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Birefringence simulation of annealed ingot of magnesium fluoride single crystal

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A B S T R A C T

We developed a method for simulating birefringence of an annealed ingot of MgF_2 single crystal for lithography optics. This method provides the optical path difference caused by crystal symmetry and residual stress existing in the crystal. The method consists of the heat conduction analysis, the residual stress analysis and the birefringence analysis. Because there exists no experimental data on the inelastic behavior of MgF_2 single crystal, the residual stress was estimated with the elastic thermal stress analysis using the finite element method by assuming a stress-free temperature. In this analysis, the temperature dependence of material properties and crystal anisotropy were taken into account. In the birefringence analysis, the distributions of optical path difference were calculated by an approximate method using the result of the residual stress analysis. This approximate method uses the average stress along the wave normal and is equivalent to the exact method in case of low stress dealt with the present study. In this analysis, it is possible to consider both the intrinsic birefringence and the stress birefringence in any crystal orientation. The distribution of the optical path difference in the annealed ingot obtained from the present calculation agrees qualitatively with that of the experiment. Its calculated value also agrees reasonably well with that of the experiment, when a stress-free temperature is adequately selected.

1. Introduction

Recently, the wavelength of light used in semiconductor lithography has become shorter and shorter for fine processing of electronic devices. Thus, magnesium fluoride (hereafter abbreviated as MgF_2) single crystal is expected as a new optical material for lithography because of its high durability and excellent transmission characteristic in vacuum ultraviolet region. When MgF_2 single crystals are used as optical material for light polarizer, we need crystals with large diameters.

Such large MgF_2 single crystals are grown by the Czochralski method or the vertical Bridgman method. Extremely high material performances are required for optical materials to achieve high resolution of lithography. In such use of MgF_2 single crystal, one of the technical issues is birefringence, which results in degrading the optical quality of the MgF_2 single crystal. The birefringence is classified into two categories, the intrinsic birefringence and the stress birefringence. The intrinsic birefringence is caused by the crystal symmetry and is necessary to use MgF_2 single crystal as a polarizing element. The stress birefringence is caused by the photo-elastic effect attributable to the residual stress of the crystal and induces the disarray of light. It is therefore important to reduce the stress birefringence by reducing the residual stress. In the Czochralski method, the residual stress is mainly induced in the crystal by the thermal stress, whereas in the vertical Bridgman method it is induced not only by the thermal stress but also by mechanical stress caused by the contact of the crystal and crucible. In general, as-grown single crystals with larger diameters have larger residual stress, which results in larger stress birefringence in as-grown crystals. Therefore, annealing after single-crystal growth is the indispensable process, when MgF_2 single crystal is used as an optical material for lithography. Such annealing reduces the residual stress and suppresses the stress birefringence to a low level, but very long annealing period is required to reduce the stress birefringence to a target value. Numerical simulations of the residual stress and the birefringence play an important role for searching effective annealing conditions.

In our previous study [1], we have already developed a method for simulating the birefringence of an annealed ingot of CaF_2 single crystal for a lens material in the wafer-stepper of the semiconductor lithography. CaF_2 single crystal is the cubic system,

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whereas MgF_2 single crystal is the tetragonal system. It is therefore expected that MgF_2 single crystal shows more complicated birefringence than CaF_2 single crystal. The analysis of birefringence due to residual stress has not been performed so far for the tetragonal crystal. In the present paper, we develop a methodology for simulating the stress birefringence of the single crystal with the tetragonal system and perform the birefringence analysis of a MgF_2 single-crystal ingot after annealing.

2. Theory of birefringence

Based on Ref. [2], we summarize the theory of birefringence.

2.1. Photo-elastic effect

The dielectric constant is changed by the stress. Such an effect is called the photo-elastic effect. In general, it is given by

$$\begin{Bmatrix} \Delta B_1 \\ \Delta B_2 \\ \Delta B_3 \\ \Delta B_4 \\ \Delta B_5 \\ \Delta B_6 \end{Bmatrix} = \begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{13} & \pi_{14} & \pi_{15} & \pi_{16} \\ \pi_{21} & \pi_{22} & \pi_{23} & \pi_{24} & \pi_{25} & \pi_{26} \\ \pi_{31} & \pi_{32} & \pi_{33} & \pi_{34} & \pi_{35} & \pi_{36} \\ \pi_{41} & \pi_{42} & \pi_{43} & \pi_{44} & \pi_{45} & \pi_{46} \\ \pi_{51} & \pi_{52} & \pi_{53} & \pi_{54} & \pi_{55} & \pi_{56} \\ \pi_{61} & \pi_{62} & \pi_{63} & \pi_{64} & \pi_{65} & \pi_{66} \end{bmatrix} \begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{Bmatrix} \tag{1}$$

where σ_i is the stress, ΔB_i the change of the inverse dielectric constant and π_{ij} the piezo-optical constant. The subscripts i and j are abbreviated forms of tensor indices, and the corresponding relations are as follows: $11 \rightarrow 1$, $22 \rightarrow 2$, $33 \rightarrow 3$, 23 and $32 \rightarrow 4$, 31 and $13 \rightarrow 5$, and 12 and $21 \rightarrow 6$.

