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**Scott et al.**

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(54) **LASER SPIDERWEB SENSOR USED WITH PORTABLE HANDHELD DEVICES**

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( * ) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

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(22) Filed: **Sep. 24, 2015**

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(51) **Int. Cl.**
***G01N 21/00*** (2006.01)
***G01J 3/02*** (2006.01)
***G01J 3/42*** (2006.01)

(52) **U.S. Cl.**
CPC ............. ***G01J 3/0291*** (2013.01); ***G01J 3/021*** (2013.01); ***G01J 3/42*** (2013.01); *G01J 3/0256* (2013.01);

(Continued)

(58) **Field of Classification Search**
CPC ............. G01N 2333/59; G01N 33/558; G02B 17/023; G02B 2027/0154; G02B 25/002;

(Continued)

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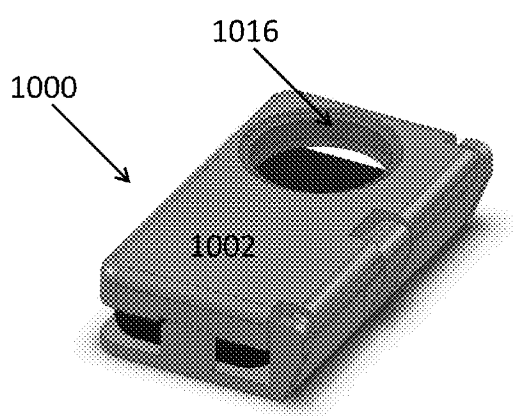
(57) **ABSTRACT**

A portable spectrometer, including a smart phone case storing a portable spectrometer, wherein the portable spectrometer includes a cavity; a source for emitting electromagnetic radiation that is directed on a sample in the cavity, wherein the electromagnetic radiation is reflected within the cavity to form multiple passes of the electromagnetic radiation through the sample; a detector for detecting the electromagnetic radiation after the electromagnetic radiation has made the multiple passes through the sample in the cavity, the detector outputting a signal in response to the detecting; and a device for communicating the signal to a smart phone, wherein the smart phone executes an application that performs a spectral analysis of the signal.

**21 Claims, 20 Drawing Sheets**



(52) **U.S. Cl.**
CPC ........ *G01J 2003/423* (2013.01); *G01N 21/00* (2013.01)

(58) **Field of Classification Search**
CPC .. G02B 25/005; G02B 25/02; G02B 27/0101; G02B 27/0149; G02B 27/027; G02B 27/028; G02B 27/04; G02B 27/2292; G02B 5/09
See application file for complete search history.

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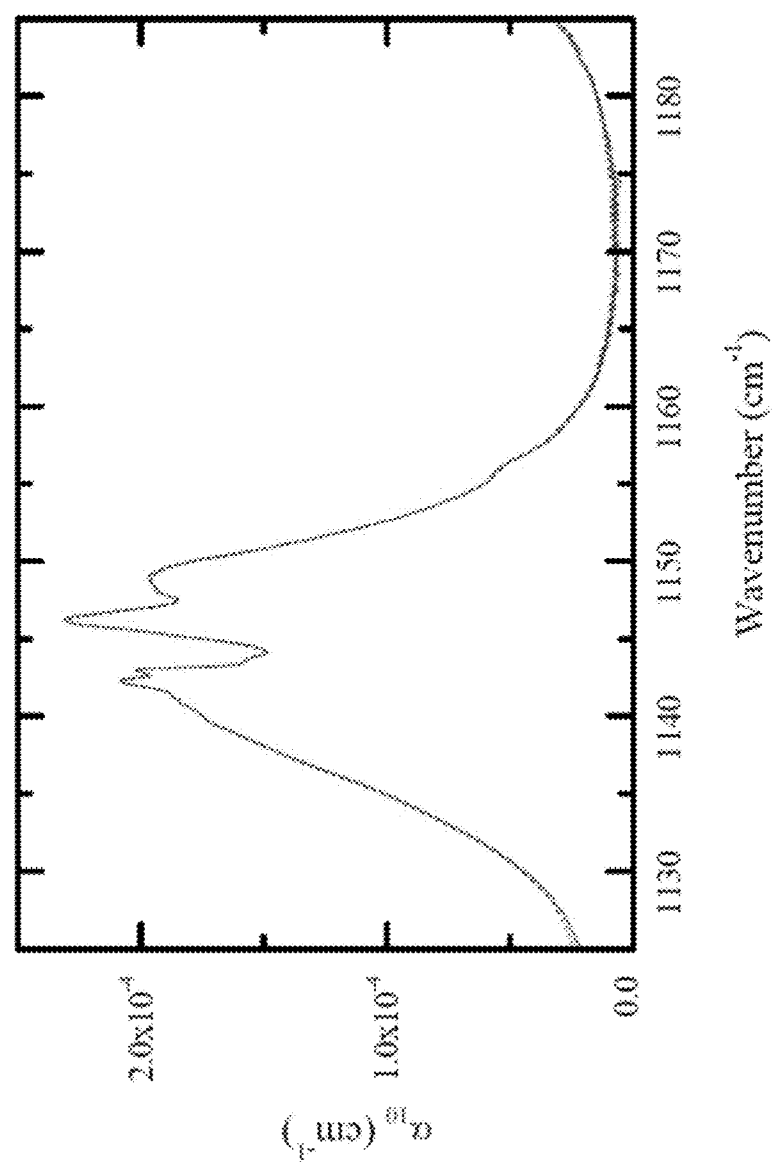

$\alpha_{10}$ (cm$^{-1}$)
2.0x10$^{-4}$
1.0x10$^{-4}$
0.0
1130
1140
1150
1160
1170
1180
Wavenumber (cm$^{-1}$)

Figure 1

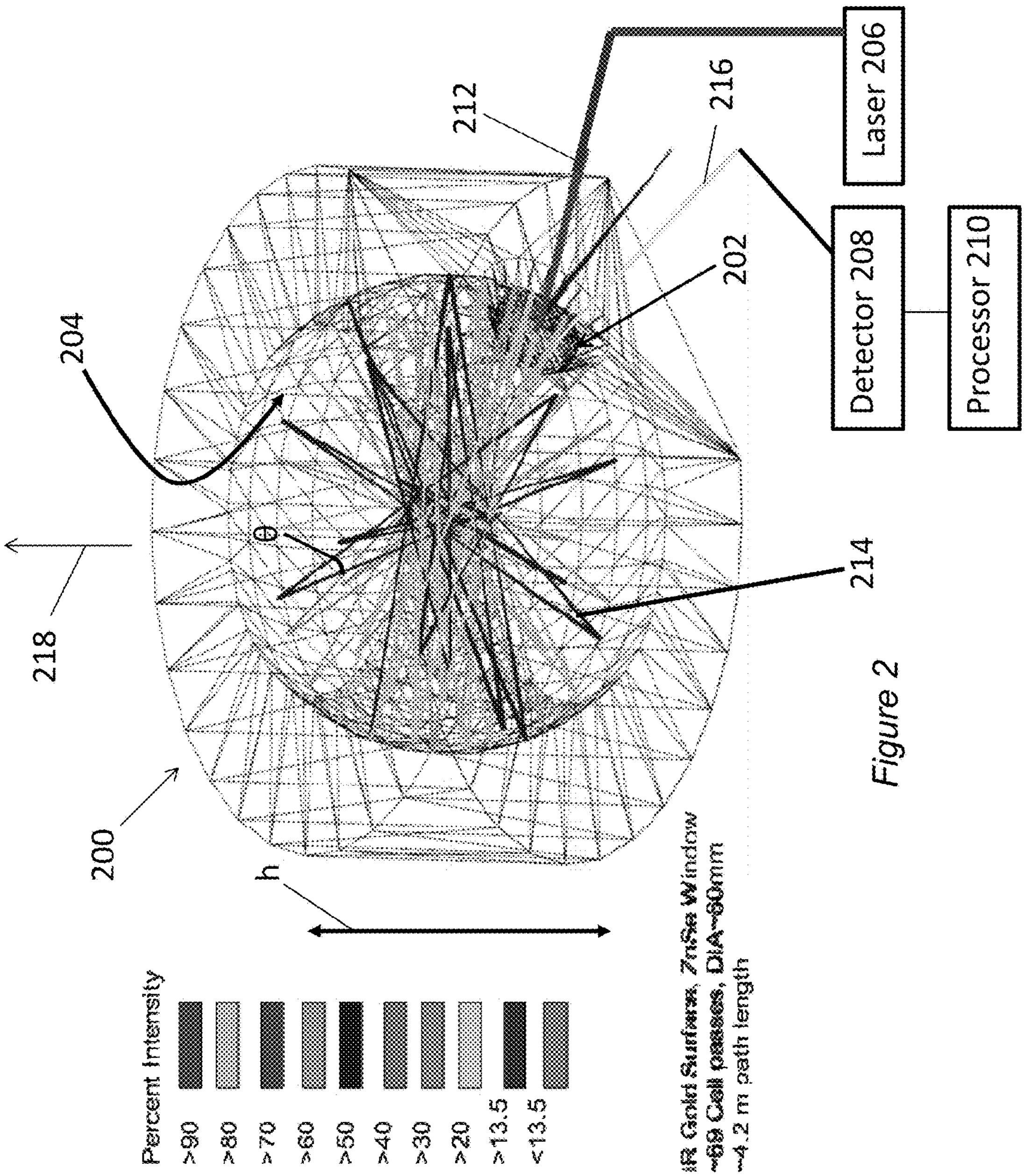

Laser 206
Detector 208
Processor 210
212
216
202
204
218
214
200
θ
h
Percent Intensity
>90
>80
>70
>60
>50
>40
>30
>20
>13.5
<13.5
IR Gold Surfaces, ZnSe Window
~69 Cell passes, DIA~80mm
~4.2 m path length

