupon each slit illuminated by light **1950** emits light **1960** and each slit illuminated by light **1952** emits light **1962**, which are then respectively focused by the array of collimating lenses **1932** into collimated beams of light **1970** from the sample **1901** and light **1972** from the reflective surface **1924**. The collimated beams **1970**, **1972** are optionally passed through a grating **1934** to spatially separate the light by wavelength as discussed with respect to FIG. 6.

The light beams **1970** and **1972** are spatially separated such that beam **1970** can be measured separately from beam **1972**, whereupon the measured characteristics of the reference beam **1972** can be used to calibrate the sensor used for light **1970** or to interpret the measurement of light **1970**. In certain embodiments, the beams **1970**, **1972** may be alternately directed to a common sensor (not shown in FIG. 19B). In certain embodiments, a sliding mask (not shown in FIG. 19) or functional equivalent is provided at a point along the optical path from the cover slip **1920** to the grating **1934** to enable a user to direct the collimated light from either the sample or the reflective surface to the detector such that the detector observes only the reflective surface rays, which provides a reference signal suitable for calibration of the system, or only the sample emission rays.

Embodiments

A1. An apparatus for analysis of a sample, comprising: a frame having a first axis; a sample holder coupled to the frame and disposed on the first axis; a transmissive diffraction grating coupled to the frame and disposed along the first axis such that light traveling along the first axis from the sample holder passes through the grating in a first direction; and a source coupled to the frame and configured to emit a

first light to pass through the grating in a second direction that is opposite the first direction.

A2. The apparatus of A1, further comprising: a lens coupled to the frame; and a spatial filter coupled to the frame; wherein the lens and spatial filter are disposed along the first optical axis.

A3. The apparatus of A1, wherein a portion of the first light emitted by the source is diffracted by the grating to travel parallel to the first optical axis.

A4. The apparatus of A3, wherein: the light emitted by the source is monochromatic; the diffracted portion of the first light comprises a mode; the light emitted by the source travels to the grating along a second optical axis that is not parallel to the first optical axis; and an angle between the first and second optical axes determines the mode of the diffracted portion of the first light.

A5. The apparatus of A4, wherein: the light source comprises a plurality of sources each emitting light at a plurality of unique frequencies; the second optical axis comprises a plurality of secondary optical axes that are respectively associated with the plurality of unique frequencies and respectively disposed at a plurality of unique angles to the first optical axis.

A6. The apparatus of A3, wherein: the light emitted by the source is white light; the diffracted portion of the white light comprises a color; the light emitted by the source travels to the grating along a second optical axis that is not parallel to the first optical axis; and an angle between the first and second optical axes determines the color of the diffracted portion of the light.

A7. The apparatus of A1, wherein: the sample holder is configured to accept the sample such that the sample is disposed on the first optical axis; the first light illuminates the sample, whereupon the sample emits a second light that enters the grating in the first direction; and a portion of the second light exits the grating as diffracted second light; the apparatus further comprises: a lens coupled to the frame and configured to focus the diffracted second light to form a Raman spectrum; a detector coupled to the frame and configured to sense the Raman spectrum and provide data related to the Raman spectrum; a processor communicatively coupled to the detector; and a non-volatile memory communicatively coupled to the processor and comprising: a reference file associated with a material; and an instruction file that, when executed by the processor, causes the processor to receive the data from the detector, compare the received data with a portion of the reference file, and determine an attribute of the sample.

A8. The apparatus of A7, wherein the attribute of the sample comprises an amount of a material component in the sample.

A9. The apparatus of A1, wherein the light passes from the source to the grating without being reflected.

B1. A method of obtaining a Raman spectrum of a sample, the method comprising the steps of: illuminating the sample with a first light, whereupon the sample emits a second light that passes through a transmissive diffraction grating in a first direction and exits the grating as diffracted second light, wherein the first light passed through the grating in a second direction opposite the first direction prior to illuminating the sample; focusing the diffracted second light to form a Raman spectrum.