MgF_2 single crystal belongs to the 4/mmm crystal point group and the tetragonal crystal, so the photo-elastic matrix can be simplified as follows, when the analysis coordinate system (x_1–x_2–x_3) is coincident with the crystal coordinate system (X_1–X_2–X_3):

$$\begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{13} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{13} & 0 & 0 & 0 \\ \pi_{31} & \pi_{31} & \pi_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{66} \end{bmatrix} \tag{2}$$

In the case where the analysis coordinate system is not coincident with the crystal coordinate system, the components of photo-elastic matrix are obtained using tensor transformation.

For the symmetric property of MgF_2 single crystal, the components of the inverse dielectric constant B_i are expressed in the crystal coordinate system by the refractive index for ordinary-ray n_o and that for extraordinary-ray n_e as follows:

$$\begin{Bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \\ B_6 \end{Bmatrix} = \begin{Bmatrix} B_1 \\ B_1 \\ B_3 \\ 0 \\ 0 \\ 0 \end{Bmatrix} = \begin{Bmatrix} 1/n_o^2 \\ 1/n_o^2 \\ 1/n_e^2 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{3}$$

2.2. Indicatrix

We consider the following indicatrix described in the analysis coordinate system (x_1–x_2–x_3) to obtain the refractive indices

$$B_1x_1^2 + B_2x_2^2 + B_3x_3^2 + 2B_4x_2x_3 + 2B_5x_3x_1 + 2B_6x_1x_2 = 1 \tag{4}$$

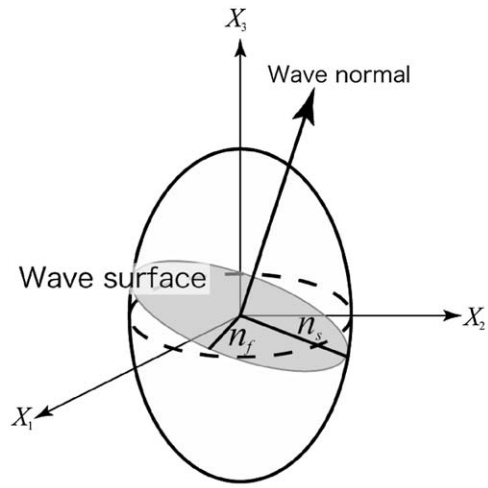

Fig. 1. An indicatrix and determination of refractive indices.

When stress is applied to single crystal, the indicatrix is expressed by adding the increment of B_i calculated from Eq. (1).

$$\begin{aligned}(B_1 + \Delta B_1)x_1^2 + (B_2 + \Delta B_2)x_2^2 + (B_3 + \Delta B_3)x_3^2 + 2(B_4 + \Delta B_4)x_2x_3 \\ + 2(B_5 + \Delta B_5)x_3x_1 + 2(B_6 + \Delta B_6)x_1x_2 \\ = 1\end{aligned} \tag{5}$$

The refractive indices are determined as follows. As shown in Fig. 1, a wave surface cuts an ellipse from the ellipsoid. Light can be decomposed into the oscillation components along the two principal axes, the long axis and the short axis, of the ellipse. The long axis and the short axis are called the slow axis and the fast axis, respectively. The lengths of the principal axes of the ellipse correspond to the refractive index along the slow axis n_s and that along the fast axis n_f.

When the wave normal coincides with the x_3-axis of the analysis coordinate system, Eq. (6) is obtained by taking $x_3 = 0$ in Eq. (5).

$$(B_1 + \Delta B_1)x_1^2 + (B_2 + \Delta B_2)x_2^2 + 2(B_6 + \Delta B_6)x_1x_2 = 1 \tag{6}$$

From this ellipse, we can calculate the birefringence $\Delta n = n_s - n_f$ defined by the difference between two refractive indices and the azimuth ρ defined by the angle between the fast axis and the x_1-axis as follows:

$$\Delta n = \frac{1}{2}\left(\frac{B_1 + \Delta B_1 + B_2 + \Delta B_2}{2}\right)^{-3/2} \times \sqrt{(B_1 + \Delta B_1 - B_2 - \Delta B_2)^2 + 4(B_6 + \Delta B_6)^2} \tag{7}$$

$$\tan 2\rho = \frac{2(B_6 + \Delta B_6)}{B_1 + \Delta B_1 - B_2 - \Delta B_2} \tag{8}$$

3. Method of analysis

In the birefringence simulation of MgF_2 single crystal after annealing, the heat conduction analysis during the annealing process is firstly performed to calculate the temperature distribution in the single crystal, then the residual stress is obtained from the thermal stress analysis, and finally the optical