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Residual stress prediction and control of Ta_2O_5/SiO_2 multilayer based on layer structure designing

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Residual stress, which can be inevitably introduced during the optical films deposition process, must be controlled in many applications since the surface deformation is caused. The residual stress is traditionally controlled by adjusting the process parameters. However, the process parameters are determined by other more desired properties in many fields. In these cases, layer structure is the only variable to change the residual stress status of the components. Ta_2O_5/SiO_2 is most commonly used material pair in visible/near infrared (VIS/NIR) region. In this letter, stress behaviors of Ta_2O_5 and SiO_2 single layers deposited by ion-assisted deposition (IAD) are studied. Stress-thickness linear correlation curves of the two materials are obtained, which agree with the commonly reported linear results. Based on these features, a kind of antireflection (AR) coating acted as back side coating is designed to control the residual stress of components by the layer structure designing. A series of AR coatings at 1 319 nm are designed, according to residual stress status desired to introduce.

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Optical films have been widely applied in industry[1], such as semiconductor device, optical communication[2], photon-electronic monitor, and all kinds of optical system. Residual stress accumulation, which is inevitable during the optical films deposition process, is one of the most important factors to obtain desired optical properties. In optical communication, filters, such as dense wavelength division multiplexing (DWDM), coarse wavelength division multiplexing (CWDM) etc.[3−5], always have very thick layer structure and residual stress accumulation can cause the deformation of the substrate, which will lead to the transmission failure of the signal.

For decades, great efforts have been made on the research of correlation between the residual stress and process parameters for different materials. The researches had been focusing on the reducing the residual stress of multilayer system by adjusting the process parameters and materials[6−8]. However, the process parameters are always determined by other more desired properties in certain specific applications. Taking the laser cavity mirror as an example, the process is set to pursue minimum loss to achieve maximum reflectivity. In these cases, layer structure designing is the only variable to change the residual stress status of the multilayer system.

This letter studies stress behaviors of Ta_2O_5 and SiO_2 single layers deposited by ion-assisted deposition (IAD). Stress-thickness correlation curves of the two materials are obtained. Based on these relations, a kind of antireflection (AR) coating is designed to control the residual stress of components. Finally, a series of AR coatings at 1 319 nm are designed, according to residual stress status desired to introduce.

The residual stress was calculated by the Stony equation[9]:

$$\sigma = \frac{4E_\mathrm{s}d_\mathrm{s}^2}{3(1-\gamma_\mathrm{s})D_\mathrm{s}^2}\frac{\Delta\mathrm{PV}}{d_\mathrm{f}}, \tag{1}$$

where σ is the residual stress of the coating; E_s and γ_s are the elastic modulus and Poisson ratio of the substrate, respectively; D_s is the diameter of the substrate; d_s is the thickness; d_f is the thickness of the film; ΔPV is the value of surface figure change which can be measured by interferometer.

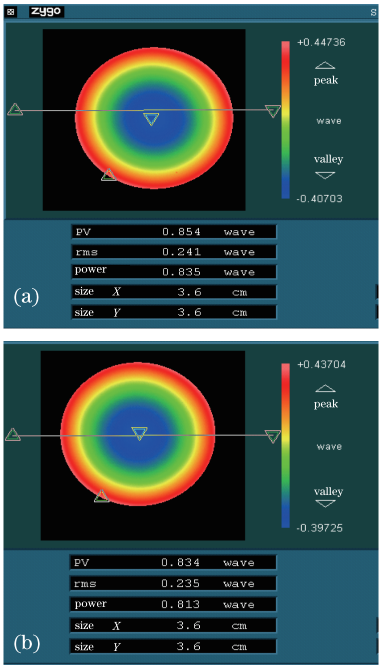
In this study, AR coating, which is commonly used as back side coating, aims to introduce desired residual stress, which can balance the residual stress from the front side coating and decrease the deformation of the whole component.

In order to introduce desired residual stress, we brought forward following AR layer structure: $\mathrm{S}|(2H)^x(mHnL)|\mathrm{A}$ or $\mathrm{S}|(2L)^x(mHnL)|\mathrm{A}$. H and L represent a quarter optical thickness high-index and low-index materials at wavelength λ and λ is the reference wavelength. $(2\mathrm{H})^x$ or $(2\mathrm{L})^x$ actually acts as absentee layer and can introduce the desired residual stress by adjusting the value of x. (mHnL) acts as the AR coating.

In this study, single crystal silicon wafers ($\phi40\times10$) were used as substrate and all samples were fabricatedby IAD. The process parameters are outlined in Table 1. For Ta_2O_5 and SiO_2 single layers, a series of samples with different thicknesses were produced. For the $(2\mathrm{L})^x0.73\mathrm{H}$ 0.59L structure, four samples were produced (x=1, 3, 6, and 10) and the reference wavelength is 1 319 nm. The thicknesses of samples were controlled by optical monitor system and crystal monitor system. The surface figure measurements were performed before and after the deposition using Zygo interferometer, respectively.