B2. The method of B1, further comprising the steps of: coupling a disposable element to an apparatus, wherein the disposable element comprises a sample holder and the

grating and the apparatus comprises a light source configured to emit the first light; and placing the sample on the sample holder.

B3. The method of B1, wherein the first light is coherent.

B4. The method of B1, wherein the first light is monochromatic.

B5. The method of B1, further comprising the step of filtering the second light to remove a portion of the first light.

B6. The method of B1, further comprising the step of evaluating the Raman spectra to determine an attribute of the sample.

B7. The method of B6, wherein the attribute of the sample comprises an amount of a material component in the sample.

C1. An apparatus for analysis of a sample of a material, comprising a holder configured to accept the sample, the holder comprising a sample plate comprising a first surface configured to contact the accepted sample; and a sample lens array coupled to the sample plate, the sample lens array comprising a plurality of focusing elements.

C2. The apparatus of C1, wherein the holder further comprises a slit array coupled to the sample lens array, the slit array comprising a plurality of slits; and a collimating lens array coupled to the slit array, the collimating lens array comprising a plurality of collimating lenses.

C3. The apparatus of C1, wherein the plurality of focusing elements are configured to collect light from a respective plurality of regions of the surface of the sample and produce a respective plurality of beams of light.

C4. The apparatus of C2, wherein a portion of the plurality of focusing elements are arranged in a first straight row that is parallel to a first slit of the plurality of slits of the slit array; and the focusing elements of the first row are configured to focus their respective beams of light on the first slit.

C5. The apparatus of C4, wherein the plurality of collimating lenses are configured to receive a portion of the plurality of beams of light that pass through the plurality of slits; and modify each of the plurality of beams of light such that all of the modified plurality of beams of light are collimated in a common direction.

C6. The apparatus of C1, wherein the holder further comprises a compartment configured to accept the sample, wherein the sample plate forms a portion of the compartment; and a lid that is coupled to the holder and configured to selectably close over the compartment and permanently prevent removal of an accepted sample from the holder.

C7. The apparatus of C1, wherein the focusing elements are holographic lenses.

C8. The apparatus of C2, wherein the collimating lenses are holographic lenses.

C9. The apparatus of C1, wherein the sample plate further comprises a channel configured to accept a liquid sample.

C10. The apparatus of C1, wherein the sample plate further comprises an actuator selected from the group of a temperature control element, a filtering element, and a stimulation element.

C11. The apparatus of C1, wherein the holder is configured to accept a beam of illuminating light and guide the accepted beam of illuminating light to a side of the sample plate that is not the first surface.

C12. The apparatus of C1, further comprising a frame configured to removably accept the holder; a detector coupled to the frame; a focusing lens coupled to the frame; and a transmissive diffraction grating coupled to the frame.

C13. The apparatus of C12, further comprising an optical filter coupled to the frame; and a spatial filter coupled to the frame.

C14. The apparatus of C12, wherein the grating comprises a first surface and a second surface that is opposite the first surface; a portion of a beam of light emitted by the accepted sample passes through the grating from the first surface to the second surface; and the frame is further configured to accept a beam of illuminating light and guide the accepted beam of illuminating light to the second surface of the grating such that a refracted portion of the beam of illuminating light is directed through the grating and exits the first surface toward the accepted sample.

C15. The apparatus of C1, wherein the holder is configured for use with only a single sample.

Headings and subheadings, if any, are used for convenience only and do not limit the invention.

Reference to an element in the singular is not intended to mean “one and only one” unless specifically so stated, but rather “one or more.” Use of the articles “a” and “an” is to be interpreted as equivalent to the phrase “at least one.” Unless specifically stated otherwise, the terms “a set” and “some” refer to one or more.

