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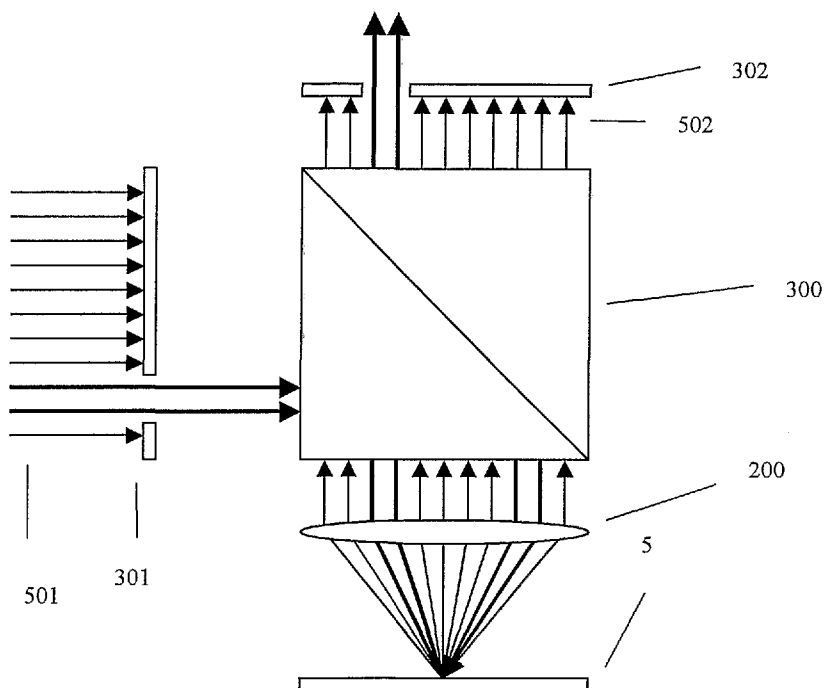
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(54) Title: MICROSCOPE PROBE FOR INVESTIGATION OF SEMICONDUCTOR STRUCTURES



(57) Abstract: A device (300-302) is described allowing simultaneous control of angles at which an optical beam is impinging a sample (5) and at which radiation emitted by the sample (5) is collected. The device (300-302) can be applied in the field of Raman spectroscopy for investigation, which can be used to identify tensor components of stress in silicon wafers. An embodiment of the invention allows scanning optical beams on the sample surface with 80 nanometer and below resolutions.

MICROSCOPE PROBE FOR INVESTIGATION OF SEMICONDUCTOR STRUCTURES

BACKGROUND OF THE INVENTION

5 The selection rules used in Raman spectroscopy of semiconductor structures often require control of the angle at which an optical beam and control of the angle at which Raman emission is collected. Often certain resonances are manifested only at particular incidence and collection angle combinations. In research and development laboratory environments this is often accomplished using separate optics for control of excitation
10 and collecting emitted radiation [1].

 In a commercially important case of Raman spectroscopy of a silicon surface [100], commonly used backscattering geometry allows observation of only one longitudinal optical (LO) phonon [1]. Bonera et al. [3], [4] notice that by using a high numerical aperture, one can break the selection rules for pure backscattering geometry
15 and one can excite vibration modes forbidden in pure backscattering geometry, and observe the presence and characteristics of other phonons. Furthermore, they discuss angular distribution and application of the polarization control to analyze and determine independently, up to three components of out of six independent strain components in silicon. Bonera et al. [3], [4] points out that the exact values of measured stress tensor
20 components depend upon model assumptions (in particular depend on assumed vanishing elements of the stress tensor).

 Loechelt et al. [2] demonstrate that by conducting an experiment in an off axis configuration and by controlling the incident angle and polarization state of the incident

and collected radiation, it is possible to determine all six independent components of a stress tensor for [100] ([100] crystallographic direction) cut surface of silicon. These types of arrangements are quite complicated and difficult to implement in a commercial tool. Furthermore, this type of lateral resolution of a spectroscopic system deteriorates, and cannot be implemented in a micro – Raman tool [3, 4].

In this disclosure we describe a novel optical probe allowing wide control of the incidence and collection angles of the excitation beam and Raman emission respectively, while preserving relatively high spatial resolutions.

Furthermore, we describe modifications of this probe allowing measurements and imaging of the features significantly smaller than the spot size of the excitation beam on the sample surface.

The present device and method of using this invention allows convenient measurement of off-axis Raman emissions without the need to realign the excitation and collection optics, and without the need to rotate the wafer during measurement (as it is described by Loechtel [1,2]). The present invention is compact and easy to implement in an industrial metrology tool.

Brief description of drawings

Figure 1 depicts the geometry of a typical Raman measurement.