Figure 2

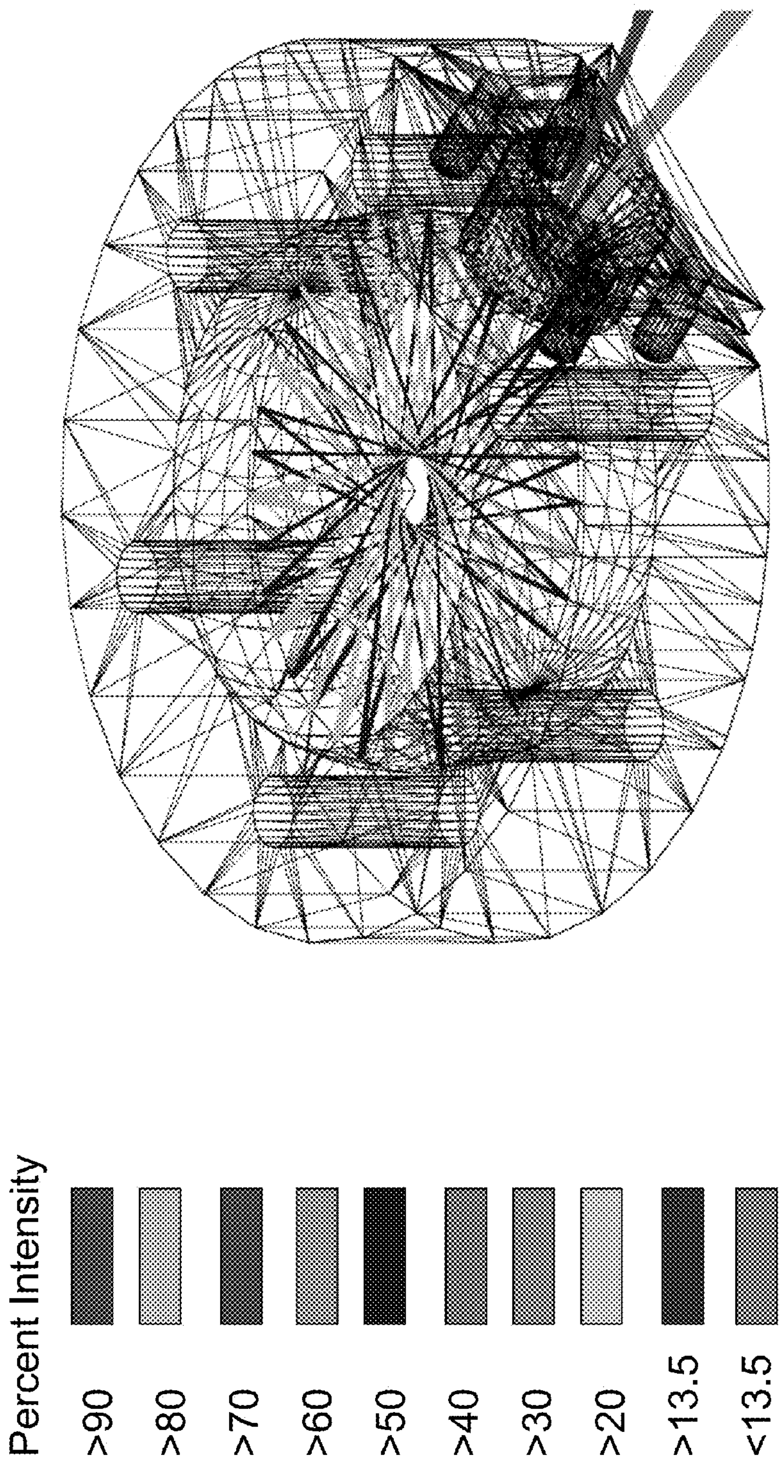



Figure 3

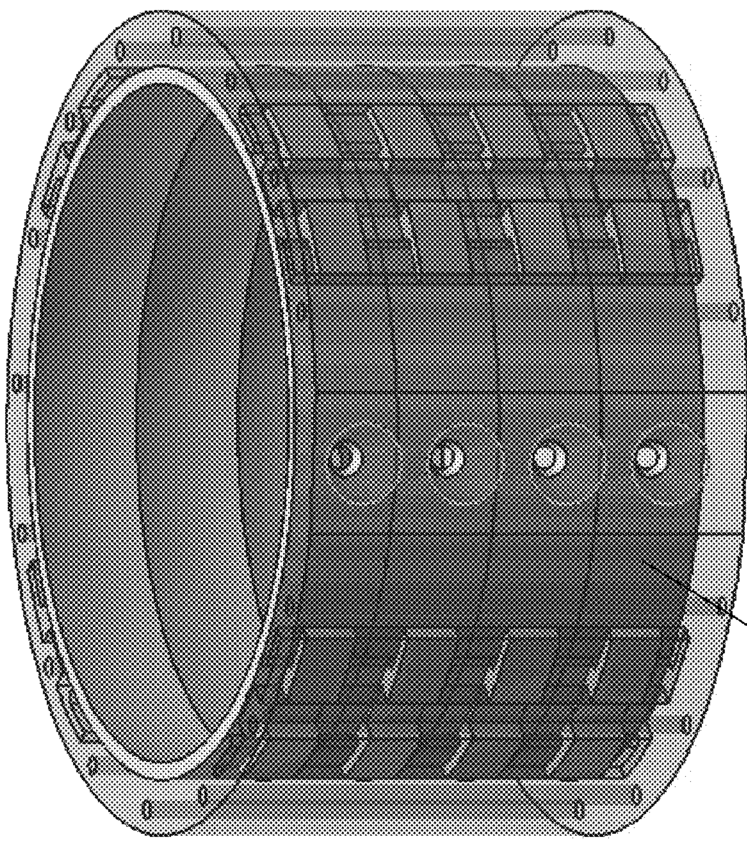



Figure 4

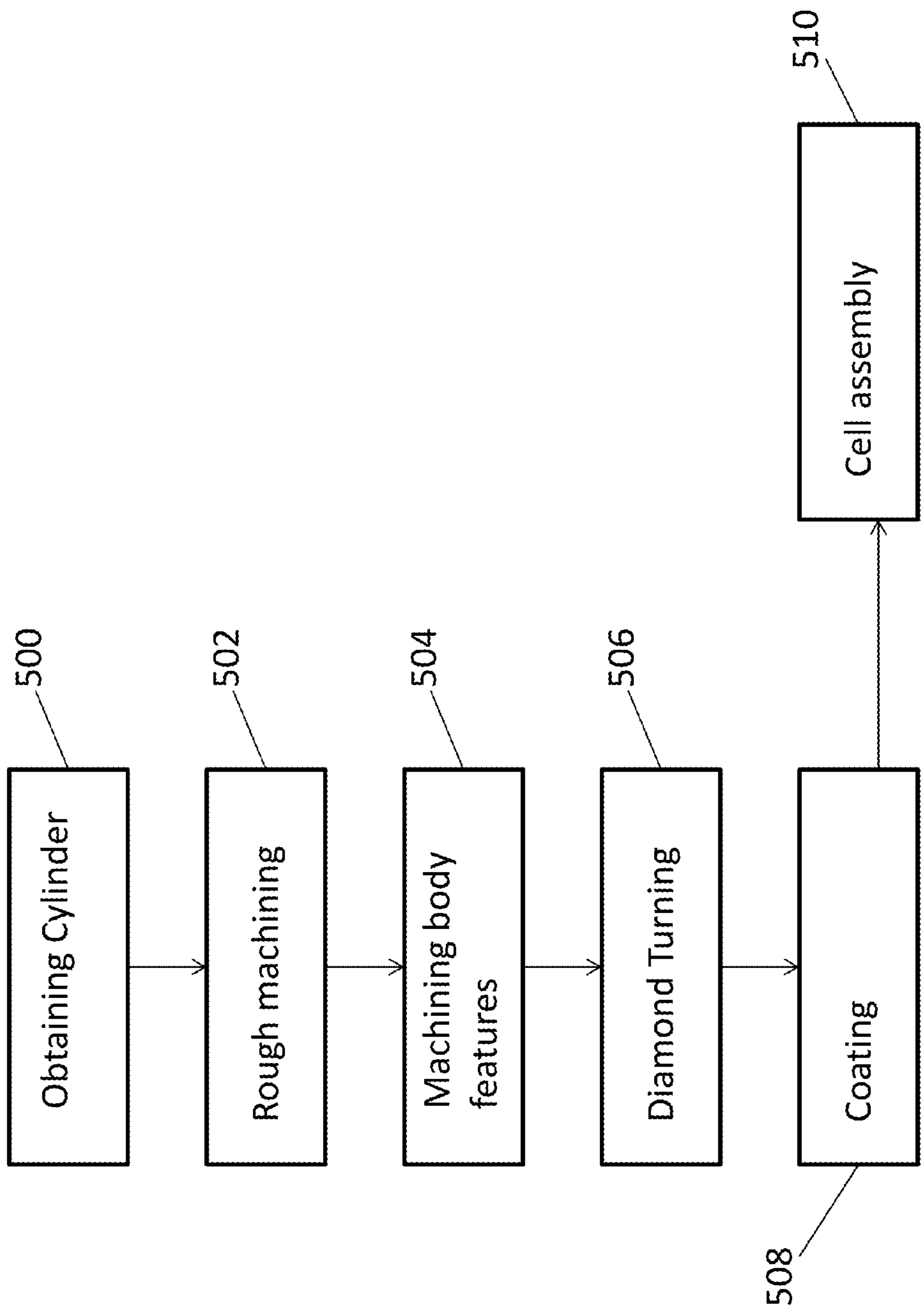

500
Obtaining Cylinder
502
Rough machining
504
Machining body features
506
Diamond Turning
508
Coating
510
Cell assembly

*Figure 5*

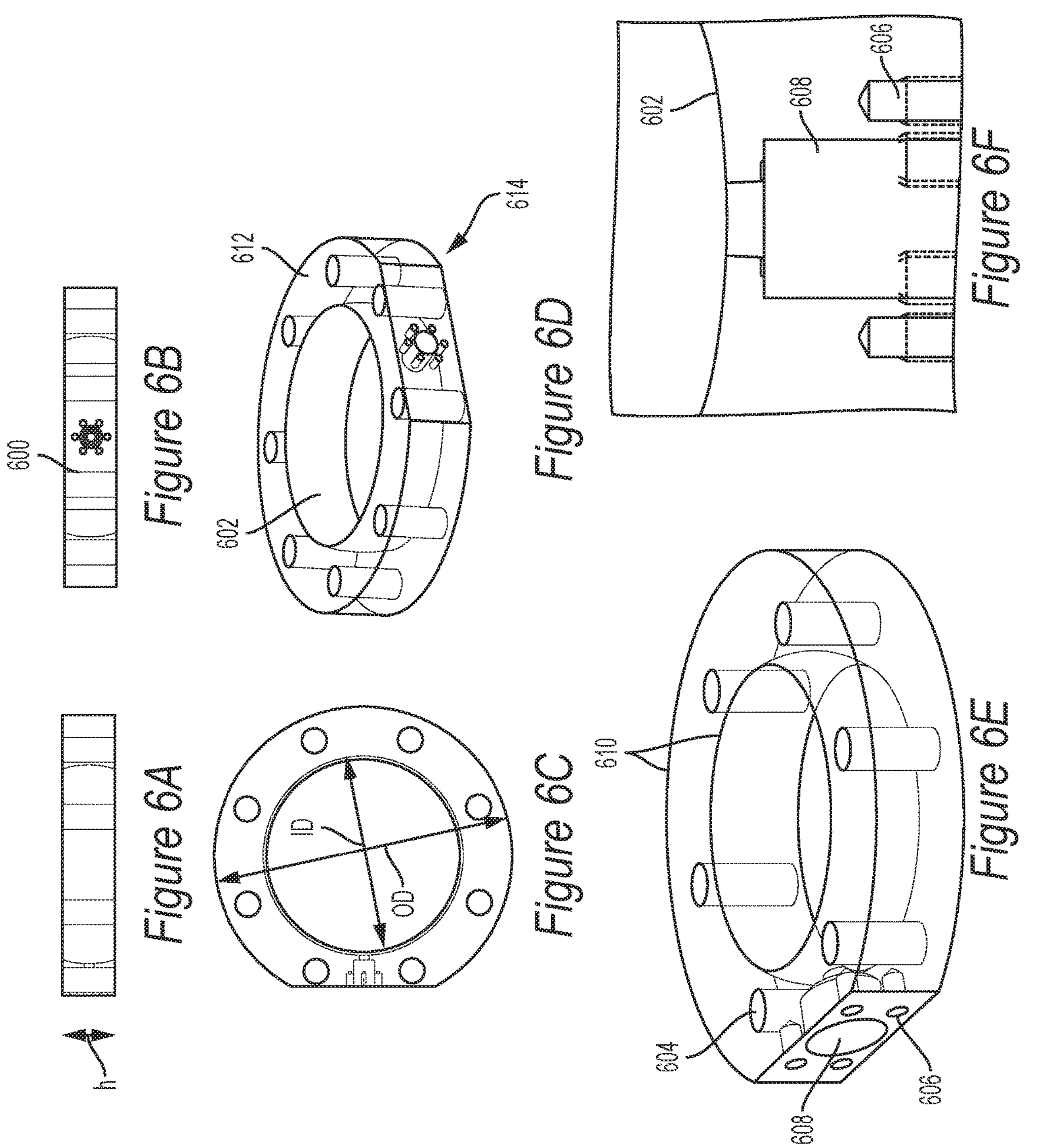



Figure 6A

Figure 6B

Figure 6C

Figure 6D

Figure 6E

Figure 6F

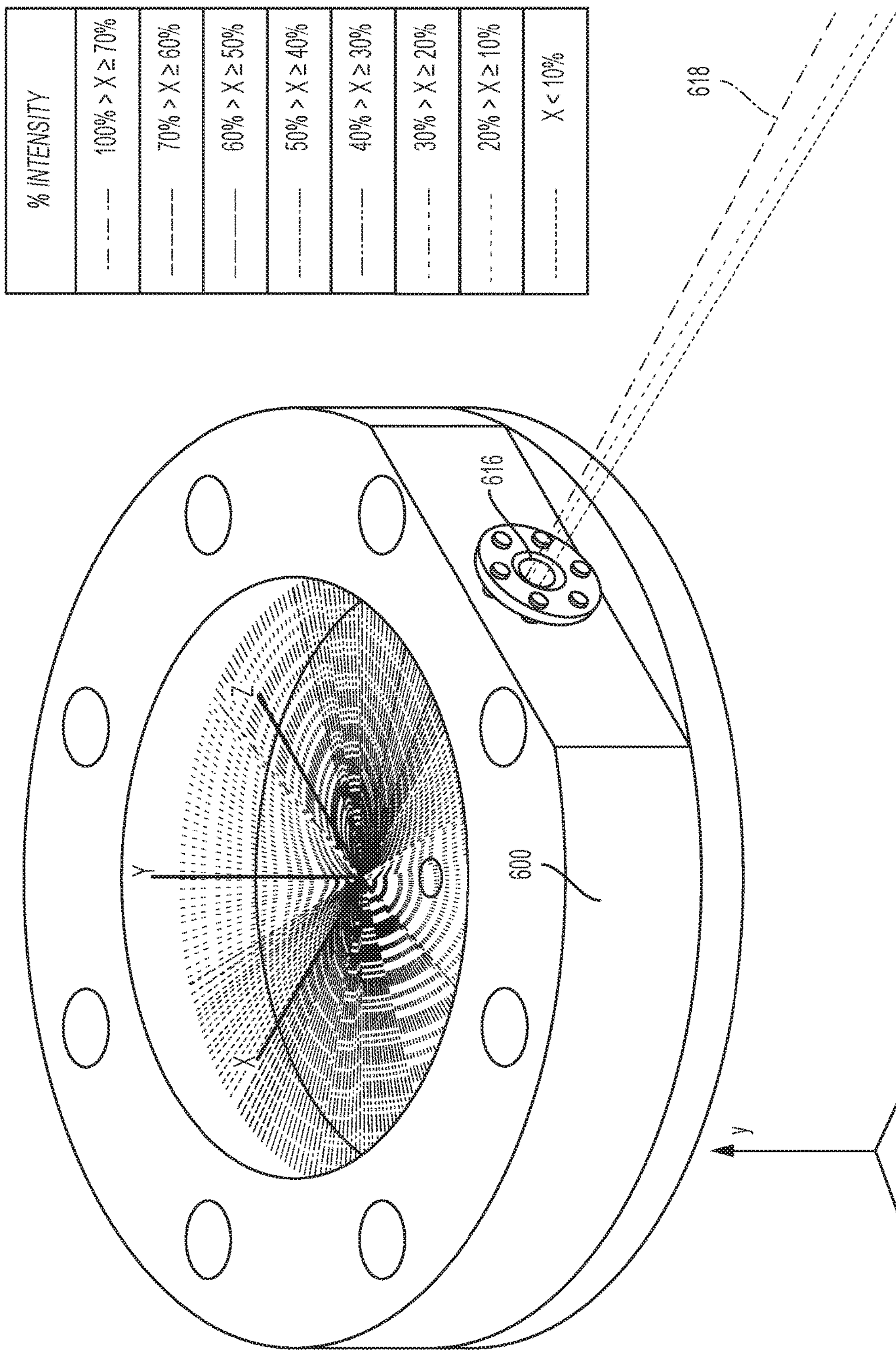
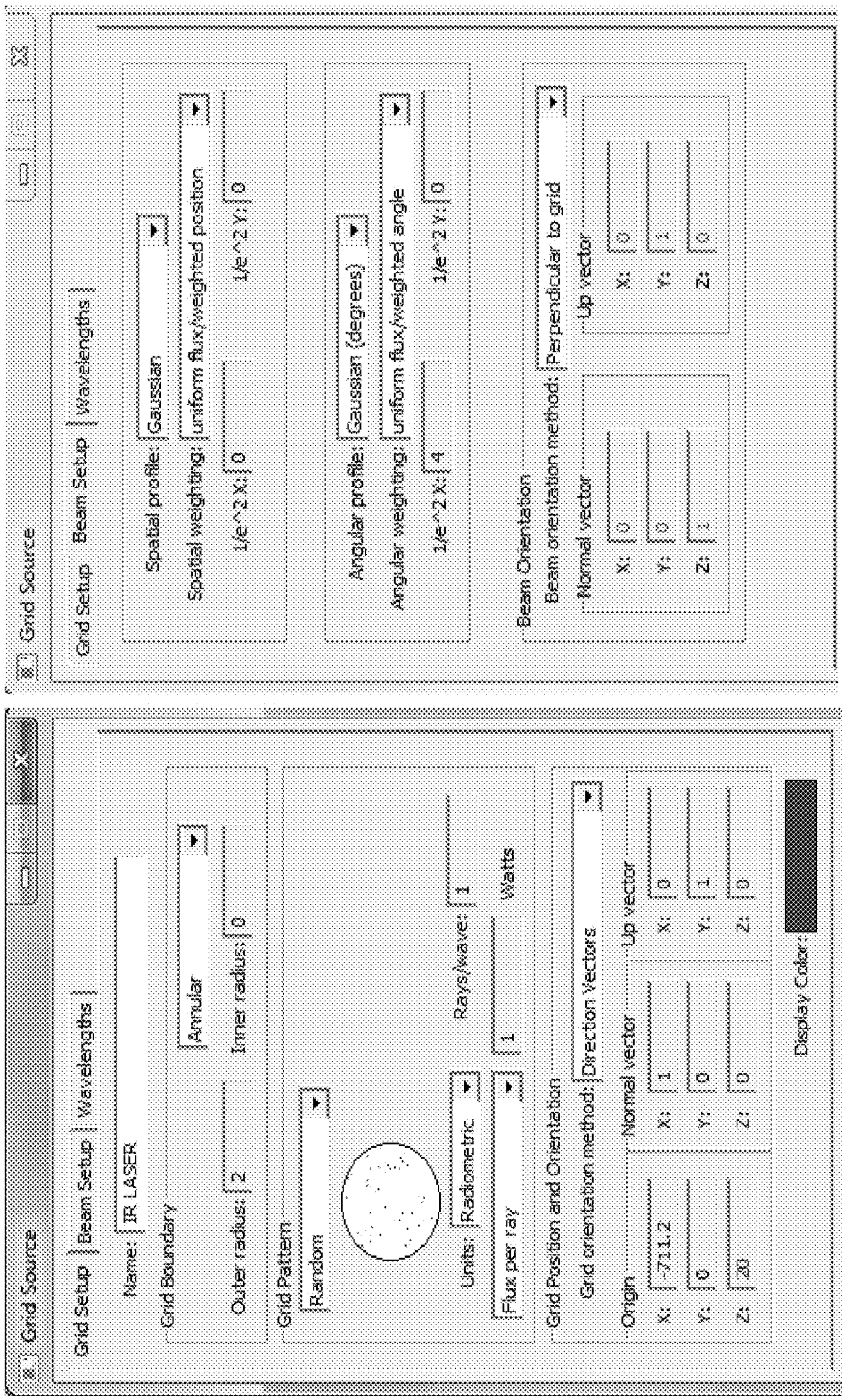

% INTENSITY
100% > X ≥ 70%
70% > X ≥ 60%
60% > X ≥ 50%
50% > X ≥ 40%
40% > X ≥ 30%
30% > X ≥ 20%
20% > X ≥ 10%
X < 10%
618
616
600
Y
Z
X
y
z
x

