Precision auto-alignment for the specimen stage of an ellipsometer

Sunglim Park, Jaewha Jung, and DaeGab Gweon
Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, 373-1 Kusung-Dong Yusong-Gu, Taejon 305-701, Korea

Young Dong Kim
Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, 1 HoeGi-Dong DongDaeMun-Gu, Seoul 130-701, Korea

(Received 26 April 2001; accepted for publication 6 May 2002)

We present a new three-step auto-alignment algorithm for the specimen stage of an ellipsometer with adjustable angle of incidence. Correction of errors in tilt angle and position of the specimen stage can be performed by locating the reflected light spot at the center of the detector at two different angles of incidence. The current method does not need auxiliary focusing equipment. The alignment algorithm works to high precision in both model simulation and practical experiments with a rotating analyzer ellipsometer. © 2002 American Institute of Physics.

DOI: 10.1063/1.1489425

I. INTRODUCTION

Ellipsometry is one of the most accurate methods for studying optical constants of many interesting materials and thin films. Though the optical constants of a material should be independent of the measurement method, there are several reports that azimuthal misalignment of components in ellipsometric measurement can make the optical constants appear to depend on the angle of incidence (AOI).1–5 Since the exact AOI value is needed to deduce the absolute value of the index of refraction of a material, precise calibration of the AOI is essential, requiring precise alignment of the specimen stage.

Most commercially available ellipsometers use a focusing microscope and three-axis stage for specimen alignment.6 Another auto-alignment method has also been reported, which uses two step motors to move the detector.7 Though this latter method can align the reflected light to the center of the detector aperture, translation errors in the specimen stage can still cause errors in the AOI. In this article, we present an auto-alignment algorithm of a specimen stage that uses a three-axis stage and the detector signal. We developed a rotating analyzer ellipsometer with a precision specimen stage8 to test our new auto-alignment algorithm to high precision.

II. SETUP

We have constructed a single-wavelength rotating analyzer ellipsometer of the type developed by Aspnes,9 whose automation was first proposed by Cahan and Spanier.10 Figure 1 shows our setup [Fig. 1(a)] and its optical layout [Fig. 1(b)]. Figure 1(b) shows the definition of angle of incidence (AOI, θ). A 2 mW HeNe laser was used as light source, and calcite (Glan–Thompson) prisms with extinction ratio <10−5 and ordinary refractive index n = 1.655 were used for both polarizer and analyzer. The analyzer prism rotates in the hollow shaft step motor at 15 revolutions/s. We inserted a 50 kHz photoelastic modulator (PEM-90, HINDS Co.) between the polarizer and specimen stage to improve data acquisition speed for in situ monitoring applications. The detector was a silicon photodiode (UDT555D). The input (incident) and output (reflected) arms are each designed as one body which contains all the optical components. These are precisely positioned at the vertical half-circular disk with magnets and ball bearings. Figure 1(a) shows several radial grooves on the vertical disk. To change the AOI, we simply move the input and output arms to the appropriate radial groove of preference. The arms can be positioned to within 0.005° in the AOI by this method.

As shown in Fig. 1(b), when we arbitrarily place a specimen on the specimen stage, three possible errors can occur: (1) h-translation error (displacement along the z axis), (2) α-tilt angle error (rotation about the y axis), and (3) β-tilt angle error (rotation about the x axis), where the origin of the x–y–z coordinate is taken to be at the specimen in the perfectly aligned case. These errors result in deviation (solid line) of the reflected light from its perfectly aligned path (dotted line). Figure 1(c) shows a schematic of our specimen stage. Three dc linear motors driven by computer make the points A, B, and C move in the vertical direction (white arrow) independently. Point A is located on the x axis, while the straight line between B and C is parallel to the y axis. (Positioning error of the centering triangle ABC onto origin O in manufacturing is about 1 μm, which causes negligible error in the current analysis.) For α tilt of the specimen stage, for example, motor A moves in the negative z direction, while motors B and C move in the positive z direction. This causes the sample at position O to have no translational motion but only rotational motion. Therefore, unlike ordinary tilt stages or kinematic mirror mounts, which are widely used as the specimen stage in commercial ellipsometers, x and y axis rotations and the z-axis translation of our stage are independent, making the auto-alignment procedure much sim-
pler. Our stage has a 25 mm translation range with 60 nm resolution and a 20° rotation range with 10^{-6} degree resolution, as described previously. The choice of specimen is irrelevant to the alignment procedure. We used a bare Si wafer for our specimen.