Figure 2 depicts the geometry of a beam focused on a wafer by means of a microscope objective.

Figure 3 depicts a definition of the angle coordinates α and θ defining collection and incidence angles.

Figure 4 depicts a device for the control of an incidence angle.

Figure 5 depicts a device for control of both incidence and collection angles.

Figure 6 depicts a device for the fine control of the position of an excitation spot.

5

DETAILED DESCRIPTION OF THE INVENTION

In Figure 1 we present an experimental arrangement usually used for off-axis Raman measurements. A laser **1** is emitting a laser beam which is filtered by a spectral filter **2**, polarization of the beam emerging from spectral filter **2** is rotated by a half wave plate **3**, ellipticity of the polarization state of the beam is controlled subsequently by a quarter wave plate **4**. The radiation emerging from the quarter wave plate **4** is focused using an optional focusing lens **400** impinging a silicon wafer **5** and is collected by a collection lens **6**, and filtered by a spectral filter **60**. The polarization state of the beam is analyzed by combination of quarter-wave plate **7** and polarizer **8**. Subsequently beam is spectrally analyzed by spectrometer **9** and detected by array detector **10**.

Similar experimental arrangement was used by Loechelt et al their work [1,2]. In their work, Loechelt et. al., [1,2] were using an incidence angle approximately equal to 60 degrees.

We propose using a device, based upon a microscope objective, to reproduce the off axis geometry. Let us consider a microscope objective (focusing lens) **200** presented in Figure 2 focusing laser beam on wafer **5** by means of microscope objective **200**. The angle between the marginal ray **201** and the chief ray **202** defines the Numerical Aperture (NA) of the system. All rays emerging from the microscope objective **200** are propagating inside a cone defined by the angle between the marginal ray and the chief ray.

The angle between the chief ray **202** and the marginal ray **201**, in case of typical commercial 60X microscope objective, is often in the range of 58 – 71 degrees (which corresponds to $NA = 0.85 - 0.95$) [5, 6]. This angle is essentially the same as the incidence angle of 60 degrees used by Loechelt et al [1, 2].

It is straightforward that one can define the angular coordinates α and θ of rays propagating from a focal point of a microscope objective **200** by introducing suitable a aperture restricting the spherical angle as shown in Figure 3. Every ray collected by the objective **200** and emerging from a focal point of the objective can be described by a pair
5 of angles α and θ .

As presented in Figure 3, it is possible to select a portion of the spherical angle within the cone, defined by marginal rays, which will correspond to the same or essentially the same geometry of measurement as that described in [2]. This can be accomplished by means of a suitable aperture partially blocking a portion of the incident
10 radiation as described in Figure 4. As seen in Figure 4, the aperture **210** partially blocks the incident beam **501** so only portion of the beam within the well defined spatial position is impinging lens **200** and is focused at well defined angles α and θ on the sample **5**.

It is straightforward to extend this idea to the geometry encountered in a typical micro Raman experiment, where the exciting laser beam and the Raman emission are
15 passing through the same beam splitter as presented in Figure 5. As shown in Figure 5, the incident beam **501** is partially blocked by aperture **301** and directed by beam-splitter **300** to microscope objective **200** and focused at incident angle defined by the aperture **301** on sample **5**. The sample emits radiation, which is collected by a microscope objective **200**, passes through the beam-splitter **300** and is partially blocked by the
20 aperture **302**. The radiation transmitted through the aperture **302** was emitted by the sample **5** at an emission angle defined by the opening in the aperture **302**.

It is important to notice that in this case, by choosing suitable apertures **301,302**, we can fully reproduce all the geometries of all measurements necessary to calculate all six independent components of stress tensor described in [2]. Apertures **301,302** can be mounted on motorized filter wheels, such as described in Thorlabs catalog [7], or other
5 suitable moving stages allowing their easy automated positioning of said apertures. Furthermore the polarization state of the incident and emitted radiation can be controlled and analyzed by standard optical tools such as polarizers, quarter-wave and half-wave plates mounted on suitable rotational stages.

Loechelt et al [1, 2] teaches that by measuring Raman emission from silicon wafer
10 oriented in **100** a crystallographic direction at various incidence angles with respect to crystallographic orientation of the wafer and at various polarization angles, one can establish all six independent components of stress tensor of the material. Loechelt et al [1, 2] provides an explicit prescription for the stress tensor calculation.

It is straightforward to anyone skilled in the arts that the results presented by
15 Loechelt et al [1, 2] can be generalized to any material possessing the same (diamond) crystal structure.