Terms such as “top,” “bottom,” “upper,” “lower,” “left,” “right,” “front,” “rear” and the like as used in this disclosure should be understood as referring to an arbitrary frame of reference, rather than to the ordinary gravitational frame of reference. Thus, a top surface, a bottom surface, a front surface, and a rear surface may extend upwardly, downwardly, diagonally, or horizontally in a gravitational frame of reference.

Although the relationships among various components are described herein and/or are illustrated as being orthogonal or perpendicular, those components can be arranged in other configurations in some embodiments. For example, the angles formed between the referenced components can be greater or less than 90 degrees in some embodiments.

Although various components are illustrated as being flat and/or straight, those components can have other configurations, such as curved or tapered for example, in some embodiments.

Pronouns in the masculine (e.g., his) include the feminine and neuter gender (e.g., her and its) and vice versa. All structural and functional equivalents to the elements of the various aspects described throughout this disclosure that are known or later come to be known to those of ordinary skill in the art are expressly incorporated herein by reference and are intended to be encompassed by the claims. Moreover, nothing disclosed herein is intended to be dedicated to the public regardless of whether such disclosure is explicitly recited in the claims. No claim element is to be construed under the provisions of 35 U.S.C. § 112, sixth paragraph, unless the element is expressly recited using the phrase “means for” or, in the case of a method claim, the element is recited using the phrase “operation for.”

A phrase such as an “aspect” does not imply that such aspect is essential to the subject technology or that such aspect applies to all configurations of the subject technology. A disclosure relating to an aspect may apply to all configurations, or one or more configurations. A phrase such as an “embodiment” does not imply that such embodiment is essential to the subject technology or that such embodiment applies to all configurations of the subject technology. A disclosure relating to an embodiment may apply to all embodiments, or one or more embodiments. A phrase such as an “embodiment” may refer to one or more embodiments and vice versa.

The word “exemplary” is used herein to mean “serving as an example or illustration.” Any aspect or design described

herein as “exemplary” is not necessarily to be construed as preferred or advantageous over other aspects or designs.

All structural and functional equivalents to the elements of the various aspects described throughout this disclosure that are known or later come to be known to those of ordinary skill in the art are expressly incorporated herein by reference and are intended to be encompassed by the claims. Moreover, nothing disclosed herein is intended to be dedicated to the public regardless of whether such disclosure is explicitly recited in the claims. No claim element is to be construed under the provisions of 35 U.S.C. § 112, sixth paragraph, unless the element is expressly recited using the phrase “means for” or, in the case of a method claim, the element is recited using the phrase “step for.” Furthermore, to the extent that the term “include,” “have,” or the like is used in the description or the claims, such term is intended to be inclusive in a manner similar to the term “comprise” as “comprise” is interpreted when employed as a transitional word in a claim.

Although embodiments of the present disclosure have been described and illustrated in detail, it is to be clearly understood that the same is by way of illustration and example only and is not to be taken by way of limitation, the scope of the present invention being limited only by the terms of the appended claims.

What is claimed is:

1. A method of analyzing a sample, comprising the steps of:

measuring a first spectral response of the sample;
selecting a reference material having a first Raman peak having a first magnitude at a first wave number;
measuring a first peak value in the first spectral response at the first wave number; and
determining an amount of the reference material in the sample based in part on a first ratio of the measured first peak value to the first magnitude of the first Raman peak of the reference material.

2. The method of claim 1, further comprising the step of: measuring a second peak value in the first spectral response at a second wave number;
wherein:

the reference material has a second Raman peak having a second magnitude at the second wave number; and
the step of determining the amount of the reference material is additionally based in part on a second ratio of the measured second peak value to the second magnitude of the second Raman peak of the reference material.

3. The method of claim 1, wherein the step of measuring the first spectral response comprises illuminating the sample with a source light having a first wavelength.

4. The method of claim 3, wherein the first magnitude of the first Raman peak of the reference material is associated with the first wavelength.