Figure 6G



Grid Source
Grid Setup
Beam Setup
Wavelengths
Name: IR LASER
Grid Boundary
Annular
Outer radius: 2
Inner radius: 0
Grid Pattern
Random
Units: Radiometric
Flux per ray
1
Rays/wave: 1
Watts
Grid Position and Orientation
Grid orientation method: Direction Vectors
Origin
X: -711.2
Y: 0
Z: 20
Normal vector
X: 1
Y: 0
Z: 0
Up vector
X: 0
Y: 1
Z: 0
Display Color:
Grid Source
Grid Setup
Beam Setup
Wavelengths
Spatial profile: Gaussian
Spatial weighting: uniform flux/weighted position
1/e^2 X: 0
1/e^2 Y: 0
Angular profile: Gaussian (degrees)
Angular weighting: uniform flux/weighted angle
1/e^2 X: 4
1/e^2 Y: 0
Beam Orientation
Beam orientation method: Perpendicular to grid
Normal vector
Up vector


Figure 6H

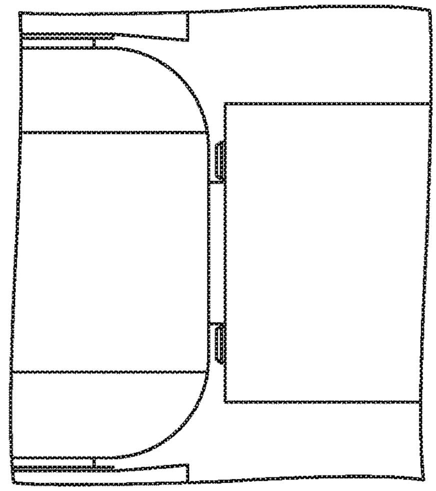


Figure 6M

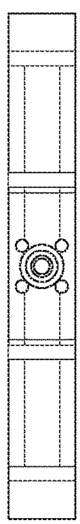


Figure 6J

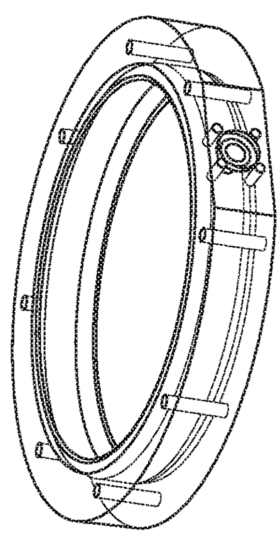


Figure 6L

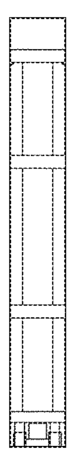


Figure 6I

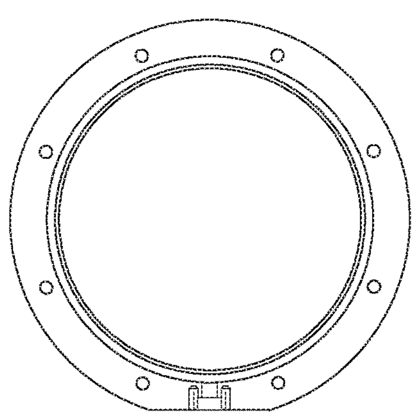


Figure 6K

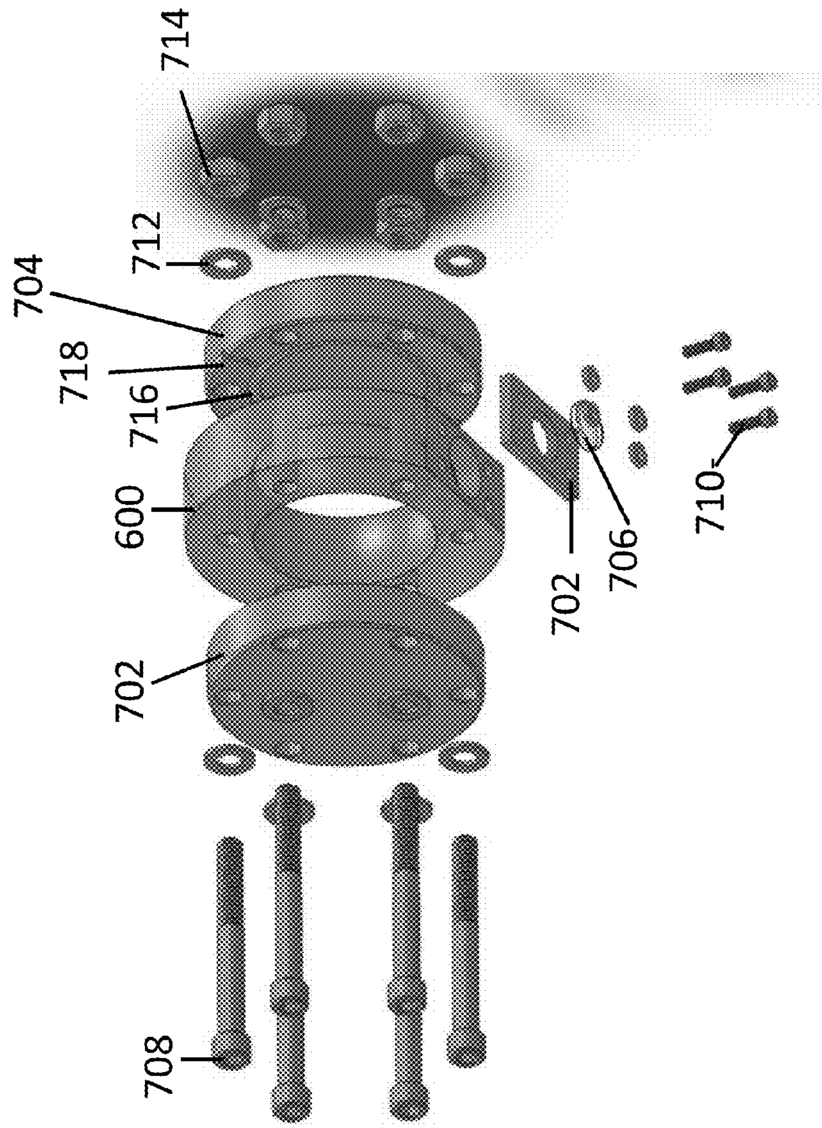



Figure 7A

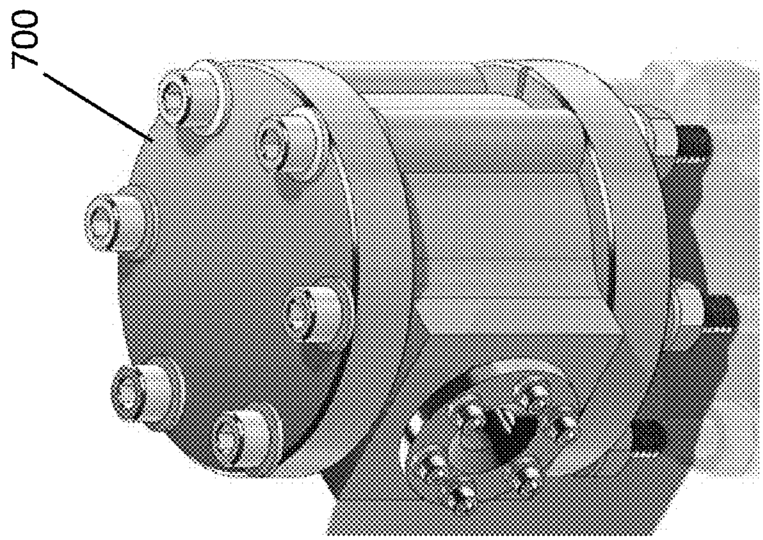
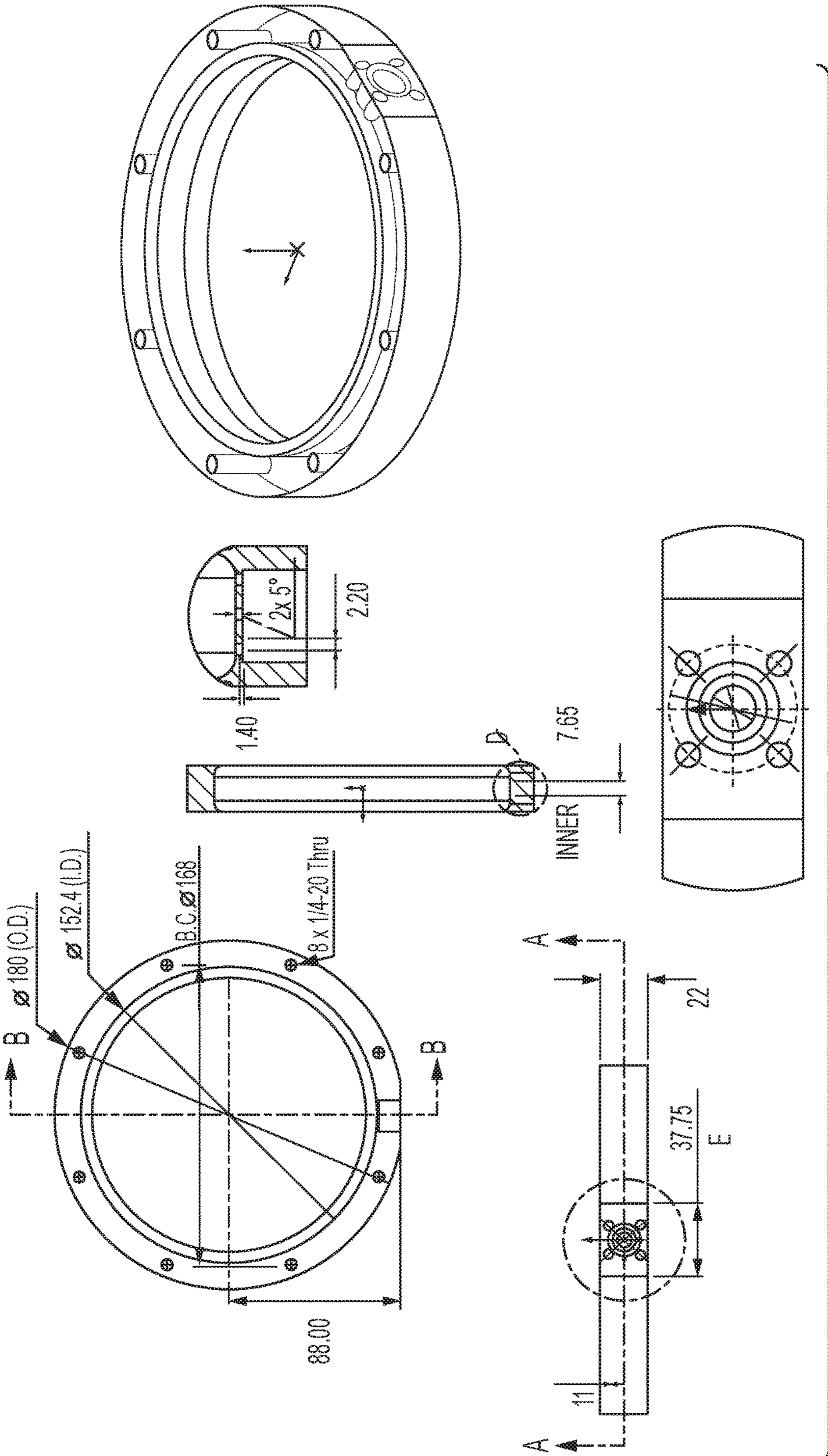



Figure 7B



B
B
ø 180 (O.D.)
ø 152.4 (I.D.)
B.C.ø168
8 x 1/4-20 Thru
88.00
A
A
22
37.75
E
11
1.40
2x 5°
2.20
D
7.65
INNER