Loecht et al [1,2] define a procedure in which they specify which combination of incidence, emission angles and polarization states for incidence and emission angle should be used in order to accurately measure all the components of stress tensor.
20 Here are the main findings presented in the Loechelt [2] patent:

“In a diamond-structure semiconductor like silicon, there are three Raman-active optical phonon modes: two transverse optical (TO) phonon modes (TO1 and TO2) and one longitudinal optical (LO) phonon mode. Because unstrained silicon has cubic

symmetry, these three phonons are degenerate in frequency at $\mathbf{k} = 0$. Non-hydrostatic crystal strain destroys this symmetry and lifts the degeneracy. The splitting in phonon frequencies and the mixing of the phonon modes contain complete information about the stress that destroyed the symmetry. However, if only one of these three phonons is
 5 observed, as in conventional backscattering Raman spectroscopy, only partial information can be obtained about the stress.

The intensity of a phonon mode for a given scattering geometry can be determined by examining the Raman polarizability tensors. For phonons with a wave number of $\mathbf{k}=0$ appropriate for Raman scattering, one can choose the polarizations of the
 10 three degenerate optical phonons to be any set of three mutually perpendicular vectors. If the three cubic axes are chosen, the Raman polarizability tensors are given

by [2]:

$$TO_1 \rightarrow \Delta_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & d \\ 0 & d & 0 \end{pmatrix},$$

$$TO_2 \rightarrow \Delta_2 = \begin{pmatrix} 0 & 0 & d \\ 0 & 0 & 0 \\ d & 0 & 0 \end{pmatrix},$$

$$LO \rightarrow \Delta_3 = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Equation 1

15

In this notation, TO_1 , TO_2 , and LO denote phonon modes polarized in the $[100]$, $[010]$, and $[001]$ directions, respectively, and d represents a nonzero number. This particular choice of phonon basis and nomenclature is useful for interpreting the results of backscattering experiments from a $[001]$ crystal surface.

The Raman polarizability tensors determine the intensity of the scattered light from the sample according to

$$I_k = \Xi |\mathbf{p}'^T \Delta_k \mathbf{p}|^2 I_0,$$

5

Equation 2

where I_k is the intensity from the k th phonon mode (TO1, TO2, or LO), Ξ is a constant related to the Raman scattering cross section, \mathbf{p}' is the polarization vector of the scattered light, Δ_k is one of the polarizability tensors given above, \mathbf{p} is the polarization vector of the incident light inside the sample, I_0 is the intensity of the incident light, and the superscript T denotes transposed vector. The signal line shape Λ_k for a given phonon mode with a frequency of ω_k is given by a Lorentzian function of the form [2]:

$$\Lambda_k(\omega; \omega_k) = \frac{I_k \Gamma}{(\omega - \omega_k)^2 + \Gamma^2}.$$

Equation 3

where ω is the difference in frequency between the incident and scattered light (Raman frequency), and Γ is the half width at half maximum of the signal. The total signal line shape $\Lambda(\omega)$ is the sum of the signals from the three contributing phonon modes,

$$\Lambda(\omega) = \sum_{k=1}^3 \Lambda_k(\omega; \omega_k).$$

Equation 4

For unstrained silicon, all three phonon modes are degenerate with a frequency of $\omega_k = \omega_0 = 520.3 \text{ cm}^{-1}$ at room temperature (22 °C).

In the presence of strain τ the phonon frequencies ω_k shift from their unstrained value ω_0 . Using degenerate perturbation theory, the new phonon frequencies and polarizations follow from the eigenvalues and eigenvectors of the following secular matrix. [2].

$$\Psi(\tau)\mathbf{d}_k = \lambda_k \mathbf{d}_k,$$

$$\Psi(\tau) = \begin{pmatrix} p\epsilon_{11} + q(\epsilon_{22} + \epsilon_{33}) & 2r\epsilon_{12} & 2r\epsilon_{13} \\ 2r\epsilon_{21} & p\epsilon_{22} + q(\epsilon_{33} + \epsilon_{11}) & 2r\epsilon_{23} \\ 2r\epsilon_{31} & 2r\epsilon_{32} & p\epsilon_{33} + q(\epsilon_{11} + \epsilon_{22}) \end{pmatrix} \quad \text{Equation 5}$$