5. The method of claim 3, further comprising the steps of: measuring a second spectral response of the sample while illuminating the sample with a source light having a second wavelength; and

measuring a third peak value in the second spectral response at the first wave number;
wherein the step of determining the amount of the reference material is additionally based in part on the measured third peak value.

6. The method of claim 3, wherein the step of measuring the first spectral response comprises guiding light reflected from a surface of the sample that is illuminated by the source

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light to a sensor that measures the intensity of the reflected light at a plurality of frequencies.

7. The method of claim 6, wherein the reflected light passes through a slit then through a collimating lens then through a grating then through a focusing lens to spatially separate the light according to wavelength on the sensor.

8. The method of claim 7, wherein:

the slit is configured as an array of parallel slits; and the collimating lens is configured as a collimating lens array of parallel cylindrical lenses arranged such that each cylindrical lens captures light that emerges from a respective slit of the array of parallel slits.

9. The method of claim 8, wherein:

the reflected light passes through a sample lens then through the slit; and

the sample lens is configured as a sample lens array of parallel cylindrical lenses that capture light reflected from respective parallel areas of the sample and focuses the light onto a respective slit of the array of parallel slits.

10. The method of claim 9, wherein:

the amount light at a particular frequency that emerges from each of the cylindrical collimating lenses is brought to a common location on the sensor; and

the intensity of the light at a particular frequency at the sensor is proportional to a total area of the parallel areas of the sample from which reflected light is captured by the sample lens array, such that the sensitivity of the determination of the amount of the reference material in the sample is proportional to the strength of the intensity of the light at the sensor.

11. The method of claim 1, wherein the reference material comprises a known amount of a component, further comprising the step of:

determining an amount of the component in the sample based in part on the known amount of the component in the reference material.

12. A holder for analyzing a sample, comprising:

a sample plate having a surface configured to be in contact with the sample and to be illuminated by a source light; a slit array comprising a plurality of slits and positioned such that light reflected from the surface is directed toward the slit array; and

a collimating lens array comprising a plurality of cylindrical lenses each configured to capture light that emerges from a respective slit of the slit array and collimate the light emerging from the plurality of cylindrical lenses in a common direction.

13. The holder of claim 12, further comprising:

a sample lens array comprising a plurality of cylindrical lenses configured to capture light reflected from respective parallel areas of the sample and focuses the captured light onto a respective slit of the slit array.

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14. The holder of claim 12, further comprising a body coupled to each of the sample plate, the sample lens array, the slit array, and the collimating lens array.

15. The holder of claim 14, wherein the body comprises an interface configured to detachably mate with a spectrometer comprising one or more of:

a sensor;

a grating configured to disperse light emerging from the plurality of collimating lenses such that light of a common frequency is collimated in a common direction; and

a focusing lens configured to focus light of a common frequency emerging from the grating onto a common location on the sensor.

16. The holder of claim 12, further comprising:

a compartment coupled to the sample plate and configured to contain the sample;

a cap configured to be coupled to the body so as to seal the compartment after a sample is placed in the compartment; and

a unique identifier;

wherein the holder is configured to be used only one time to contain a sample.

17. A tamper-evident holder, comprising:

a body comprising:

an access opening;

a closure compartment;

a latch opening into the closure compartment; and

a window that provides visibility into the closure compartment; and

a cap comprising a non-return fitment;

wherein:

the cap is configured to seal the access opening when the cap is placed in a closure position;

the fitment passes through the latch opening to a latched position when the cap is placed in the closure position;

the fitment is visible through the window while in the latched position;

the fitment is configured to separate from the cap when the cap is dislodged from the closure position; and

a separated fitment is retained in the closure compartment.

18. The tamper-evident holder of claim 17, wherein the body further comprises a sample compartment coupled to the access opening.

19. The tamper-evident holder of claim 18, wherein the window also provides visibility into the sample compartment such that the sample can be optically analyzed without dislodging the cap from the closure position.

20. The tamper-evident holder of claim 17, wherein the window comprises a transparent material such that the sample is protected from contamination.

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