*Figure 8*

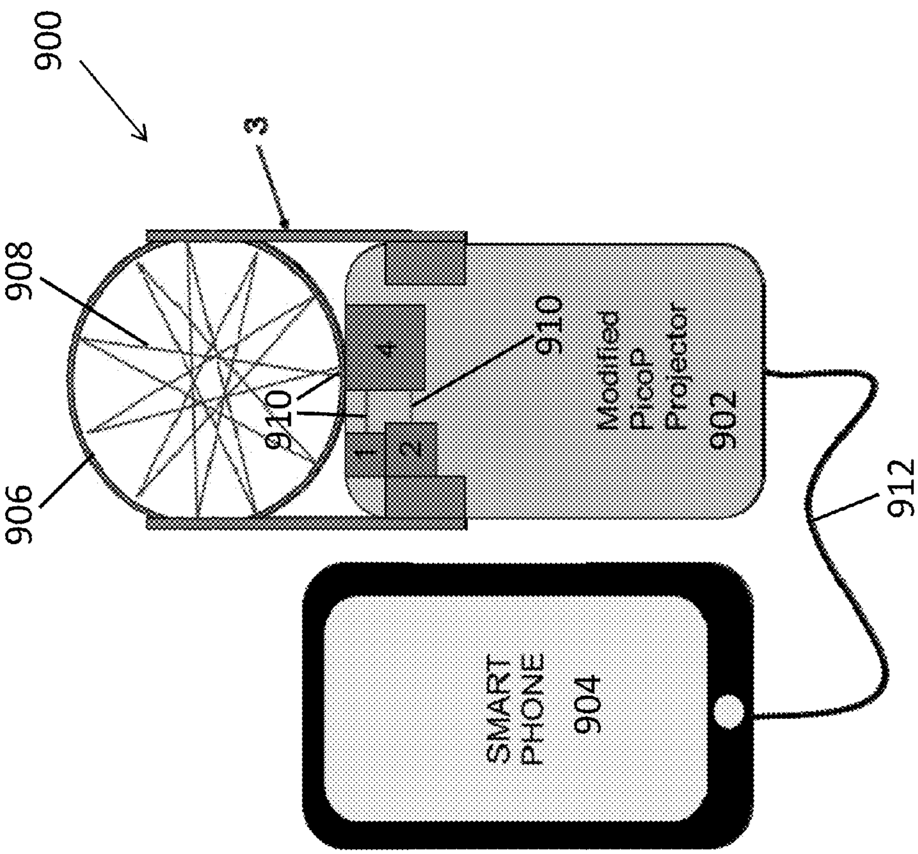

900
3
908
906
910
910
1
2
4
Modified
PicoP
Projector
902
912
SMART
PHONE
904

Figure 9

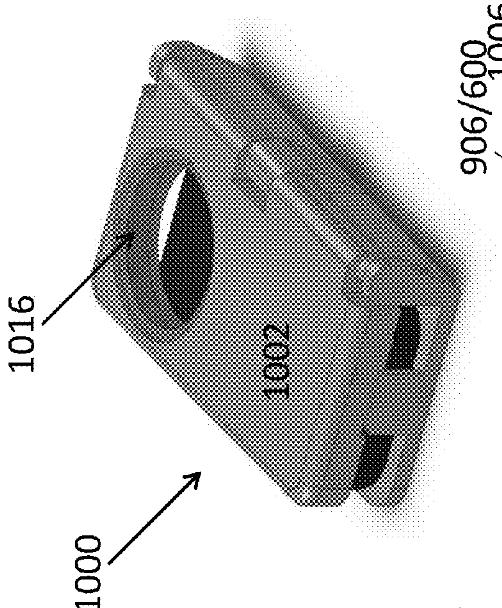



Figure 10A

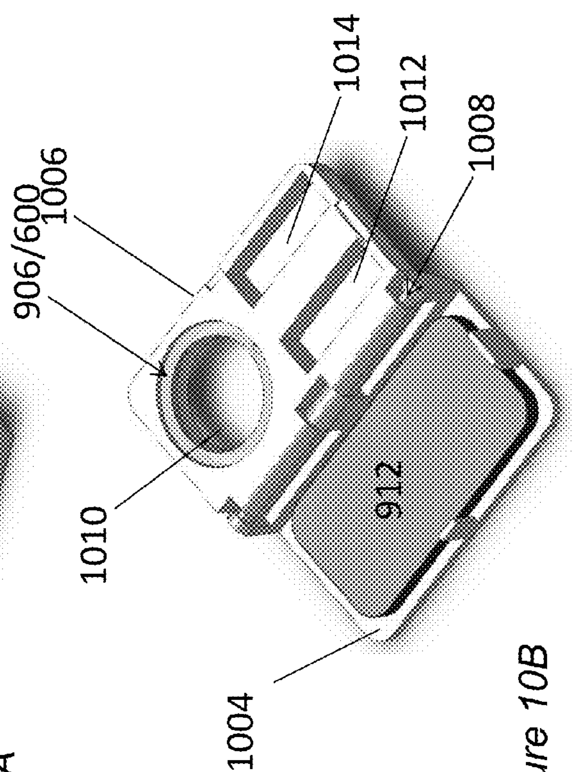



Figure 10B

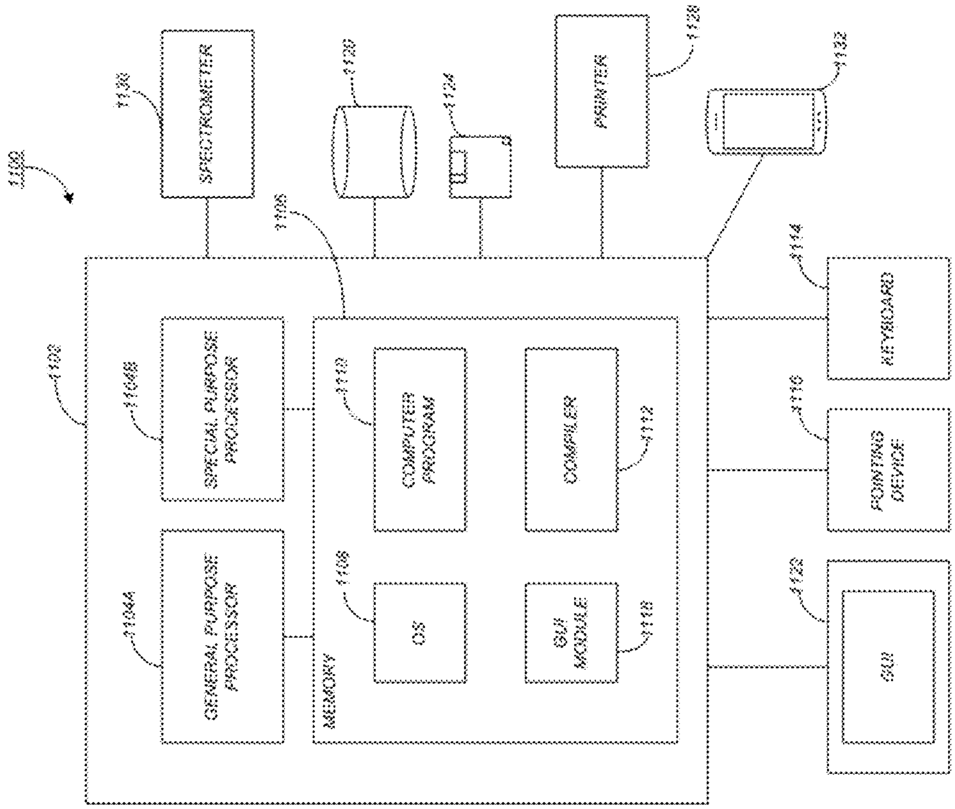

1100
1102
GENERAL PURPOSE PROCESSOR
1104A
SPECIAL PURPOSE PROCESSOR
1104B
MEMORY
1106
OS
1108
COMPUTER PROGRAM
1110
COMPILER
1112
GUI MODULE
1118
SPECTROMETER
1130
1120
1124
PRINTER
1128
1132
KEYBOARD
1114
POINTING DEVICE
1116
GUI
1122

Figure 11

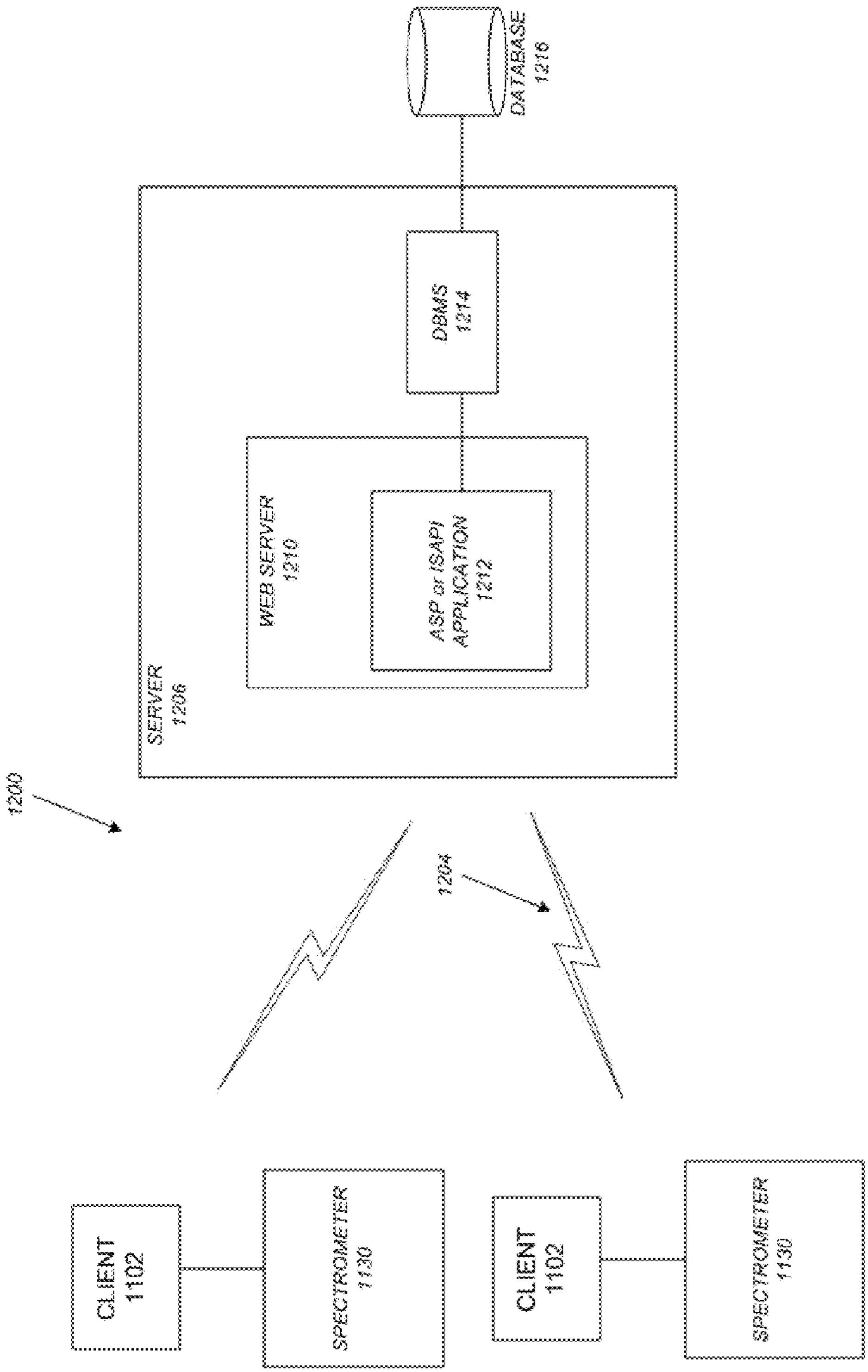

1200
SERVER
1206
WEB SERVER
1210
ASP or ISAPI
APPLICATION
1212
DBMS
1214
DATABASE
1216
1204
CLIENT
1102
SPECTROMETER
1130
CLIENT
1102
SPECTROMETER
1130

Figure 12

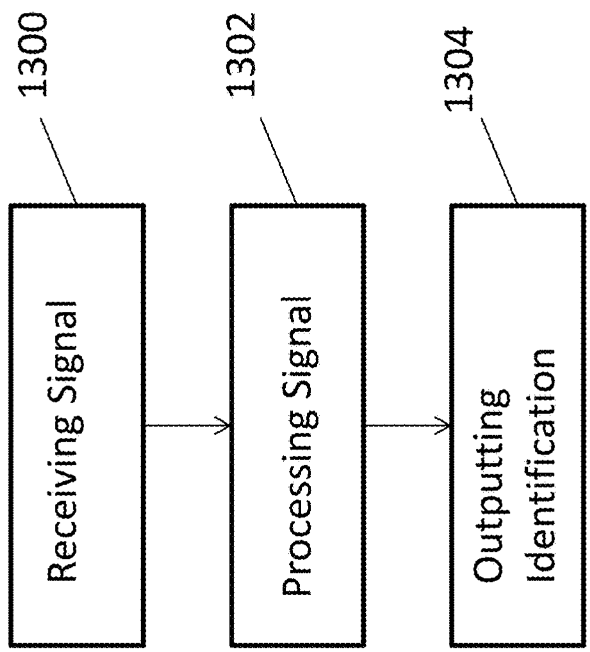

1300
Receiving Signal
1302
Processing Signal
1304
Outputting Identification

*Figure 13*

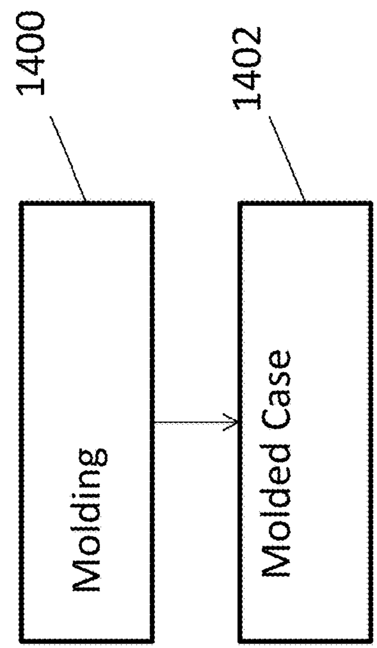



Figure 14

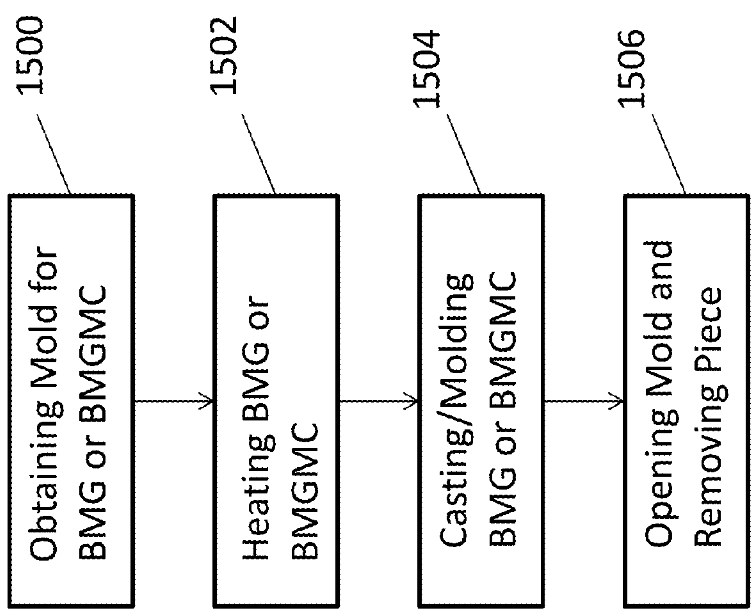

1500
Obtaining Mold for BMG or BMGMC
1502
Heating BMG or BMGMC
1504
Casting/Molding BMG or BMGMC
1506
Opening Mold and Removing Piece

*Figure 15*

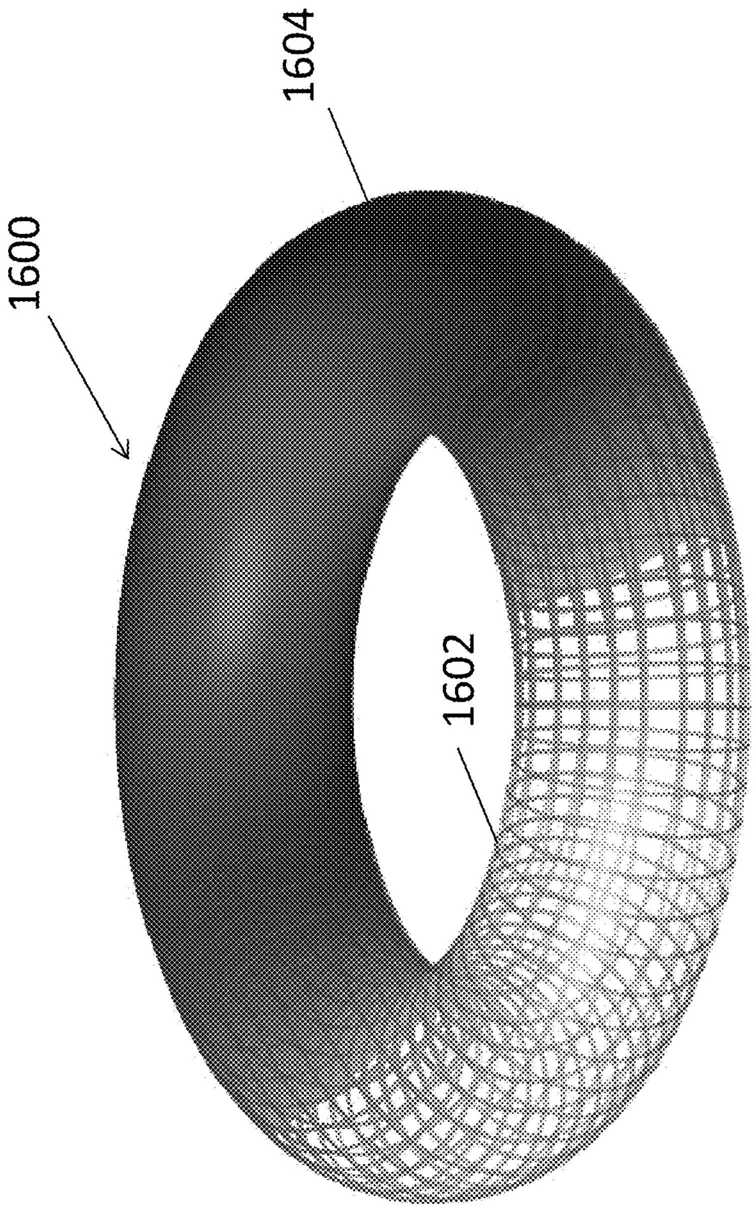



Figure 16

# LASER SPIDERWEB SENSOR USED WITH PORTABLE HANDHELD DEVICES

## CROSS REFERENCE TO RELATED APPLICATIONS

This application claims the benefit under 35 U.S.C. Section 119(e) of co-pending and commonly-assigned U.S. Provisional Patent Application Ser. No. 62/054,800, filed on Sep. 24, 2014, by David C. Scott, Alexander Ksendzov, Warren P George, Richard L. Baron, James A. Smith, Abdullah S. Aljabri, Joel M. Steinkraus, and Rudi M Bendig, entitled "LASER SPIDERWEB SENSOR USED WITH PORTABLE HANDHELD DEVICES," which application is incorporated by reference herein.

## STATEMENT REGARDING FEDERALLY SPONSORED RESEARCH AND DEVELOPMENT

The invention described herein was made in the performance of work under a NASA contract, and is subject to the provisions of Public Law 96-517 (35 USC 202) in which the Contractor has elected to retain title.