These eigen values and eigenvectors are related to the shifted phonon frequencies ω_k in the following fashion:

$$\lambda_k = \omega_k^2 - \omega_0^2 = (\omega_k + \omega_0)(\omega_k - \omega_0) \approx 2\omega_0(\omega_k - \omega_0),$$

$$\omega_k \approx \omega_0 + \frac{\lambda_k}{2\omega_0}.$$

Equation 6

Since the Raman tensors are the derivatives of the system's electronic polarizability relative to the phonon normal coordinates, and the normal coordinates under stress are linear combinations of the normal coordinates for the unstressed material, as is apparent from Eq. (5), the Raman polarizability tensors for the perturbed phonons can be easily written as linear combinations of the tensors, in the first order approximation in Eq. (1) as [2]

$$D_k = \sum_{i=1}^3 \Delta_i (\mathbf{d}_k)_i.$$

Equation 7

In the preceding equations, $\Psi(\tau)$ is a 3x3 secular matrix whose components are linear functions of the strain tensor ϵ , which is ultimately related to the stress tensor σ through the compliance tensor s . The parameters p , q , and r are deformation potential constants [2]. The strain tensor ϵ is related to the stress tensor σ by Hooke's law, which states that ϵ
 5 $= s \sigma$. For crystalline silicon, s has only three different components. Also, $(\mathbf{d}_k)_i$ represents the i th component of the k th normalized eigenvector. The approximations in Eq.(6) are valid since ω_k are close to ω_0 ."

Further, it has been demonstrated by Loechtel in [2] that the incident light is tilted away from the normal axis, the scattered light is collected normally, and both beams are
 10 polarized. By allowing the incident light to deviate from normal incidence, all three active optical phonon modes are accessible for measurement. Furthermore, the polarizers enable the experimenter to vary the relative contribution of these three modes to the measured signal intensity. This combination of off-axis illumination with polarization is more powerful and general than polarized backscattering methods, which can only
 15 determine the in-plane stress components for special crystal orientations. If one judiciously selects the various angles of the apparatus, a given phonon mode can be selectively studied. By analyzing the results of several selective measurements, all six components of the stress tensor can be determined.

As it is shown in [2] further simplification can be achieved by efficiently relating
 20 the secular matrix to the components of the stress tensor σ . First, the symmetry of $\Psi(\sigma)$ implies that there are only six independent components and said matrix has form

$$\Psi(\sigma) = \begin{pmatrix} \phi_1 & \phi_6 & \phi_3 \\ \phi_6 & \phi_2 & \phi_8 \\ \phi_3 & \phi_8 & \phi_5 \end{pmatrix}$$

Equation 8

where vector ψ is given by

$$\psi = \Pi s \sigma \quad \text{Equation 9}$$

where Π is a matrix of deformation potential constants s in compliance matrix, and σ is a stress tensor expressed in six component vector form convention. In a linear model stress
 5 σ is given as a linear form with vector of adjustable parameters (model parameters) \mathbf{x} .

$$\sigma = T\mathbf{x} \quad \text{Equation 10}$$

From Eq. 9 and Eq. 10 we see that ψ is also a linear function of vector \mathbf{x} .
 Loechtel in [2] at all has shown that it is possible to find all relevant stress components from the experiment in which incidence θ angle is constant, the angle between the [100]
 10 axis of the crystal (in plane of the surface) and the projection of the incidence beam direction on the surface of crystal ϕ , and angles α , β describing direction of linear polarizers inserted in the incident and scattered beam paths and defined in [2]. Angles are α , β varied by rotating said polarizers, angle ϕ can be changed by means of rotating crystal with respect to axis normal or by means of selecting suitable aperture proposed in
 15 this invention 301. The four angle combination $(\theta, \phi, \alpha, \beta)$ describe configuration of off-axis Raman measurement. The full measurement comprises of series of experiments in r configurations defined by angles $(\theta, \phi_j, \alpha_j, \beta_j)$ where $j=1, \dots, r$. Specific examples of such angles combinations are presented in [2].

The calculation of model vector parameter \mathbf{x} is performed by means of fitting predicted
 20 line shapes given by equation 4 to experimentally observed line shapes for every experiment j . This is accomplished by minimizing parameter χ^2 as a function of its arguments (\mathbf{x} , and Ξ):

$$\chi^2(\mathbf{x}, \Xi) = \sum_{j=1}^r \chi^2(\mathbf{x}, \Xi, \theta, \alpha_j, \phi_j, \beta_j) \quad \text{Equation 11}$$

where we implicitly assumed that all experiments $j = 1, \dots, r$ have been performed under the same or similar experimental conditions (same apparatus, same exposure times etc), where

$$\chi^2(x, \Xi, \theta, \alpha_j, \varphi_j, \beta_j) = \frac{\sum_{i=1}^n [\Lambda_{\text{exp},j}(\omega_i) - \Lambda_j(\omega_i)]^2}{n} \quad \text{Equation 12}$$

where ω_i is frequency at which observation is performed and corresponds to one point of n points comprising Raman emission spectrum.

By finding absolute minimum of the function $\chi^2(x, \Xi)$ we find value of x vector optimizing fit, and stress tensor components in the sample using Equation 10.