III. ALIGNMENT ALGORITHM

It is clear that errors in the tilt angles and the vertical (z-axis) position of the specimen cause significant error in the AOI (θ), which results in incorrect analysis of optical properties of the specimen. Note that since the β tilt angle and the h translation of the specimen stage make the reflected beam move in the plane of incidence (y–z plane), the β-tilt error and the h-translation error have a significant effect on the error of AOI. On the other hand, the α-tilt angle error has a smaller effect, since α tilt of the specimen stage leads to a reflected beam motion perpendicular to the plane of incidence. Our alignment method at two different AOIs, which consists of three steps with accessing and centering subprocesses, can separate the effects of these errors. We explain the subprocesses first.

A. The accessing and centering processes

If any amount of reflected light is reaching the detector, the system can maximize the optical signal relatively easily. However, a system with auto-alignment ability should be able to find the optical signal, even when the light spot is far from the detector aperture. We call this an “accessing process,” which has not been dealt with previously. In this process the two tilting motions are used without translational motion along the z axis. Figure 2(a) shows the accessing trajectory (dashed line) of the reflected light spot (small circle), which moves in a spiral of increasing radius (R_s). Not to miss the detector’s entrance aperture [Fig. 2(a), large bold circle], we have to carefully choose the parameters (R_s and φ) of the spiral. Figure 2(b) shows the geometry of the light spot, which barely misses the detector aperture. This sets the maximum possible value of the step size (Δφ) for catching the aperture. The radius R_s of the spiral is, therefore,
and the light spot, respectively. We define a new coordinate process stops and a centering process, shown in Fig. 3, be-
given by 11,12 where the actual movement of the α- and β-tilt angles are given by11,12

\[
\Delta \phi = 2 \cos^{-1} \left( \frac{2R^2 + 2Rr - 2Rr - r^2}{2R^2 + 2Rr} \right),
\]

(2)

where the actual movement of the α- and β-tilt angles are given by11,12

\[
\Delta \alpha = \tan^{-1} \left( \frac{R_s \cos \phi}{d_s} \right),
\]

\[
\Delta \beta = \tan^{-1} \left( \frac{R_s \sin \phi}{d_s} \right) / \sin \theta.
\]

Once the detector finds the light signal the accessing process stops and a centering process, shown in Fig. 3, begins. We define a new coordinate ξ-η in Fig. 3 at the detector aperture. The ξ axis is perpendicular to the plane of incidence, while the η axis is parallel to the plane of incidence. The large and small circles represent the detector aperture and the light spot, respectively. The intensity of the detector signal is correspondingly shown together at the right side of Fig. 3 for each position of the light spot. When the entire light spot is inside the detector aperture, the signal intensity is maximized.

Figure 3(a) shows the initial position of light spot in the centering process, which would be around the edge of the detector aperture. We denote this position by ξ₀ in the ξ direction with the light intensity signal given by I₀. By changing the α-tilt angle we can move the light spot until the signal passes the maximum (I_max) value, reaching half of the maximum (I_max/2) at position ξ₁ [Fig. 3(a)]. (A few parameters in the centering algorithm are set to select the direction of movement. At the ξ₀ point, the change of light signal along positive and negative ξ directions should be checked to select the right direction.) Once reaching the ξ₁ position, the spot moves in the reverse direction until it reaches ξ₂ where the light intensity is I_max/2 again [Fig. 3(b)]. The spot then moves to the (ξ₁ + ξ₂)/2, which is the center position of the detector aperture in the ξ direction [Fig. 3(c)]. At this point, the α-tilt angle error is completely removed. Because our specimen stage has independent movements along the α and β tilts as discussed above, for the η direction which lies inside the plane of incidence, we repeat the same procedure, changing only the β-tilt angle about the x axis. This completes the centering process.

It should be emphasized that in the centering process the detector’s signal was not simply maximized. Rather, the light spot was set at the midpoint between I_max/2, which is the center of detector aperture. Note that even if the aperture size is smaller than that of the light spot, these accessing and centering algorithms still work. We have only assumed that the image of the reflected light and detector aperture are perfect circles, and also that the light intensity inside the circular light spot is uniform. These are reasonable approximations to their real shape and characteristics.