## BACKGROUND OF THE INVENTION

1. Field of the Invention

This invention relates to a spectrometer and method of fabricating a spectrometer.

2. Description of the Related Art

(Note: This application references a number of different publications as indicated throughout the specification by one or more reference numbers within brackets, e.g., [x]. A list of these different publications ordered according to these reference numbers can be found below in the section entitled "References." Each of these publications is incorporated by reference herein.)

Detection of chemicals important in the global carbon cycle and climate monitoring are of paramount importance to the Department of Energy (DOE), the Environmental Protection Agency (EPA), the Department of Transportation (DOT) and NASA. The mission of the Biological and Environmental Research (BER) program at the DOE is to understand complex biological, climatic, and environmental systems across spatial and temporal scales ranging from sub-micron to the global, from individual molecules to ecosystems, and from nanoseconds to millennia. This is accomplished by discovering the physical, chemical, and biological drivers of climate change; and seeking the molecular determinants of environmental sustainability and stewardship.

Chemical detection also has application in medicine, for example, in identification of disease markers.

## SUMMARY OF THE INVENTION

One or more embodiments of the invention disclose a portable spectrometer, comprising a smart phone case or portable computer case storing a portable spectrometer, wherein the portable spectrometer includes a cavity; a source for emitting electromagnetic radiation that is directed on the sample in the cavity, wherein the electromagnetic radiation is reflected within the cavity to form multiple passes of the electromagnetic radiation through the sample; and a detector for detecting the electromagnetic radiation after the electromagnetic radiation has made the multiple passes through the sample in the cavity, the detector outputting a signal in response to the detecting and communicating the signal to a smart phone or portable computer, and the smart phone or portable computer executing an application that performs a spectral analysis of the signal. Thus, one or more processors in the smart phone can form an output identifying a composition of the sample (e.g., the sample that enters, is contained in, is enclosed by, or is defined by, the cavity).



The cavity can include a ring having an elliptical inner surface. The cavity can include an inner surface substantially described by the equation:

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{c^2} = 1,$$

wherein x, y, and z are Cartesian coordinates, a is an equatorial radius comprising a maximum value of x and y, c is a distance along the z- axis from coordinate (x=0, y=0, z=0) to a pole of the spheroid described by the equation, and $a \neq c$.

The electromagnetic radiation incident on the inner surface can be reflected from multiple regions of the inner surface such that the multiple passes of the electromagnetic radiation through the sample in the cavity are formed.

The cavity can be dimensioned such that a volume of the cavity comprising the sample is between 33 $mm^3$ and 905000 $mm^3$. The cavity can have a height in a range of 2 millimeters (mm)-20 mm, a width of 2 mm-60 mm, and a length of 2 mm-60 mm, for example. In one or more embodiments (referring to the equation as a function of x, y, and z above), $z<c$, z is in a range of 2 mm-20 mm, and a is in a range of 2 mm-60 mm. In one or more embodiments, an angle of incidence of the electromagnetic radiation, at a first reflection within the cavity, is between more than 0 degrees and 45 degrees, a is less than 60 mm, z is less than 20 mm, and the angle of incidence, a, and z are such that a total path length of the electromagnetic radiation transmitted through the sample includes a distance of 30 meters. An angle of incidence of the electromagnetic radiation at a first reflection within the cavity, a, and z can be selected such that the spectrometer can identify the sample having a relative concentration in the cavity of 50 parts-per-billion by volume (ppbv).

The cavity can further comprise one or more windows through which the electromagnetic radiation is inputted into the cavity and through which the electromagnetic radiation exits the cavity after a last pass of the electromagnetic radiation through the sample, the detector positioned to receive the electromagnetic radiation after the last pass.

The smart phone case further comprise a first wing storing the smart phone; a second wing storing the portable spectrometer; and a hinge connecting the first wing to the second wing, wherein the hinge folds the smart phone case so that the second wing is superposed on the first wing when the smart phone case is closed. The first wing can have substantially a same surface area as the smart phone and the second wing has substantially a same size as the portable spectrometer. When the smart phone case is closed, the smart phone case can have a length of 30 centimeters (cm) or 15 cm or less, a width of 30 cm or 15 cm or less, and a thickness of 4 cm or less.

The second wing can comprise a first opening or attachment for holding the cavity, a second opening or attachment for holding the source, a third opening or attachment for holding the detector, and one or more additional openings through which the laser beam is transmitted to the cavity from the source and from the cavity to the detector.

The portable spectrometer can further comprise an optical interfacing system, wherein the optical interfacing system guides the electromagnetic radiation into the cavity at an appropriate angle to achieve a desired number of the multiple passes, guides the electromagnetic radiation after the number of passes onto the detector, and is stored in the smart phone case.

The spectrometer can further comprise support electronics for the detector and support electronics for the laser.

The cavity and/or case assemblies can comprise or consist essentially of bulk metallic glass or bulk metallic glass matrix composite.

One or more embodiments of the invention further disclose a method of fabricating a smart phone case, comprising molding a material (e.g., bulk metallic glass or bulk metallic glass composite) into a smart phone case wherein the smart phone case is capable of holding the smart phone and the portable spectrometer such that the portable spectrometer can operate and perform a spectral analysis of the sample. For example, the molding can comprise molding the smart phone case wherein the cavity comprises a molded surface of the smart phone case and the electromagnetic radiation is reflected from the molded surface to form the multiple passes of the electromagnetic radiation through the sample during operation of the spectrometer.

One or more embodiments of the invention further disclose an article of manufacture or spectrometer comprising a ring cavity, the ring/ring cavity comprising a reflective inner surface described by the equation:

$$\frac{x^2+y^2}{a^2}+\frac{z^2}{c^2}=1,$$

wherein x, y, and z are Cartesian coordinates, a is an equatorial radius comprising a maximum value of x and y, c is a distance along the z- axis from coordinate (x=0, y=0, z=0) to a pole of the spheroid described by the equation, and $a \neq c$. One or more openings are cut in the inner surface for one or more windows. A laser beam incident on the elliptical inner surface through the one or more windows is reflected from multiple regions of the reflective inner surface such that multiple passes of the laser beam through a sample surrounded by the elliptical inner surface are formed, and detection of the laser beam reflected from the multiple regions and received on a detector through the one or more windows can be used to identify the sample.

## BRIEF DESCRIPTION OF THE DRAWINGS

Referring now to the drawings in which like reference numbers represent corresponding parts throughout:

FIG. **1** shows a high resolution absorption spectrum of 10 parts per million (ppm) Freon-125, wherein the solid red line is the absorption spectrum measured using the External Cavity Quantum Cascade Laser (EC-QCL) and a Herriott cell configured for a path length of 47 m and the dashed blue line is a reference absorption spectrum obtained from the spectral library;

FIG. **2** illustrates a laser intensity model for three dimensional injection into a Laser Spider Web Sensor (LSS) according to one or more embodiments of the invention, wherein, for this configuration, the radius of curvature of the interior surface is greater than the internal diameter of the ring, generating an elliptical surface enabling a greater path length than a planar ring pattern (the intensity pattern is calculated using Tracepro™ optical ray trace software);

FIG. **3** illustrates a ray trace illustrating a specific condition for a 2 degree injection angle of a laser beam into a spherical ring according to one or more embodiments of the invention, wherein the number of round trips inside the spherical ring can be varied by changing the laser beam injection angle;

FIG. **4** illustrates an ultralight four channel system developed for chemical detection and according to one or more embodiments of the invention, comprising aluminum rings coated with gold on chrome and encased in a carbon fiber shell;

FIG. **5** is a flowchart illustrating a method of fabricating a ring cavity and absorption cell according to one or more embodiments of the invention;

FIGS. **6**A-**6**F illustrate a laser ring spectrometer geometry, according to one or more embodiments of the invention, wherein FIG. **6**A illustrates a first side view, FIG. **6**B illustrates a second side view, FIG. **6**C illustrates a top view, FIG. **6**D and FIG. **6**E illustrate perspective views, FIG. **6**F shows a magnified view of a section of the ring;

FIG. **6**G shows a Tracepro™ optical analysis of the fabricated ring illustrated in FIGS. **6**A-**6**F, according to one or more embodiments of the invention;

FIG. **6**H illustrates a computer screenshot showing profile, positioning, power, and radius of the laser beam (units in mm) used for the Tracepro™ analysis in FIG. **6**G, according to one or more embodiments of the invention;

FIGS. **6**I-**6**M illustrate a laser ring spectrometer geometry designed for spaceflight, according to one or more embodiments of the invention, wherein FIG. **6**I illustrates a first side view, FIG. **6**J illustrates a second side view, FIG. **6**K illustrates a top view, FIG. **6**L illustrates a perspective view, and FIG. **6**M shows a magnified view of a section of the ring;

FIG. **7**A illustrates an LSS assembly for testing of chemical detection signal levels in the Jet Propulsion Laboratory (JPL) Optical Metrology Laboratory, and FIG. **7**B illustrates the assembled LSS, according to one or more embodiments of the invention;

FIG. **8** illustrates specifications for a 6 inch Spherical Super Cell, according to one or more embodiments of the invention;

FIG. **9** illustrates an architecture for the LSS comprising a smart phone, wherein the showing a configuration wherein the LSS is integrated into a Modified PicoP projector according to one or more embodiments of the invention;

FIGS. **10**A and **10**B illustrate a smart phone architecture for the LSS including a case for housing the smart phone and the LSS, according to one or more embodiments of the invention;

FIG. **11** is an exemplary hardware and software environment used to implement one or more embodiments of the invention;

FIG. **12** schematically illustrates a typical distributed/cloud-based computer system using a network to connect client computers to server computers, according to one or more embodiments of the invention;

FIG. **13** is a flowchart illustrating a method of processing a signal according to one or more embodiments of the invention;

FIG. **14** illustrates a method of molding a smart phone case according to one or more embodiments of the invention;

FIG. **15** illustrates a method of molding the ring cavity and/or spectrometer case using bulk metallic glass, according to one or more embodiments of the invention; and

FIG. **16** illustrates a toroidal mold that can be used to mold a BMG ring cavity according to one or more embodiments of the invention.

## DETAILED DESCRIPTION OF THE INVENTION

In the following description of the preferred embodiment, reference is made to the accompanying drawings which form a part hereof, and in which is shown by way of illustration a specific embodiment in which the invention may be practiced. It is to be understood that other embodiments may be utilized and structural changes may be made without departing from the scope of the present invention.

Technical Description

Introduction Current state of the art systems using Gas Chromatography—Mass Spectrometry (GC/MS), Surface Acoustic Wave (SAW) sensors, Ion Mobility Spectrometers (IMS), Laser Induced Fluorescence (LIF), and other systems, are large, use consumables, and require large quantities of power. Laser spectrometers offer a tremendous improvement over the current state of the art chemical detection systems in that they can be configured in an open path system that does not require inlet systems and pumps to introduce the sample to be analyzed into the spectrometer. Extensive work with the infrared spectral libraries funded by the National Nuclear Security Administration (NNSA), Defense Advanced Research Projects Agency (DARPA), and other government agencies enables direct comparison with the library data in real time to enable extremely high confidence detection of analytes.

In one or more embodiments, a laser spectrometer comprises a laser electromagnetically coupled to a cavity comprising a gaseous chemical sample or analyte, wherein the laser beam emitted from the laser has a frequency resonant with one or more known vibrational modes or one or more known absorption frequencies of one or more known chemical elements or compounds. A detector is electromagnetically coupled to the cavity to measure the laser beam after the laser beam has interacted with the sample. If the detector measures absorption corresponding to the known absorption frequency of the known compound, then the sample can be identified.

Recent advancements in laser spectrometers enable these systems to be implemented for facile detection of chemicals. Specifically, research for the NNSA has demonstrated the feasibility of detection of chemical weapons agents via that of simulants (Freons) with similar spectroscopic features [2]. This has been achieved using Freon-125 as a simulant, a tunable laser, and a Herriott cell-based sensor based on flight proven designs developed at the Jet Propulsion Laboratory (JPL) for use in earth and planetary exploration.

The experimentally obtained spectrum of this simulant shown in FIG. **1** matches that found in the spectral library extremely well, demonstrating the ability of this technique to detect the exact shape of the spectral feature, which in turn indicates the ability to recognize the simulant even in the presence of significant interference. It has also been demonstrated that the detected features of a typical interferent, namely water, are so different in shape and width as compared to the simulant, that they are easily recognized and separated from such a measurement.

Judging from the signal-to-noise ratio (SNR) of the experimental data obtained, the noise equivalent absorption sensitivity is estimated to be $0.5\times10^{-7}$ to $1\times10^{-6}$ $cm^{-1}$. For the particular feature of the simulant examined in this work, this corresponds to a relative concentration of 50 to 25 parts-per-billion by volume (ppbv). For applications requiring higher sensitivity, longer path lengths can be obtained using advanced spherical ring optical cavity designs. The corresponding relative concentrations of other chemical targets would differ depending on the particular transition strengths, and would thus have to be scaled accordingly. Targets of specific interest are $CO_2$, CO, $H_2O$, $CH_4$, $N_2O$ and $O_2$.

The first set is under observation for its role in global warming and its contribution to the greenhouse effect. Having a global network of portable detectors can yield invaluable information about the bulk movement and presence of greenhouse gases through observation of their localized behavior. Currently NASA's Orbiting Carbon Observatory (OCO-2) is taking similar measurements but from the vantage point of space. For this project, ground based data would be invaluable for validation.

In addition, detection of $O_2$ (and other other compounds and elements) is important when monitoring healthy working conditions. Low levels of $O_2$ in a room decrease productivity levels and create a health hazard. Having portable monitors that can take precision measurements of both fluctuations and relative amounts of $O_2$, $CO_2$, CO and $H_2O$ levels in a building would allow for a safer and more comfortable work place.

Cavity Design

FIG. **2** illustrates a spectrometer according to one or more embodiments of the invention including a cavity **200** (e.g., into which a gaseous chemical sample or analyte is placed), one or more windows **202** in the cavity; a laser **206** electromagnetically coupled to the cavity **200**; a detector **208** electromagnetically coupled to the cavity; and one or more processors **210** connected to the detector **210**. A laser beam **212** (e.g., emitting infrared or terahertz electromagnetic radiation), outputted from the laser **206** and incident on the inner surface **204** through the one or more windows **202**, is reflected from multiple regions of the inner surface **204** such that multiple passes of the laser beam **214** through a sample in the cavity are formed. The detector **208** (e.g., InGaAs detector) outputs a signal in response to detecting the laser beam **216** reflected from the multiple regions and received on the detector **208** through the one or more windows **202**. The detector can be positioned to receive the electromagnetic radiation **216** after the last pass.

The laser beam **212** has a frequency resonant with one or more known vibrational modes or one or more known absorption frequencies of one or more known chemical elements or compounds. If the detector **208** measures absorption corresponding to the known absorption frequency of the known compound, then the sample can be identified. Thus, one or more processors connected to the detector can process the signal (by comparing the absorption of the sample to the absorption of a known compound) to form an output identifying the sample.

The laser can comprise a broadly tunable laser, e.g., quantum cascade laser, that can be tuned to emit electromagnetic radiation over a wavenumber range up to 65 $cm^{-1}$ or up to 100 $cm^{-1}$ from a center frequency corresponding to a wavelength in a range of 1 micrometer to 20 micrometers. The quantum cascade laser can use a grating to tune the frequency. The inner surface can comprise a mirror reflective surface (e.g., including a coating or optical coating, such as a gold coating) that can reflect over this frequency range.