Furthermore, we present a second embodiment of the invention where the angle of the incident beam is controlled by means of a steering mirror as shown in Figure 6 where shows how the incident beam **501** is deflected by steering mirror **600**, subsequently is partially blocked by aperture **301** and directed by the beam-splitter **300** to a microscope objective **200** and focused at an incident angle defined by the aperture **301** on the sample

5. The sample emits radiation, which is collected by the microscope objective **200** passes through the beam-splitter **300** and is partially blocked by the aperture **302**. The radiation transmitted through the aperture **302** was emitted by the sample **5** at an emission angle defined by the opening in the aperture **302**. The exact position of the focal spot is defined by the angle of steering mirror.

The steering mirror angle is controlled by piezo-electric actuators (for example, a mirror mounted on a mirror mount KC-1PZ [8]). Since the focal length of the typical microscope objective described above is of the order of 1-3 mm, and resolution of this

mirror mount is 6 arc sec, this arrangement permits positioning the center of the optical beam with a resolution of the order of 20 nm. It is possible to construct a mirror stage having a resolution one order of magnitude higher and achieve control of the position of the center of the optical beam with a resolution of the order of 20 nm. This allows us to
5 further enhance the spatial resolution of our optical system. Resolution is achieved by modulation of the position of center of the optical beam, which can be at least an order of magnitude higher than the waist of the beam.

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<http://www.edmundoptics.com/onlinecatalog/DisplayProduct.cfm?productid=1720> (2 of 3) 7/18/2005 6:40:29 AM, **Copyright 2005, Edmund Optics Inc. 101 East Gloucester Pike, Barrington, NJ/USA 08007-1380**
- 15 **Phone: (800) 363-1992, Fax: (856) 573-6295**
- [6] **Nikon:** <http://www.microscopyu.com/articles/optics/objectiveproperties.html> (3 of 8) 7/19/2005 10:55:25 AM
- [7] http://www.thorlabs.com/Visual/Nav.cfm?Guide_ID=80&Visual_ID=91
- [8] Thorlabs mirror KC1-PZ
- 20 http://www.thorlabs.com/NewGroupPage9.cfm?Category_ID=26&ObjectGroup_ID=231

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CLAIMS

What is claimed:

1. An optical device for exciting a sample surface by an optical beam at a predetermined and controlled angle for collecting radiation emitted by a sample at other than, but not necessarily, the same angle comprising:

an entrance aperture partially blocking exciting radiation, and being mounted in front of, and to, an optical beam-splitter directing exciting radiation towards the focusing element and being mounted in front of a focusing element, directing focused exciting radiation on the surface of a sample being in optical communication with the focusing element and the sample is mounted to a wafer chuck mechanically connected to the focusing element, at an incidence angle predetermined by the opening in the aperture, and

a second aperture mounted on another side of the optical beam splitter in such way that said aperture is partially blocking the radiation emitted by the sample, which was collected and collimated by the focusing element, where the opening of the second aperture defines the collection angle.
2. The device described in claim 1 where the apertures are replaceable.
3. The device described in claim 1 where the apertures are positioned by motion stages and positioning devices.
4. The device described in claim 3 where the positioning devices are filter wheels.
5. The device described in claim 1 where the polarization state, of the incident and emitted radiation, is controlled by quarter wave plates and polarizers mechanically connected to the apertures.

6. The device described in claim 1 used as an optical probe incorporated in a Raman spectrometer.
7. The device described in claim 1 where the exciting beam is directed to the entrance aperture by a steering mirror which is optically with the entrance aperture, which deflects the exciting beam at a user controlled angle which defines the position of the spot where the exciting beam is impinging the measured sample.
8. A method of measuring stress tensor components in materials possessing crystallographic diamond structure using the apparatus described in claim 1 comprising:
 - performing a series of off-axis Raman measurements with different configurations defined by an excitation incidence angle, a polarization angle of an excitation beam, a collection angle, and a polarization of collection emission conditions in the spectral proximity of (LO) phonon,
 - calculation of the root mean square sum of the deviation of the spectra observed in each of the off-axis Raman measurements and spectra calculated using a model assuming the presence of three nearly degenerate phonons and taking into account linear corrections to the phonon frequencies due to the presence of stress, where stress is a model fitting parameter,
 - calculating the sum of the mean square sum of the deviations for all spectra,
 - minimizing said sum by changing the value of an assumed stress model fitting parameter by iterating the last two steps until the value of the stress model fitting parameter does not change more than a prescribed tolerance, and

reporting the value of the model fitting parameter minimizing the sum as a stress tensor.