B. First step

When the initial accessing and centering processes are completed at an arbitrary AOI (θ₁), the light path is as shown in Fig. 4. Since all the optical components are fixed on both the input and the output arms as explained in Fig. 1, adjustments are only made at the specimen stage. Therefore, we consider misalignment only along the output light path. We assume, as shown in Fig. 4, that the reflecting surface of the specimen has a translation error h from the origin (O) [which is the same coordinate in Fig. 1(b)] and a tilt angle error β₁. Note that the origin coincides with the reflecting point at perfect alignment. The dashed bold line is the optical light path of perfect alignment, while the solid bold line represents the misaligned case. The misaligned optical light path is refracted and offset by d₁ at the analyzer prism, which has thickness t_p and refractive index n.

The offset is given by

\[
d_1 = t_p \left( \tan \beta_1 - \frac{\sin \beta_1}{\sqrt{\sin^2 \beta_1 - \sin^2 \beta_0}} \right) \cos \beta_1.
\]

This offset of the optical light path causes an additional apparent translation error of the specimen stage as shown in the inset of Fig. 4,

\[
\delta_1 = \frac{d_1}{2 \cos \beta_1 \sin (\theta_1 - \beta_1)},
\]

where θ₁ is the AOI at the first step. The relation between the tilt angle error and the translation error is then
C. Second step

In the second step, shown in Fig. 5, the input and output arms are set at a second AOI ($\theta_2$). The second AOI must be different from the first but does not have to be the angle of final ellipsometric measurement. If the initial translation error $h$ of the specimen stage is not zero, the light spot at this new AOI will not be at the center of the detector aperture, but shifted along the $h$-axis direction of Fig. 3. (Once the $\alpha$-tilt angle error was corrected in the initial centering process, no more adjustment in the $\xi$ direction is needed.) Therefore, only the $\beta$ tilt needs to be adjusted. Afterward, the optical light path follows the solid line of Fig. 5, which is again refracted and offset at the analyzer prism. The second offset $d_{p2}$ is not shown in Fig. 5 for simplicity but is defined the same as $d_{p1}$ in Fig. 4 via Eq. (4), this time in terms of $\beta_2$, which is the second tilt angle error of the specimen stage. The second apparent translation error caused by this offset is called $\delta_2$, and has the form of Eqs. (5) and (6) with $\beta_1 \rightarrow \beta_2$. Here, again, the translation error depends only on $\beta_2$.

D. Third step

Since thickness varies from sample to sample, the $\beta_1$ value obtained in the first step is general. However, the difference between the first and second tilt angle errors, $\beta = \beta_2 - \beta_1$, is absolute. Thus, $\beta_2$ is determined by $\beta_1$, which means that $h + \delta_2$ can also be expressed in terms of $\beta_1$ only. Since both $\delta_1$ and $\delta_2$ are determined by $\beta_1$, we can get the two unknown errors, $h$ and $\beta_1$, from the Eq. (6). Therefore, in the final (third) step, we complete the alignment by moving the specimen stage to the origin according to the calculated values of $h$ and $\beta_1$.

IV. SIMULATION AND EXPERIMENT

To check our alignment algorithm, we made a simulation using a homogeneous transformation matrix (HTM). The HTM is a $4 \times 4$ matrix consisting of rotation and translation matrices, which describes not only the spatial position and orientation of an object in three-dimensional space but also coordinate transformations. It is widely used in modeling geometric errors. We have developed a model to describe the light path in a general ellipsometer, whose details were reported elsewhere.

The radii of the detector aperture and light spot were set to be 4 and 1 mm, respectively. The $d_s$ was 300 mm, and the translation error $h$ was $-1.0$ mm. The $\alpha$- and $\beta$-tilt angle errors were set to 0.015 and $-0.015$ rad, respectively. We assumed that the light spot was initially away from the center of the detector aperture by 12.5 mm. In this configuration the initial value of $\Delta \phi$ was 30.0° and decreased to smaller values according to Eq. (2). As shown in Fig. 6, the light spot (thin open circle) followed a spiral trajectory during the accessing process to find the detector aperture (bold open circle), and finished the centering process perfectly. (We show only every tenth step in Fig. 6 for clarity.) Figure 7 shows the change of intensity at the detector during the simulated alignment procedure together with changes of the error parameters. Here, ST1, ST2, and ST3 represent the first, the second, and the
third steps of alignment algorithm, respectively, while AP and CP stand for accessing and centering processes, respectively. Figure 7(a) is the normalized signal at the detector, showing a clear increase of the light intensity between iteration Nos. 0–20 of the accessing process. During this process, the $\alpha$ and $\beta$-tilt angles vary simultaneously, as shown in Figs. 7(b) and 7(c), according to Eq. (3). The first centering process was carried out between iteration 20 and 470. The centering process along the $\xi$ direction (iteration number from 20 to 250) used only $\alpha$-tilt adjustment, while that along $\eta$ direction (iteration number from 250 to 470) used only $\beta$-tilt adjustment, as shown in Figs. 7(b) and 7(c). As explained above, the $\alpha$-tilt causes the light spot to move in and out of the plane of incidence. Therefore, once the centering process along the $\xi$ direction is over, the $\alpha$-tilt angle error was corrected to be zero with no more change during the rest of the alignment procedure.