In one or more embodiments of the invention, the resonate laser traces in the cavity form a web of coherent light ensuring complete sampling of the air in the target volume, and/or the multipass ring cell maps a linear cavity into a ring or circular cavity. As is the case with traditional Herriott cells, the inner surface comprising mirror surface in one or more examples can be entirely spherical or astigmatic, which produces dense Lissajous-type patterns that enable large path lengths. Like stable Herriott designs, the ring multipass cell according to one or more embodiments of the invention is self-imaging and constantly re-focuses the propagating beam as it reflects from surface to surface within the cavity.

FIG. **2** further illustrates an example of a ring cell with elliptical surfaces **204**. For this configuration the radius of curvature of the interior surface **204** is greater than the internal diameter of the ring. This generates an elliptical surface **204** enabling a greater path length than a planar ring pattern (illustrated in FIG. **3**) [13]. Specifically, FIG. **2** illustrates the inner/interior surface **204** of the cavity **200** comprising an elliptical surface of revolution about an axis **218** (e.g., wherein the generatrix is an ellipse or portion of an ellipse rotated 360 degrees about the central axis **218** passing through a center of the cavity). In this way, the surface of revolution can comprise a section of a spheroid/truncated spheroid/ellipsoid of revolution that can be bisected into two equal parts by a bisecting plane comprising one of the two semi-diameters of the spheroid.

In one or more embodiments of the invention, the inner/interior surface can be described by the equation:

$$\frac{x^2+y^2}{a^2}+\frac{z^2}{c^2}=1,$$

wherein x, y, and z are Cartesian coordinates in a Cartesian coordinate system having x, y, and z axes, a is a real number representing the equatorial radius (a maximum value of x and y), c is a real number representing a distance along the z-axis from coordinate (x=0, y=0, z=0) to a pole of the spheroid described by the equation, and $a \neq c$. In one or more embodiments, $z<c$, z is in a range of 2 mm-20 mm, and/or a is in a range of 2 mm-60 mm.

The cavity height (h) can be made quite thin (<10 mm) to allow for modular units for different wavelengths of interest, and the shallow cell depth can avoid wall effects sometimes encountered with cells of the linear configuration.

The angle at which the laser beam **212** is inputted into the cavity (e.g., the angle with respect to the input surface of the window **202**), the angle of incidence of the electromagnetic radiation on the inner surface **204** (at first and/or subsequent reflections within the cavity), and the angle θ between an incident beam and the subsequently reflected beam, can be selected to obtain a desired number of passes through the cavity. Together with the angle of incidence, a, and z can also be selected such that the spectrometer can identify the sample having a relative concentration in the cavity of 50 parts-per-billion by volume (ppbv) and/or such that a total path length of the electromagnetic radiation transmitted through the sample includes a specified minimum distance (e.g., 4 meters, 30 meters). For example, the angle of incidence of the electromagnetic radiation, at a first reflection within the cavity, can be between more than 0 degrees and 45 degrees, a can be less than 60 mm, and z can be less than 20 mm, such that a total path length of the electromagnetic radiation transmitted through the sample includes a distance of 4 meters or 30 meters.

The colors or shading of the beams **214** in FIG. **2** (and FIG. **3**) show how the intensity of the laser beam is attenuated as it is reflected by the inner surface **204** and as the number of passes/reflections **214** through the cavity is increased. At the input, the laser beam **212** has more than 90% of the initial intensity (at the laser output). At the output, the laser beam **216** has more than 20% of the initial intensity (calculated for an inner surface **204** comprising a gold surface coated for an infrared laser beam **206**, a ZnSe window **202**, a cavity **200** having an inner diameter of 2a=60 mm, and an angle θ wherein the laser makes ~69 passes through the cell before exiting the cell, corresponding to a ~4.2 meter (m) path length of the laser beam through the cavity **200**). In FIG. **3**, the ray trace analysis is for an inner surface comprising a gold surface coated for an infrared (IR) beam, a ZnSe window, and a cavity having an inner diameter of 50 mm, and the ray trace analysis shows the laser beam inputted into the cavity makes ~37 passes through the cell before exiting the cell (corresponding to a ~1.85 m path length of the laser beam through the cavity).

Stacking multiple rings allows tailoring the detection suite of chemicals to meet the given application. Using interchangeable modular designs it is possible to tailor the detection system to cover a broad range of chemicals important to global climate change or other applications. FIG. **4** is a modular multichannel system in which four rings **400** (theoretically operating four different wavelengths) are stacked together in order to detect multiple gas species as the airflow passes through.

Manufacturing and Assembly Procedure

FIG. **5** illustrates a method of fabricating the ring cavity **600** (illustrated in FIGS. **6A**-**6F**) and calibration cell **700** (illustrated in FIGS. **7A**-**7B**), according to one or more embodiments of the invention.

Block **500** represents obtaining a 6061 Aluminum metal cylinder. However other metal or materials could be used.

Block **502** represents rough machining the ring reflecting surface **602** with a 5 axis computer numerical control (CNC) mill, wherein the rough cut should leave a maximum of 0.005" of material in excess of the final dimensions. However, in one or more embodiments, a different maximum of material in excess of the final dimensions could be used.

Block **504** represents machining all additional body features including mounting holes **604**, **606**, and window hole **608**, etc., with the exception of the final ring surface **602** and the knife edges **610**.

Block **506** represents diamond turning the inner surface/final ring surface **602** and knife edges **610** (e.g., at NiProOptics™).

Block **508** represents applying (e.g., at NiProOptics) a gold surface coating across the inner face/final ring surface **602** of the ring **600**. The surface can be shaped according to the elliptical surface **204** illustrated in FIG. **2** (or surface in FIG. **3**), for example. The rings can be used as the rings **400** in FIG. **4**.

FIG. **6G** shows a Tracepro™ optical analysis of the fabricated ring, showing intensity X as a percentage of the input intensity of the laser beam, and as a function of reflections in the cavity. In FIG. **6G**, the laser beam makes **218** bounces between input and output from the cavity, corresponding to a path length of 33.22 meters, and the output intensity of the laser beam outputted from the cavity is 5% of the input intensity. For the Tracepro™ analysis of FIG. **6G**, the window **616** is a ZnSe window, the inner surface of the ring has an IR gold coating, the laser is aligned such that an input angle of the laser beam **618** is 4 degrees with respect to the surface normal of the window, and the laser's output is positioned at a coordinate (−711.2 mm, 0, 20) where the origin is taken as the center of the ring (the distance of 711.2 mm or 28" is the value used for characterization of the cell in the lab), as shown in the screenshot of FIG. **6**H. The window **616** in the cavity **600** is a window through which electromagnetic radiation **618** (or **212**) can be inputted into the cavity **600** and through which electromagnetic radiation exits the cavity after a last pass of the electromagnetic radiation through the cavity (or through a sample if the cavity contains a sample).

For the embodiment illustrated in FIGS. **6**A-F the calculated volume enclosed by the inner surface **602** of the cavity **600** is 789,855.56 $mm^3$ (according to Solidworks™), the ring **600** has a 6" inner diameter ID, a ~9.84" Outer Diameter (250 mm), ¾" flange through hole **604** diameter (×8), #10-32 tapped holes **606** for the window (×6), a 16 mm diameter, 20 mm deep window extrusion **608**, an O-ring groove **716** for AS568A-011, and 40 mm cell height h.

FIGS. **6**I-**6**M illustrate an embodiment of the ring that can be used in spaceflight, wherein the calculated volume enclosed by the inner surface **602** of the cavity **600** is 175,188.42 $mm^3$ (according to Solidworks™), the ring **600** has a 6" inner diameter ID, a ~7.086" Outer Diameter (180 mm), ¼-20" flange through hole **604** diameter (×8), #10-32 tapped holes **606** for the window (×4), a knife edge for a copper gasket, a cell lip over the inner diameter, a 16 mm diameter, 11 mm deep window extrusion **608**, and 22 mm cell height h.

Block **510** represents further assembly. The step can include adding in all threaded inserts, assembling the calibration cell assembly (as illustrated in FIG. **7**A) to obtain an assembled calibration cell **700** (as illustrated in FIG. **7**B), and aligning all components (e.g., laser and detector). FIGS. **7**A-**7**B illustrate a gas frequency reference cell comprising non-spherical ring **600**, non-spherical face plate **702**, non-spherical outer disk **704**, window **706** with antireflective AR coating, bolts **708** for insertion in holes **604**, bolts **710** for insertion in holes **606**, washers **712**, hex nuts **714** for fastening bolts **708**, O-ring groove **716**, and gasket **718**. The cell can further comprise flanges. In one or more embodiments, a metrology laser system uses an acetylene gas frequency reference cell, wherein the all-metal non-spherical ring cavity **600** and cell **700** contain acetylene gas (e.g., for airborne applications).

Extra care must be taken with the inner surface **602** of the ring **600** to protect from scratching and contamination. The critical surfaces are the inner reflecting surface **602** and whatever surface the optics are mounted to. Secondarily, the laser injection hole **608** as well as top face **612** and bottom face **614**, are critical because they must be sealed to prevent gas leakage.

The cell **700** can further comprise one or more sealable openings for inputting an analyte or sample into the cavity.

In one or more embodiments, the cavity has a height h in a range of 2 mm-20 mm, a width of 2 mm-60 mm, and a length of 2 mm-60 mm, and/or the cavity is dimensioned such that a volume of the cavity comprising the sample is between 33 $mm^3$ and 905000 $mm^3$. However, the dimensions can be scaled up or down. The ring **600** can have a height h as small as the laser beam (e.g., half a millimeter).

Different shapes for the inner surface and ring can be used. FIG. **8** illustrates an example comprising a 6 inch Spherical Super Cell.

The cavity or ring **600** can be fabricated from other materials such as pyrex or bulk metallic glass [8]. The cavity or ring can comprise or consist essentially of bulk metallic glass (BMG) or bulk metallic glass matrix composite (BMGMC). The inner reflecting surface **204**, **602** can consist essentially of the BMG or BMGC or an optical coating can be applied to the BMG or BMGC surface. The BMG or BMGC ring or cavity can be fabricated by injection molding or casting, for example.

Laser Spider Web Sensor (LSS) Coupled to Portable Device

A portable laser system for use as a projector with iPhones or laptop computers can be used with a laser sensor according to one or more embodiments of the invention. The Microvision SHOWWX™ Laser Pico Projector (LPP) is an ideal platform for integration with the LSS.

In one or more embodiments, the laser intensity model for injection into the LSS coupled to the iPhone is that shown in FIG. **2** (wherein the intensity pattern is calculated using Tracepro optical ray trace software). However, the model of FIG. **3** could also be used. In one or more embodiments, the laser ring spectrometer geometry shown in FIG. **6**A-**6**E can be designed to fit into Microvision© Laser Picoprojector (LPP) architecture for interface to mobile devices.

The LPP can be modified to connect directly to a portable device or smart phone. FIG. **9** shows an apparatus/package **900** comprising a modified pico projector **902** (e.g., modified picoP projector), wherein the modified pico projector **902** condenses a detector (e.g., diode detector such as Vigo model PV-4TE-10.6) **1**, one or more lasers **2** (e.g., three lasers such as quantum cascade lasers, QCLs such as Alpes Lasers, models sbcw5701, sbcw2922 (1280.3 $cm^{-1}$), sbcw3055 (2205.4 $cm^{-1}$), and (1043.9 $cm^{-1}$), supporting optics bus **4**, a laser controller, external interface (e.g., for communicating with the smart phone **904**), and power source, into a handheld package **902**. Thus, the modified picoprojector can comprise components **1**, **2**, **4**, laser controller, external interface, and power source. The package **902** can further comprise the lasers (e.g., QCL) wired into the PicoP projector's amplifier and supporting electronics for the diode detector. The apparatus **900** further comprises ring cavity/multipass cell **906** (e.g., ring cavity **600**) and LSS integration fixture **3** for attaching/coupling/mechanically interfacing the ring cavity/multipass cell **906** to the modified Pico projector **900**.

In one or more embodiments, the cavity or ring **906** can further comprise top and bottom plates or attachments to sealably enclose the sample or analyte in the ring cavity **906**/**600**. Moreover, the plates or attachments can further comprise one or more sealable openings for inputting the analyte or sample into the cavity **600**/**906**. However, the ring **906** can be open on the top and/or bottom as illustrated in FIG. **9** to allow the ambient atmosphere to enter into the ring cavity **600**/**906** comprising the laser beam **908** for analysis.

The optics bus **4** can comprise an optical interfacing system (e.g. deformable mirror system) that injects or guides the laser beam **910** generated by laser **2** into the ring cavity at the appropriate angle to achieve the desired number of passes of the laser beam **908** in the cavity/multipass cell **600**/**906**. Optical bus **4** can further guide the laser beam **910** that exits the ring cavity **600**/**906**, after multiple passes through the cell **600**/**906**, into the detector **1**.

In one or more embodiments, the apparatus **900** has a height (H): 14 mm (0.55 in); width (W): 60 mm (2.36 in); length (L): 118 mm (4.64 in); weight: 122 g (4.3 oz); power: 400 mA 12 3.7 V (1.5 Watts); and battery life: 10 hours (e.g,. using Tekkeon MP1800 (4000 mAh 12 3.7V)).

The assembly/apparatus **900** can also be connected (e.g., via a wire **912** or wirelessly) to a smart phone **904**. For example, the package **902** can comprise a Universal Serial Bus (USB) connection for connecting to the phone **904** or an antenna and supporting electronics for connecting to the phone **904** wirelessly (e.g., via WIFI or bluetooth or radio waves). In this way, absorption data (measured by the detector for the laser beam **908** transmitted through the sample in the cavity **600,906**) can be transmitted/communicated to the smart phone **904** for spectral analysis and identification of the sample.

FIGS. **10A-10B** illustrate a handheld detection system **1000** incorporating the apparatus **900** into a case like device **1002** which has the ability to house the phone **904** as well as the spectrometer system/apparatus **900**. As shown in FIGS. **10A-10B**, this system **1002** is only slightly larger than a smart phone **904** when closed (as shown in FIG. **10B**) and is the size of a small book when opened (as shown in FIG. **10A**) and in use. In this regard, the smart phone case **1002** comprises a first wing/section **1004** storing the smart phone **904**; a second wing/section **1006** storing the portable spectrometer (package **902** and cavity **600/906**); and a hinge or folding mechanism **1008** connecting the first wing **1004** to the second wing **1006**, wherein the hinge/folding mechanism **1008** folds the smart phone case **1002** so that the second wing **1006** is superposed on the first wing **1004** when the smart phone case **1002** is closed.

FIG. **10B** shows the case **1002** comprises an opening **1010** comprising the ring cavity **906/200** or housing/structure for holding/securing the ring cavity **906/200/600**, an opening **1012** for housing the detector **1** and detector electronics, and an opening **1014** for housing the laser **2** and laser electronics.

Further openings for optical bus **4** and other interfacing electronics can also be provided in the case **1002**. For example, the second wing/section **1006** can comprise a first opening **1010**, hole, part, or attachment for holding the cavity **600/906**, a second opening **1014**, hole, part, or attachment for holding the source of electromagnetic radiation (e.g., laser **2** and laser controller), a third opening **1012**, hole, part, or attachment for holding the detector **1** and supporting electronics, one or more additional openings through which the laser beam is transmitted to the cavity from the source and from the cavity to the detector, and one or more openings, parts or attachments for storing/holding an optical interfacing system **4**, wherein the optical interfacing system guides the electromagnetic radiation into the cavity at an appropriate angle to achieve a desired number of the multiple passes, and guides the electromagnetic radiation after the number of passes onto the detector.