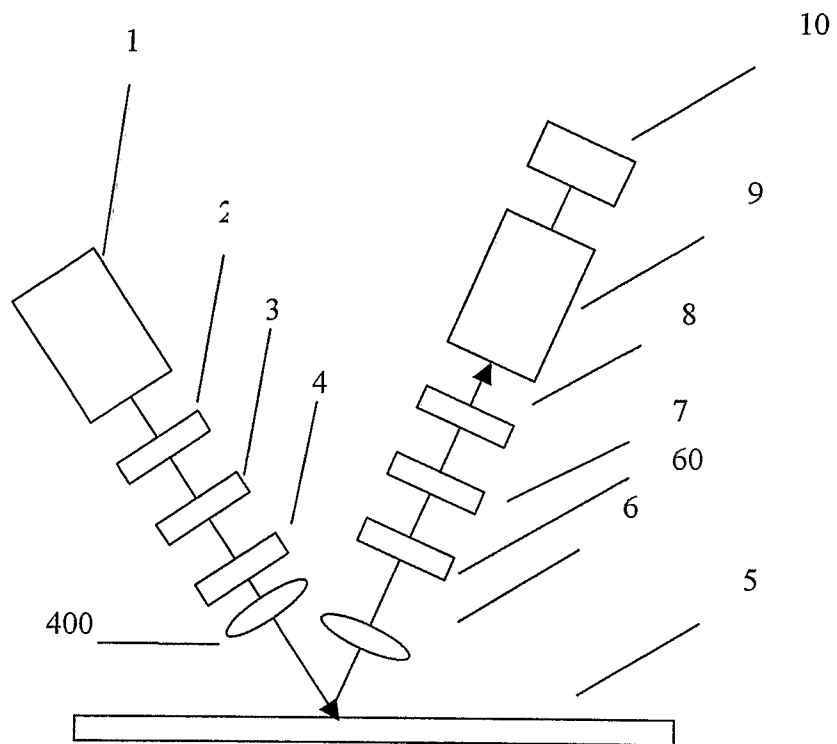


Figure 1

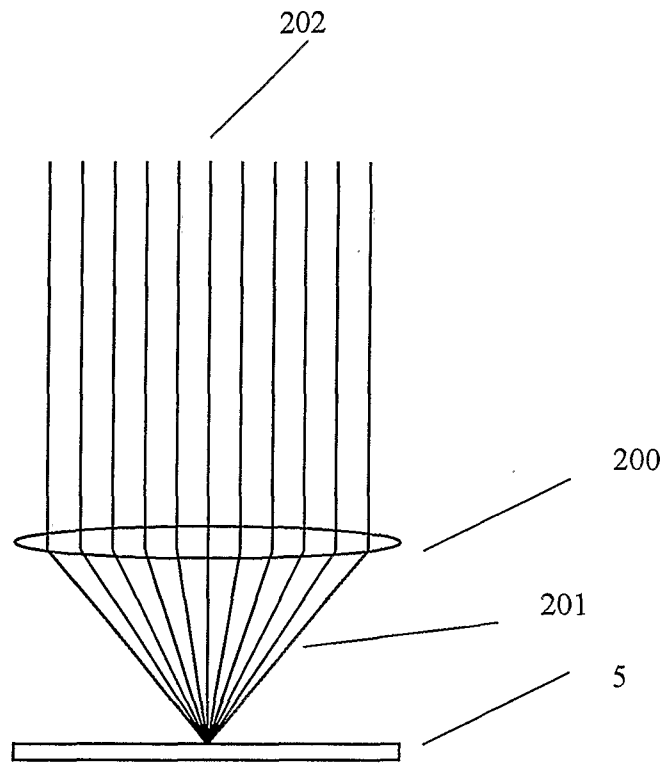


Figure 2

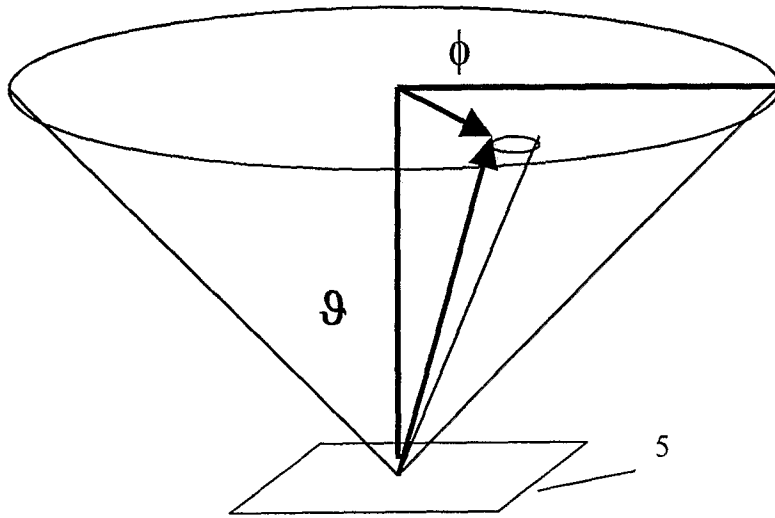


Figure 3

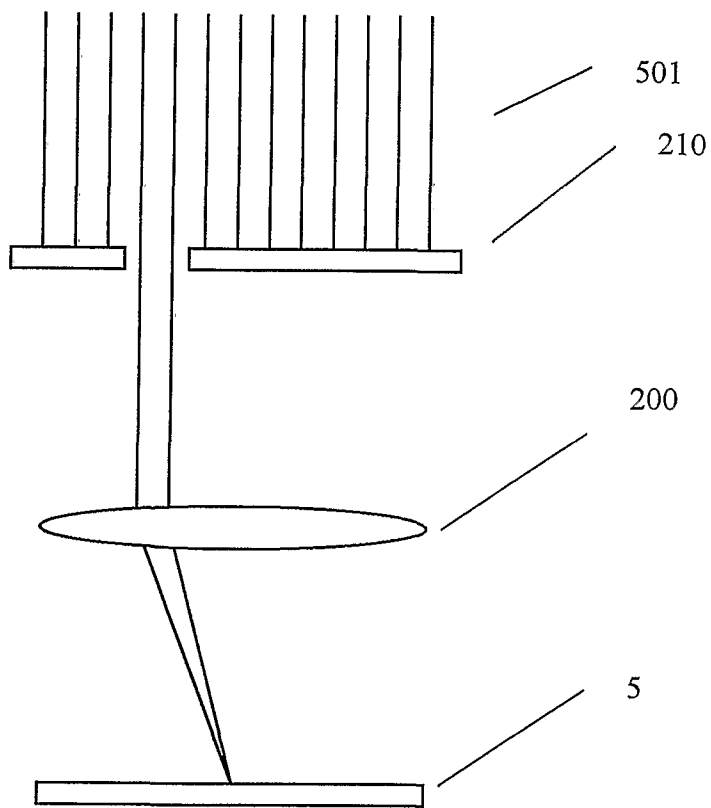


Figure 4

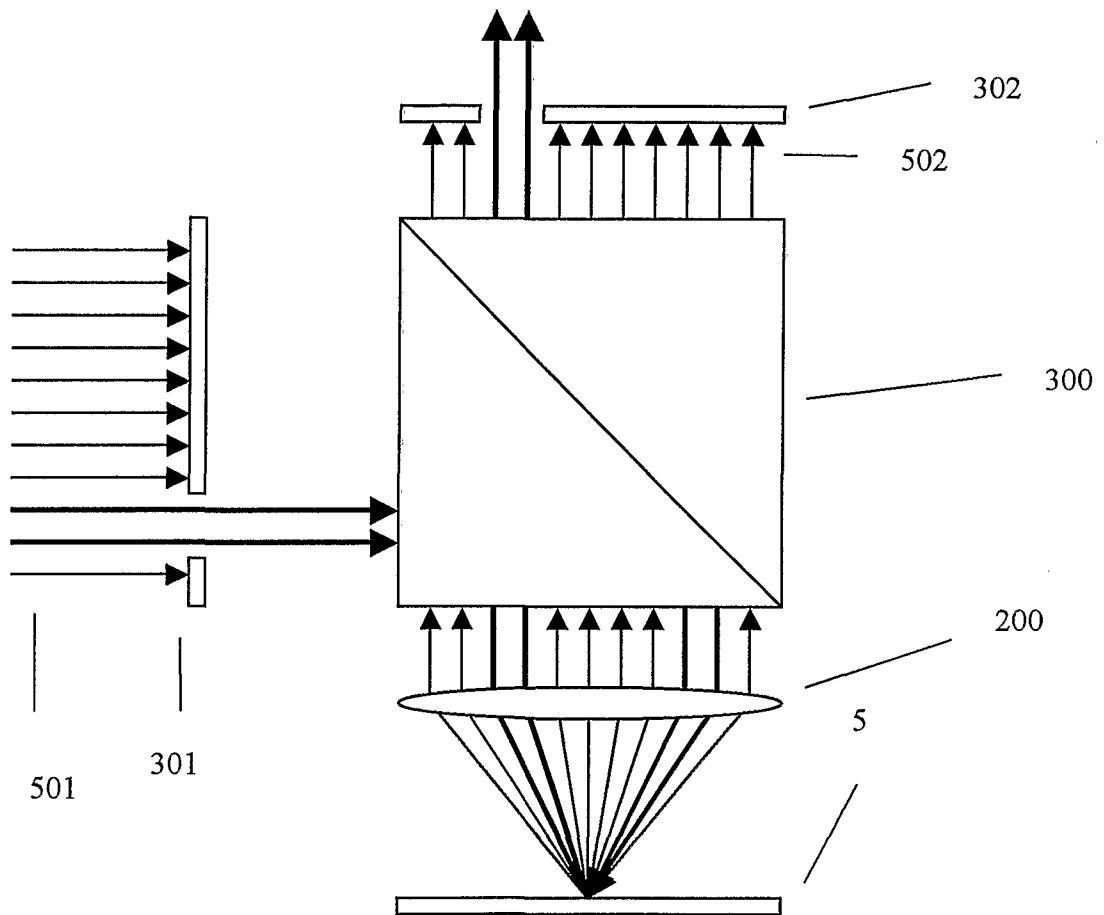


Figure 5

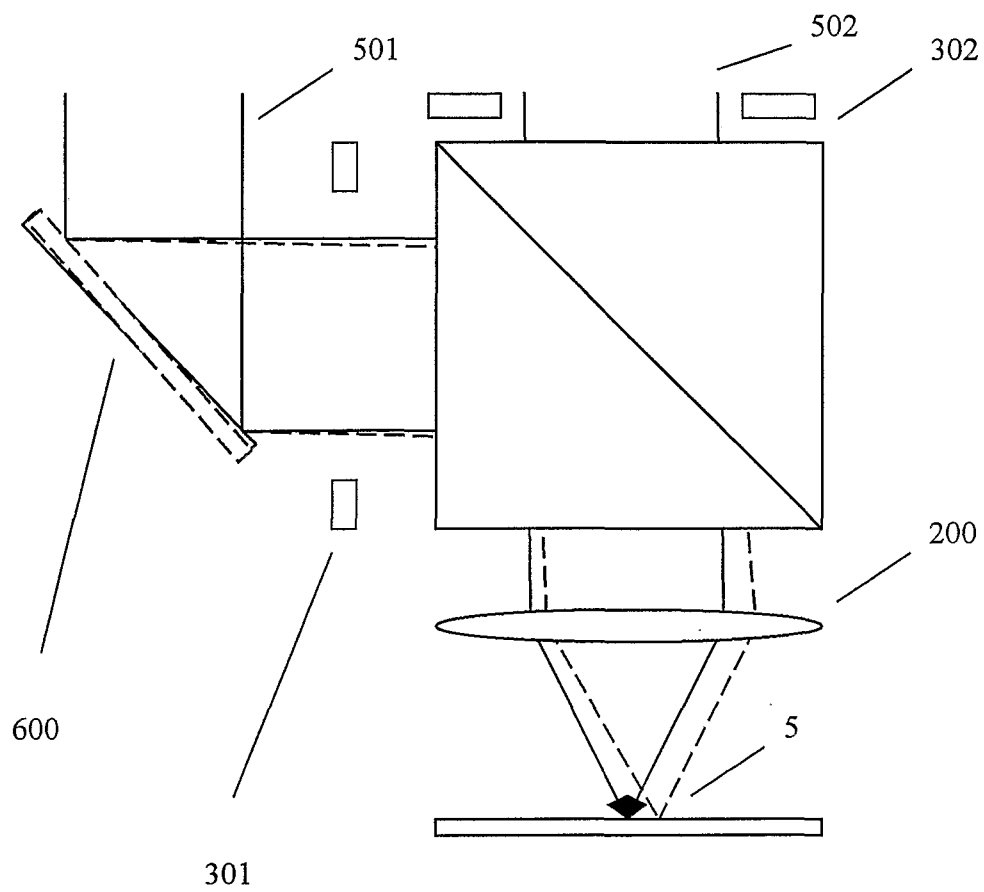


Figure 6

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US05/34127

A. CLASSIFICATION OF SUBJECT MATTER IPC: G01J 3/44(2006.01);G01N 21/65(2006.01) USPC: 356/301 According to International Patent Classification (IPC) or to both national classification and IPC		
B. FIELDS SEARCHED Minimum documentation searched (classification system followed by classification symbols) U.S. : 356/301, 317, 317, 318, 445, 446 Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Continuation Sheet		
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Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
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Y	US 2002/0039184 A (SANDUSKY) 04 April 2002 (04.04.2002), see the entire document.	1-6
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Continuation of B. FIELDS SEARCHED Item 3:
EAST
search terms: Raman, angle, aperture, tensor, stress, wafer