At the starting point of the second step (iteration Nos. 470–700), the AOI was set at a different value, and the light spot could be out of detector aperture. However, in our simulation, the given translation error (1 mm) was not large enough to cause this effect. The signal stayed at 1.0 even if we changed the AOI. (This means that we had a much bigger aperture than the light spot.) However, the centering process was still performed by changing the $\beta$-tilt angle. After the second step, translation error $h$ and tilt error $\beta_2$ were calculated in the third step to move the specimen stage to the final position [Figs. 7(c) and 7(d)]. Careful inspection of the final step tells that the signal stayed at 1.0 after iteration No. 700, even if the $\beta$-tilt angle error was still being corrected. The reason is that the size of the detector aperture was much bigger than the light spot, as shown in Fig. 6. It is very important to note again that our centering process works regardless of the relative size of the light spot to the detector aperture, because we do not simply maximize the signal at the detector for the best alignment but try to find the midpoint between the opposite edges of the detector aperture.

Practical testing of the auto-alignment algorithm was performed with our ellipsometer, shown in Fig. 1. The result is shown in Fig. 8, whose notations are the same as those in Fig. 7 except for the intensity at the detector on an absolute scale. In the experiment, the initial error values of $\alpha$, $\beta$, and $h$ are set to be zero, since the perfectly aligned coordinates are not known at the beginning. The diameters of the light spot (laser beam) and the detector aperture were 0.8 and 3.0 mm, respectively, and $d_s$ was 207 mm.

The initial accessing process took much longer than in simulation. Judging from the oscillation number of $\alpha$- and $\beta$-tilt angle adjustments in Fig. 8, the search spiral required at least five rotations. However, these results confirm that our algorithm could perform the alignment procedure perfectly, even when the light spot was far from the detector aperture. The first AOI was $45^\circ$, and gave a relatively small reflected signal of 1.8 in Fig. 8(a). For the second step the AOI was changed to $70^\circ$, and the signal at detector increased to 4.0, which is reasonable because a larger AOI gives a bigger reflected signal. One anomaly we observed was a sudden drop of the detector signal at iteration 1150 after the starting point of the second step in Fig. 8(a). This indicated that the detector lost the light spot after changing the AOI, and the auto-alignment program performed accessing automatically [by changing only $\beta$-tilt angle in Fig. 8(c)]. This proves its ability to find the signal under any circumstances.

Another observation was that the light spot moved out of
the detector aperture completely during the correction process of the translation error $h$ during the third step, even if the detector aperture was bigger than the light spot. This is because the translation error $h$ was very large. As stated above, the size of the detector aperture is unimportant. To screen out stray light for the best possible measurements, the aperture size should be as small as possible. Once the auto-

alignment is complete, the aperture size can be reduced without affecting light path of perfect alignment. Time taken for each iteration in this experiment was approximately 60 ms. The whole alignment procedure with 2000 iterations took about 2 min.

It should be noted that applications of this algorithm are not restricted to alignment of monowavelength ellipsometers. It can be applied to many different types of multichannel ellipsometers, in which case the detector aperture is replaced by the entrance slit of a spectrometer. Even if the shape of the slit is rectangular instead of circular, the centering algorithm of Fig. 3 still works. So this alignment procedure can be widely used. It can also be used for any kind of alignment of a flat surface using only a light source and detector, for example, a lithographic system.

ACKNOWLEDGMENTS

This work was supported by Grant No. 98-0200-05-01-3 from the Basic Research Program of the Korea Science and Engineering Foundation.