In one or more embodiments, the first wing has substantially a same surface area as the smart phone and the second wing has substantially a same size as the portable spectrometer. For example, when the smart phone case is closed, the smart phone case can have a length of 30 cm or less or 15 cm or less, a width of 30 cm or less or 15 cm or less, and a thickness of 4 cm or less. In one or more embodiments, the smart phone case is dimensioned such that a total volume occupied by the smart phone case including the phone and the portable spectrometer (package **902** and cavity **906**) is no more than 15% larger than a volume occupied by the smart phone.

In one or more embodiments, the smart phone case can be fabricated from plastic, metal, BMG, or BMG composite, for example. In one or more embodiments, the ring and cell phone case assemblies are manufactured out of BMG or BMGMC by a molding process wherein the ring cavity is formed into the case **1002** (i.e., the cavity comprises a surface of the case **1002** shaped or molded to form a ring cavity including an inner reflecting surface **1016** (e.g., a molded surface shaped as surface **204** illustrated in FIG. **2**) that reflects the electromagnetic radiation/laser beam **214** (e.g., as in FIG. **2**) such that the electromagnetic radiation makes/forms multiple passes through the sample). In this way the ring cavity can be an integral part of the case **1002**. Moreover, openings **1012**, **1014**, hinge **1008**, and other housings for the support electronics, smart phone **904**, and optics bus **4**, as discussed above, can also be formed during the same molding process.

The handheld detection system design accounts for major system needs but specifics of each subsystem can also be implemented. In one or more embodiments, the system/apparatus **900/1000** can tailor the laser and optics subsystems for the specific detection of $CO_2$ or to fabricate a spectrometer allowing real-time analysis with unprecedented sensitivity for multiple target species enabling real time in situ validation for the OCO. The portable form factor makes the apparatus ideal for support of human space flight, the monitoring of crew cabin conditions, and for use in future planetary exploration missions, or medical applications, for example.

Hardware Environment

FIG. **11** is an exemplary hardware and software environment **1100** used to implement one or more embodiments of the invention. The hardware and software environment includes a computer **1102** and may include peripherals. Computer **1102** may be a user/client computer, server computer, or may be a database computer. The computer **1102** comprises a general purpose hardware processor **1104A** and/or a special purpose hardware processor **1104B** (hereinafter alternatively collectively referred to as processor **1104**) and a memory **1106**, such as random access memory (RAM). The computer **1102** may be coupled to, and/or integrated with, other devices, including input/output (I/O) devices such as a keyboard **1114**, a cursor control device **1116** (e.g., a mouse, a pointing device, pen and tablet, touch screen, multi-touch device, etc.) and a printer **1128**. In one or more embodiments, computer **1102** may be coupled to, or may comprise, a portable or media viewing/listening device **1132** (e.g., an MP3 player, IPOD, NOOK, portable digital video player, cellular device, personal digital assistant, etc.). In yet another embodiment, the computer **1102** may comprise a multi-touch device, mobile phone, gaming system, internet enabled television, television set top box, or other internet enabled device executing on various platforms and operating systems.

In one embodiment, the computer **1102** operates by the general purpose processor **1104A** performing instructions defined by the computer program **1110** under control of an operating system **1108**. The computer program **1110** and/or the operating system **1108** may be stored in the memory **1106** and may interface with the user and/or other devices to accept input and commands and, based on such input and commands and the instructions defined by the computer program **1110** and operating system **1108**, to provide output and results.

Output/results may be presented on the display **1122** or provided to another device for presentation or further processing or action. In one embodiment, the display **1122** comprises a liquid crystal display (LCD) having a plurality of separately addressable liquid crystals. Alternatively, the display **1122** may comprise a light emitting diode (LED) display having clusters of red, green and blue diodes driven together to form full-color pixels. Each liquid crystal or pixel of the display **1122** changes to an opaque or translucent state to form a part of the image on the display in response to the data or information generated by the processor **1104** from the application of the instructions of the computer program **1110** and/or operating system **1108** to the input and commands. The image may be provided through a graphical user interface (GUI) module **1118**. Although the GUI module **1118** is depicted as a separate module, the instructions performing the GUI functions can be resident or distributed in the operating system **1108**, the computer program **1110**, or implemented with special purpose memory and processors.

In one or more embodiments, the display **1122** is integrated with/into the computer **1102** and comprises a multi-touch device having a touch sensing surface (e.g., track pod or touch screen) with the ability to recognize the presence of two or more points of contact with the surface. Examples of multi-touch devices include mobile devices (e.g., IPHONE, NEXUS S, DROID devices, etc.), tablet computers (e.g., IPAD, HP TOUCHPAD), portable/handheld game/music/video player/console devices (e.g., IPOD TOUCH, MP3 players, NINTENDO 3DS, PLAYSTATION PORTABLE, etc.), touch tables, and walls (e.g., where an image is projected through acrylic and/or glass, and the image is then backlit with LEDs).

Some or all of the operations performed by the computer **1102** according to the computer program **1110** instructions may be implemented in a special purpose processor **1104**B. In this embodiment, the some or all of the computer program **1110** instructions may be implemented via firmware instructions stored in a read only memory (ROM), a programmable read only memory (PROM) or flash memory within the special purpose processor **1104**B or in memory **1106**. The special purpose processor **1104**B may also be hardwired through circuit design to perform some or all of the operations to implement the present invention. Further, the special purpose processor **1104**B may be a hybrid processor, which includes dedicated circuitry for performing a subset of functions, and other circuits for performing more general functions such as responding to computer program **1110** instructions. In one embodiment, the special purpose processor **1104**B is an application specific integrated circuit (ASIC).

The computer **1102** may also implement a compiler **1112** that allows an application or computer program **1110** written in a programming language such as C, C++, Assembly, SQL, PYTHON, PROLOG, MATLAB, RUBY, RAILS, HASKELL, or other language to be translated into processor **1104** readable code. Alternatively, the compiler **1112** may be an interpreter that executes instructions/source code directly, translates source code into an intermediate representation that is executed, or that executes stored precompiled code. Such source code may be written in a variety of programming languages such as JAVA, JAVASCRIPT, PERL, BASIC, etc. After completion, the application or computer program **1110** accesses and manipulates data accepted from I/O devices and stored in the memory **1106** of the computer **1102** using the relationships and logic that were generated using the compiler **1112**.

The computer **1102** also optionally comprises an external communication device such as a modem, satellite link, Ethernet card, or other device for accepting input from, and providing output to, other computers **1102**.

In one embodiment, instructions implementing the operating system **1108**, the computer program **1110**, and the compiler **1112** are tangibly embodied in a non-transitory computer-readable medium, e.g., data storage device **1120**, which could include one or more fixed or removable data storage devices, such as a zip drive, floppy disc drive **1124**, hard drive, CD-ROM drive, tape drive, etc. Further, the operating system **1108** and the computer program **1110** are comprised of computer program **1110** instructions which, when accessed, read and executed by the computer **1102**, cause the computer **1102** to perform the steps necessary to implement and/or use the present invention or to load the program of instructions into a memory **1106**, thus creating a special purpose data structure causing the computer **1102** to operate as a specially programmed computer executing the method steps described herein (e.g., the spectral analysis of the absorption spectrum measured by the portable spectrometer **1130**). Computer program **1110** and/or operating instructions may also be tangibly embodied in memory **1106** and/or portable spectrometer **1130**, thereby making a computer program product or article of manufacture according to the invention. As such, the terms "article of manufacture," "program storage device," and "computer program product," as used herein, are intended to encompass a computer program accessible from any computer readable device or media.

The computer **1102** can be stored in a smart phone case **1002** or computer case/enclosure and connected to the portable spectrometer **1130** (e.g., as illustrated in FIGS. **2** and **10A-10B**). In one or more embodiments, the portable spectrometer **1130** includes a cavity **600** into which a sample is placed; a source (e.g., including laser **2**, laser controller/support electronics (e.g., for the laser), and/or optics bus **4**) for emitting electromagnetic radiation that is directed on the sample in the cavity **600**, wherein the electromagnetic radiation is reflected within the cavity **600** to form multiple passes of the electromagnetic radiation through the sample; a detector (e.g,. detector **1** and/or support electronics (e.g,. for the detector)) for detecting the electromagnetic radiation after the electromagnetic radiation has interacted with the sample in the cavity, the detector outputting a signal/data stream in response to the detecting; and a device **1202** for (e.g., digitally) communicating the (e.g,. digital) signal/data stream to a smart phone or computer **1102**, wherein the smart phone/computer **1102** executes an application or program **1110** that performs a spectral analysis of the signal. In one or more embodiments, the portable spectrometer **1130** comprises the computer **1130** or the computer **1130** is integrated into the portable spectrometer **1130** as one or more processors or chips configured to perform one or more functions (e.g., spectral analysis of the absorption spectrum, wirelessly transmit the data from the detector **1** to another computer). The computer case or smart phone case can store the portable spectrometer **1130**.

Of course, those skilled in the art will recognize that any combination of the above components, or any number of different components, peripherals, and other devices, may be used with the computer **1102**.

FIG. **12** schematically illustrates a typical distributed/cloud-based computer system **1200** using a network **1204** to connect client computers **1202** to server computers **1206**. A typical combination of resources may include a network **1204** comprising the Internet, LANs (local area networks), WANs (wide area networks), SNA (systems network architecture) networks, or the like, clients **1202** that are personal computers or workstations (as set forth in FIG. **11**), and servers **1206** that are personal computers, workstations, minicomputers, or mainframes (as set forth in FIG. **11**). However, it may be noted that different networks such as a cellular network (e.g., GSM [global system for mobile communications] or otherwise), a satellite based network, or any other type of network may be used to connect clients **1202** and servers **1206** in accordance with embodiments of the invention.

A network **1204** such as the Internet connects clients **1202** to server computers **1206**. Network **1204** may utilize ethernet, coaxial cable, wireless communications, radio frequency (RF), etc. to connect and provide the communication between clients **1202** and servers **1206**. Further, in a cloud-based computing system, resources (e.g., storage, processors, applications, memory, infrastructure, etc.) in clients **1202** and server computers **1206** may be shared by clients **1202**, server computers **1206**, and users across one or more networks. Resources may be shared by multiple users and can be dynamically reallocated per demand. In this regard, cloud computing may be referred to as a model for enabling access to a shared pool of configurable computing resources.

Clients **1202** may execute a client application or web browser and communicate with server computers **1206** executing web servers **1210**. Such a web browser is typically a program such as MICROSOFT INTERNET EXPLORER, MOZILLA FIREFOX, OPERA, APPLE SAFARI, GOOGLE CHROME, etc. Further, the software executing on clients **1202** may be downloaded from server computer **1206** to client computers **1202** and installed as a plug-in or ACTIVEX control of a web browser. Accordingly, clients **1202** may utilize ACTIVEX components/component object model (COM) or distributed COM (DCOM) components to provide a user interface on a display of client **1202**. The web server **1210** is typically a program such as MICROSOFT'S INTERNET INFORMATION SERVER.

Web server **1210** may host an Active Server Page (ASP) or Internet Server Application Programming Interface (ISAPI) application **1212**, which may be executing scripts. The scripts invoke objects that execute business logic (referred to as business objects). The business objects then manipulate data in database **1216** through a database management system (DBMS) **1214**. Alternatively, database **1216** may be part of, or connected directly to, client **1202** instead of communicating/obtaining the information from database **1216** across network **1204**. When a developer encapsulates the business functionality into objects, the system may be referred to as a component object model (COM) system. Accordingly, the scripts executing on web server **1210** (and/or application **1212**) invoke COM objects that implement the business logic. Further, server **1206** may utilize MICROSOFT'S TRANSACTION SERVER (MTS) to access required data stored in database **1216** via an interface such as ADO (Active Data Objects), OLE DB (Object Linking and Embedding DataBase), or ODBC (Open DataBase Connectivity).

Generally, these components **1200-1216** all comprise logic and/or data that is embodied in/or retrievable from device, medium, signal, or carrier, e.g., a data storage device, a data communications device, a remote computer or device coupled to the computer via a network or via another data communications device, etc. Moreover, this logic and/or data, when read, executed, and/or interpreted, results in the steps necessary to implement and/or use the present invention being performed.

Although the terms “user computer”, “client computer”, and/or “server computer” are referred to herein, it is understood that such computers **1202** and **1206** may be interchangeable and may further include thin client devices with limited or full processing capabilities, portable devices such as cell phones, notebook computers, pocket computers, multi-touch devices, and/or any other devices with suitable processing, communication, and input/output capability.

Embodiments of the invention are implemented as a software application on a client **1202** or server computer **1206**. Further, as described above, the client **1202** or server computer **1206** may comprise a thin client device or a portable device that has a multi-touch-based display.

Of course, those skilled in the art will recognize that any combination of the above components, or any number of different components, peripherals, and other devices, may be used with computers **1202** and **1206**.

FIG. **13** is a flowchart illustrating a method of processing the signal using the computer **1102**.

Block **1300** represents receiving, in the computer **1102**, the signal/data (e.g., absorption as a function of frequency of the laser beam **908**, **216**) from the detector **208** in the portable spectrometer **1130** of FIG. **2** or FIGS. **9-10**, when the cavity **200**, **600** comprises a sample. One or more processors or chips/devices can be configured and included in the spectrometer to wirelessly transmit the data to a computer **1102**.

Block **1302** represents processing the signal/data to identify the sample. The step can comprise comparing the absorption spectrum of the laser beam **216** with the absorption features of known compounds/species/elements, as illustrated in FIG. **1**. The step can comprise comparing an amount of absorption of the laser beam **216** at a given frequency with an amount of absorption at the given frequency for a known chemical species. If the absorption spectrum or amount of absorption of the laser beam **216** matches that of the known species, the sample in the cavity can be identified by the processor as comprising that known species.

Block **1304** represents outputting, from the computer **1102**, an identification of the sample (e.g., as a graphical output on the display **1122** or using a voice signal, for example).

Molding Process Fabricating The Ring Cavity And/Or Casing

FIG. **14** illustrates a method of fabricating a smart phone/computer case/spectrometer case.

Block **1400** represents molding a material (e.g., plastic, BMG, BMGMC), using the mold, into a smart phone case or computer case wherein the smart phone case/computer case is capable of holding a smart phone/computer and the portable spectrometer. The molding can comprise die casting or injection molding, for example. The mold can include portions/parts capable of molding attachment(s), mount(s), accessories, holes, openings, screw holes, or other features capable of holding the portable spectrometer (including the cavity, the laser, the detector, and power source). The mold can be designed to mold the case **1002** illustrated in FIG. **10**A-**10**B, for example.

Block **1402** represents the end result, a smart phone or portable computer case molded to hold a smart phone or portable computer and portable spectrometer.

The molding of Block **1400** forms the case that holds the portable spectrometer such that the cavity, the source (e.g., laser), and the detector are operably coupled during operation of the spectrometer—i.e., the case holds the cavity and the source such that the electromagnetic radiation emitted and directed from the source is reflected within the cavity to form multiple passes of the electromagnetic radiation through a sample in the cavity. Moreover, the case can hold the detector such that the detector detects the electromagnetic radiation after the multiple passes and outputs a signal that can be spectrally analyzed (by the smart phone or computer) to identify the sample.

In one or more embodiments, the smart phone/computer case can include additional features/components to secure the source, cavity, and detector (e.g., adhesive, screws, etc) during operation of the spectrometer. In one or more embodiments, the computer can comprise a chip/processor/integrated circuit held in the case.

Manufacturing Using Bulk Metallic Glass (BMG) and Bulk Metallic Glass Matrix Composite (BMGMC)

Die-casting BMGs or BMGMCs from a liquid state can be used to fabricate the ring cavity **200/906** and/or smart phone case **1002** (or portable computer case). The technique involves heating the liquid BMG or BMGMC up in a crucible (through radio frequency (RF) heating, resistance heating, oven heating, etc.) and then injecting the liquid into a mold using a shot-sleeve and die under typically tens of tons of force. The high processing temperature of the liquid and the extreme forces used in casting allow for extremely complex molds to be filled using the process. By reducing the flow velocity (to limit turbulence), or by using a counter-gravity casting variant, parts with mirror finishes can be replicated using the processes. This can be done by fabricating a mirror-polished piece of steel or carbide and then die-casting BMGs over the mold at high pressure and low flow velocity. With the correct application of temperature and pressure, a one-step process can be used to fabricate an optical finish. However, an optical coating can also be applied if desired.

FIG. **15** is a flowchart illustrating a method of fabricating a ring cavity and/or portable spectrometer case from BMG or BMGMC materials using die casting or injection molding.

Block **1500** represents obtaining, designing, and/or fabricating a mold. The mold part for molding the ring cavity can comprise a surface that is the negative of the inner reflective surface (e.g., **204** in FIG. **2** or **1016** in FIG. **10**A) of the ring cavity (e.g., **200** in FIG. **2**), so that once removed from the mold, the inner reflective surface **204/1016** has the desired (e.g., elliptical) shape. For example, the mold can comprise a torus, elliptic torus, **1600** or toroidal/doughnut shaped mold having a cross-section that is an ellipse **1602**, as illustrated in FIG. **16**. The torus can be fabricated from steel or carbide, for example, and have a smooth mirror polished outer surface **1604** so that casting of the BMG or BMGMC over the outer surface **1604** of the mold forms an optically finished mirror surface **1016/204** of a BMG/BMGMC ring cavity part. Furthermore, the torus shaped mold having the mirrored outer surface can comprise a multi-component piece so that the mold can also be broken apart or disassembled (e.g., using hydraulics) after the mirror surface **204/1016** is cast, thereby allowing easy removal of the mold from the BMG/BMGMC mirror surface **204/1016** while preventing damage to the mirror surface **204/1016** (the disassembly prevents trapping of the BMG or BMGMC material on the mold).

A mold part can also be designed to mold the BMGMC or BMG to form the case (e.g., **1002** in FIG. **10**A) including attachments, housings, mount(s), accessories, holes, openings (e.g., **1012**, **1014**), screw holes, or other features capable of holding the smart phone and portable spectrometer (including the cavity, the laser, the detector, power source, support electronics, and optics bus), as well as hinge **1008**, as illustrated in FIG. **10**A-**10**B. Thus, the mold can comprise multi-component pieces for molding the mirror surface **204** of the ring cavity as well as mold part(s) for molding the case **1002**.

Block **1502** represents heating a BMG or BMGMC ingot to above the liquidus to form a BMG or BMGMC liquid. The BMG or BMGMC can be heated in a crucible, for example.

Block **1504** represents casting or molding the heated and liquid BMG or BMGMC. The step can comprise injecting the BMG or BMGMC liquid into the mold obtained in Block **1400** (e.g., the multi-component toroidal piece and/or the mold part for the case **1002**) under pressure. The BMG or BMGMC liquid can be injected or cast into the mold using a plunger or other external force (including counter gravity). The step can comprise pressing the heated liquid BMGMC or BMG into the mold from a shot-sleeve, at a die-casting pressure between 0.1-200 tons, at a processing a temperature between 600-1500° C., and at a flow velocity of the liquid into the molds that is laminar. The inlet for injecting or introducing the BMG or BMGMC into the mold can be placed so as to not interfere with the mirror surface. The molds are massive and act as a thermal heat sink for the alloy, which allows vitrification.

Block **1506** represents, after the casting/molding, opening the mold and removing the molded piece comprising the ring cavity **200**, or the case **1002** comprising the ring cavity having inner surface **1016** integrated into the case **1002**. The opening of the mold can comprise disassembling the multi-component torus/toroidal piece to allow easy removal of the mold from the mirror surface **204/1016**, thereby preventing damage to the mirror surface **204/1016**. An injection system can also be used to remove the finished part to reduce damage to the finished part. The torus/toroid/mold can be disassembled such that it can also be reassembled (e.g., using hydraulics) for reuse in another ring cavity casting process.

The end result is a ring cavity and/or smart phone case comprising or consisting essentially of bulk metallic glass or bulk metallic glass matrix composite. In one or more embodiments where the molding monolithically integrates the ring cavity with the smart phone case, the cavity comprises/is defined by a molded surface of the smart phone case (comprising or consisting essentially of BMG/BMG composite) such that the electromagnetic radiation emitted and directed from the laser can be reflected from the molded surface to form the multiple passes of the electromagnetic radiation through the sample in the cavity during operation of the portable spectrometer. Specifically, the molded surface is of sufficient quality such that the signal, outputted by the detector in response to detecting the electromagnetic radiation after the multiple passes reflected from the molded surface, can be spectrally analyzed (by the smart phone or computer) to identify the sample.

Thus, Blocks **1400-1402** and **1500-1506** illustrate how the cavity can be formed to comprise a molded surface of the smart phone case, wherein the electromagnetic radiation can be reflected from the molded surface to form the multiple passes of the electromagnetic radiation through the sample.

Thus, Blocks **1400-1402** and **1500-1506** illustrate molding a material into a smart phone case wherein the smart phone case is capable of holding a smart phone and a portable spectrometer, the portable spectrometer including a cavity; a source for emitting electromagnetic radiation that is directed on the sample in the cavity, wherein the electromagnetic radiation is reflected within the cavity to form multiple passes of the electromagnetic radiation through the sample; and a detector for detecting the electromagnetic radiation after the electromagnetic radiation has made the multiple passes through the sample in the cavity, the detector outputting a signal in response to the detecting and communicating the signal to the smart phone, and the smart phone executing an application that performs a spectral analysis of the signal.

Advantages and Improvements

Diode lasers are a technology that has allowed relatively easy access to the molecular fingerprint region of the infrared spectrum. They are robust monopolar semiconductor laser devices that can be fabricated to operate at specific wavelengths virtually anywhere in the 2- to 20-micron range. The Herriott cell used in these sensors has evolved from designs flown on the U-2 spy plane [3], Unmanned Aerial Vehicle (UAVs) [4], and planetary probes [5]. Light is passed into the cell through a hole in one mirror, which is then bounced multiple times between the mirrors, to finally exit at the same hole through which it entered, but at a complimentary angle. There are several different configurations for Herriott cells depending on the relationship between the curvature of the mirrors and their separation, resulting in different bounce patterns or geometric modes. The chosen mode of the Herriott cells currently in use is the C-3 mode, as this affords stability against lateral movement of the mirrors with respect to one another. Research into alternative configurations for these optical systems has led to a spherical ring design for the absorption cell. Using a spherical ring design enables the facile integration of these systems into common air intake and exhaust systems. Other benefits of this new design allows for higher laser path length per absorption volume ratios, allowing for a greater sensitivity in detection for a given volume. The monolithic nature of the new absorption ring design allows for alignment stability for a wide range of vibrational and thermal changes, making it ideal for handheld and field deployable gas detection.

In particular the integration of the ring design into the exhaust systems of vehicles, trucks, busses, trains, ships, factories, and power plants will allow efficient real time monitoring of green house chemicals. Using either a hard line or wireless interface, data from these detectors can be easily collected and processed to better understand the concentrations, sources and sinks of greenhouse gasses. Aside from the environmental benefits of a multi spectrum trace gas detection system, air quality monitoring in both business and residential buildings could be used to improve the general health of the inhabitants. Spectrometers could be used to monitor $CO_2$, CO, $O_2$ and humidity levels by integrating the spherical ring designs into existing heating, ventilating, and air conditioning (HVAC) systems, the detection capability could be easily installed maintained.

Thus, one or more embodiments of the new technology developed at the Jet Propulsion Laboratory now enables real time in situ measurements of key chemicals important in global climate change including $CO_2$, $N_2O$, $CH_4$, CO, $H_2O$, and many other species of interest. Emergence of mobile smart phone technology presents an ideal opportunity to deploy multiple ($>1.0\times10^9$) sensors around the globe and form a network of in situ sensors to help map out sources and sinks of $CO_2$ and other important greenhouse gases. A network of sensors on land, ships, and aircraft would provide needed verification and validation for the Orbiting Carbon Observatory 2 (OCO-2) [1]. FIG. **12** shows a network of portable spectrometers **1130** in communication with a server.

The spectrometer according to one or more embodiments of the invention can also be used in medical applications, e.g., to identify biomarkers or disease markers in exhaled breath/breath condensate such as nitric oxide, carbon monoxide, and volatile organic compounds or other species identified by canines as being related to disease. Such breath markers can be used to measure hypoxia, oxidative stress, and inflammation in a spectrum of clinical conditions ranging from asthma, cancer, heart disease, transplant rejection (e.g., lung allograft rejection), for example.

## REFERENCES

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## CONCLUSION

This concludes the description of the preferred embodiment of the present invention. The foregoing description of one or more embodiments of the invention has been presented for the purposes of illustration and description. It is not intended to be exhaustive or to limit the invention to the precise form disclosed. Many modifications and variations are possible in light of the above teaching. It is intended that the scope of the invention be limited not by this detailed description, but rather by the claims appended hereto.

What is claimed is:

**1**. A portable spectrometer, comprising:

a smart phone case or portable computer case holding a portable spectrometer, wherein the portable spectrometer includes:

a cavity;

a laser source for emitting electromagnetic radiation that is directed on a sample in the cavity, wherein the electromagnetic radiation is reflected within the cavity to form multiple passes of the electromagnetic radiation through the sample; and

a detector for detecting the electromagnetic radiation after the electromagnetic radiation has made the multiple passes through the sample in the cavity, the detector outputting a signal in response to the detecting and communicating the signal to a smart phone or portable computer, and the smart phone or portable computer executing an application that performs a spectral analysis of the signal; and

wherein the smart phone case or the portable computer case further comprises a first opening comprising the cavity, a second opening holding the laser, and a third opening holding the detector.

**2**. The portable spectrometer of claim **1**, wherein the cavity includes a ring having an elliptical inner surface.

**3**. The portable spectrometer of claim **1**, wherein:

the cavity includes an inner surface substantially described by the equation:

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{c^2} = 1,$$

wherein:

x, y, and z are Cartesian coordinates,

a is an equatorial radius comprising a maximum value of x and y,

c is a distance along the z- axis from coordinate (x=0, y=0, z=0) to a pole of the spheroid described by the equation, and

$a \neq c$,

the electromagnetic radiation incident on the inner surface is reflected from multiple regions of the inner surface such that the multiple passes of the electromagnetic radiation through the sample in the cavity are formed, and

one or more processors in the smart phone form an output identifying a composition of the sample.

**4**. The spectrometer of claim **3**, wherein $z<c$.

**5**. The spectrometer of claim **3**, wherein:

z is in a range of 2 mm-20 mm, and

a is in a range of 2 mm-60 mm.

**6**. The spectrometer of claim **3**, wherein:

an angle of incidence of the electromagnetic radiation, at a first reflection within the cavity, is between more than 0 degrees and 45 degrees,

a is less than 60 mm,

z is less than 20 mm, and

the angle of incidence, a, and z are such that a total path length of the electromagnetic radiation transmitted through the sample includes a distance of 30 meters.

**7**. The spectrometer of claim **3**, wherein an angle of incidence of the electromagnetic radiation at a first reflection within the cavity, a, and z are selected such that the spectrometer can identify the sample having a relative concentration in the cavity of 50 parts-per-billion by volume (ppbv).

**8**. The spectrometer of claim **1**, further comprising:

one or more windows in the cavity through which the electromagnetic radiation is inputted into the cavity and through which the electromagnetic radiation exits the cavity after a last pass of the electromagnetic radiation through the sample, the detector positioned to receive the electromagnetic radiation after the last pass.

**9**. The spectrometer of claim **1**, wherein the cavity is dimensioned such that a volume of the cavity comprising the sample is between 33 $mm^3$ and 905000 $mm^3$.

**10**. The portable spectrometer of claim **1**, wherein the smart phone case further comprises:

a first wing for storing the smart phone;

a second wing comprising the first opening, the second opening, and the third opening; and

a hinge connecting the first wing to the second wing, wherein the hinge folds the smart phone case so that the second wing is superposed on the first wing when the smart phone case is closed.

**11**. The portable spectrometer of claim **10**, wherein the first wing has substantially a same surface area as the smart phone and the second wing has substantially a same size as the portable spectrometer.

**12**. The portable spectrometer of claim **10**, wherein, when the smart phone case is closed, the smart phone case has a length of 15 cm or less, a width of 15 cm or less, and a thickness of 4 cm or less.

**13**. The portable spectrometer of claim **10**, wherein the second wing comprises

the first opening holding the cavity, and

one or more additional openings through which the laser beam is transmitted to the cavity from the laser and from the cavity to the detector.

**14**. The spectrometer of claim **1**, wherein:

the portable spectrometer further comprises an optical interfacing system, and

the optical interfacing system:

guides the electromagnetic radiation into the cavity at an appropriate angle to achieve a desired number of the multiple passes,

guides the electromagnetic radiation after the number of passes onto the detector, and

is stored in the smart phone case.

**15**. The spectrometer of claim **1**, wherein the cavity comprises or consists essentially of bulk metallic glass or bulk metallic glass matrix composite and the cavity is a ring cavity having a spherical or elliptical inner surface.

**16**. A spectrometer, comprising:

a source of electromagnetic radiation;

a cavity receiving electromagnetic radiation emitted from the source; and

a detector detecting the electromagnetic radiation after multiple passes of the electromagnetic radiation through the cavity;

wherein the cavity comprises a molded surface of a smart phone case or a portable computer case, and

the electromagnetic radiation is reflected from the molded surface to form the multiple passes of the electromagnetic radiation.

**17**. The spectrometer of claim **16**, wherein the smart phone case or the portable computer case consists essentially of molded bulk metallic glass or a composite comprising molded bulk metallic glass.

**18**. A method of fabricating a smart phone case, comprising:

molding a material into a smart phone case wherein the smart phone case is capable of holding a smart phone and a portable spectrometer, the portable spectrometer including:

a cavity;

a laser for emitting electromagnetic radiation that is directed on the sample in the cavity, wherein the electromagnetic radiation is reflected within the cavity to form multiple passes of the electromagnetic radiation through the sample; and

a detector for detecting the electromagnetic radiation after the electromagnetic radiation has made the multiple passes through the sample in the cavity, the detector outputting a signal in response to the detecting and communicating the signal to the smart phone, and the smart phone executing an application that performs a spectral analysis of the signal; and

wherein the smart phone case comprises a first opening comprising the cavity, a second opening holding the laser, and a third opening holding the detector.

**19**. The method of claim **18**, wherein the material consists essentially of bulk metallic glass or a composite comprising bulk metallic glass such that the smart phone case consists essentially of the bulk metallic glass or the composite.

**20**. An apparatus, comprising:

a source of electromagnetic radiation;

a cavity receiving electromagnetic radiation emitted from the source;

a detector detecting the electromagnetic radiation after multiple passes of the electromagnetic radiation through the cavity;

a case for a mobile device, wherein the case holds the source comprising a laser, the cavity, and the detector; and

a wired or wireless connection communicating a signal outputted from the detector in response to the detecting, wherein:

the mobile device, connected to the wired or wireless connection and receiving the signal, executes an application that performs a spectral analysis of the signal, and

the mobile device comprises a tablet, a smart phone, or a laptop.

**21**. The apparatus of claim **20**, wherein the source is a quantum cascade laser and the cavity is a ring cavity.

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