Table 1. Process Parameters for Ta_2O_5 and SiO_2 Single Layers

Films	Ta_2O_5	SiO_2
Base Pressure (Pa)	2×10^{-4}	2×10^{-4}
Chamber Pressure (Pa)	1.7×10^{-2}	1.1×10^{-2}
Deposition Rate (nm/s)	0.3	0.6
Substrate Temp. (°C)	200	200



(a)
PV 0.854 wave
rms 0.241 wave
power 0.835 wave
size X 3.6 cm
size Y 3.6 cm

(b)
PV 0.834 wave
rms 0.235 wave
power 0.813 wave
size X 3.6 cm
size Y 3.6 cm

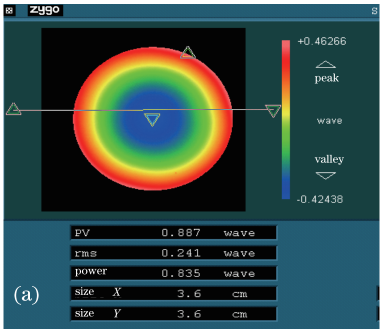
Fig. 1. Surface figure (a) before and (b) after Ta_2O_5 single layer deposition.

Table 2. Results of Single Layers

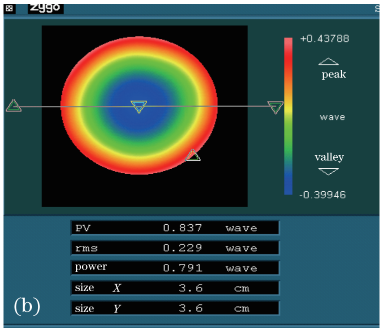
No.	Thickness (nm)	ΔPV (nm)	σ (MPa)
Ta_2O_5 Single Layer			
1	500	6.96	197.37
2	1 000	12.656	358.86
SiO_2 Single Layer			
No.	Thickness (nm)	ΔPV (nm)	σ (MPa)
1	500	9.39	269.14
2	1 000	20.88	592.12
3	1 500	31.64	897.15

Figures 1 and 2 show the typical surface figures of the samples before and after the two coating, respectively. Table 2 gives all the results of surface figure change and residual stress calculated from Eq. (1). For single crystal silicon substrate, E_s=130 GPa and γ_s=0.23 were used in the calculation.

As shown in Figs. 1 and 2, both materials introduced compress stress. For Ta_2O_5 single layer, the residual stress and thickness exhibited a linear relationship within 1 000 nm and SiO_2 also showed linear relationship with in 1 500 nm, which agree with commonly reported linear relationship between the two variables[10]. This correlation made it easy to control the residual stress by adjusting the thickness of the films. Two stress-thickness models were the built up by linear regression.



(a)
PV 0.887 wave
rms 0.241 wave
power 0.835 wave
size X 3.6 cm
size Y 3.6 cm



(b)
PV 0.837 wave
rms 0.229 wave
power 0.791 wave
size X 3.6 cm
size Y 3.6 cm

Fig. 2. Surface figure (a) before and (b) after SiO_2 single layer deposition.

For Ta_2O_5 single layer:

$\sigma = (5.98 + 0.35886d)$ MPa,

for SiO_2 single layer:

$\sigma = (0.60289d - 12.56)$ MPa,

where d (nm) is the thickness of the film. Figure 3 is the linear regression results. For SiO_2 single layer having a wide range of stress-thickness linear correlation, we choose S|$(2L)^x(mHnL)$|A in the following study.

In order to study the stress behavior of $(mHnL)$ in the $(2L)^x(mHnL)$ multilayer system, $(2L)^x(2H2L)$ multilayer were chosen to examine the residual stress behavior of the last two layers and the reference wavelength is 1 319 nm. For the AR coating S|$(2L)^x(mHnL)$|A at 1 319 nm, it can easily get from the classical films optics that m=0.73 and n=0.59.

Table 3 gives all the results of residual stress behavior of $(2L)^x(0.73H0.59L)$ multilayer system, which exhibit non-linear correlation between x and residual stress introduced by last two layers. This might be the couple effects of two different materials. For x=1, $d_{Ta_2O_5}$=111.8 nm and d_{SiO_2}=133.2 nm. According to the linear model mentioned above, the residual stresses are 40.1 and 67.37 MPa for single Ta_2O_5 and SiO_2 layers. This means the coupled effects of two materials can increase the accumulation of the stress. Based on this result, we believe the affection of last two layers becomes smaller dramatically with x increases. Based on the datum of Table 3, an exponential model was used to fit the datum and following result was gotten: $\sigma = 861.7e^{-1.397x} + 185.2e^{-0.1236x}$ and Fig. 4 shows the fitted results.

Based on datum analysis mentioned above, a series of AR coatings working at 1 319 nm were designed in order to introduce desired residual stress. This kind of

Table 3. Stress Introduced by (0.73H0.59L)

No.	X	Δ PV (nm) (Last Two Layers)	σ (MPa) (Last Two Layers)
1	1	13.29	376.80
2	2	3.79	197.37
3	5	2.54	100.65
4	10	1.90	53.83

Table 4. Residual Stress of AR Coatings

No.	x	σ (MPa)
1	1	563.04
2	2	582.40
3	3	724.70
4	4	898.84

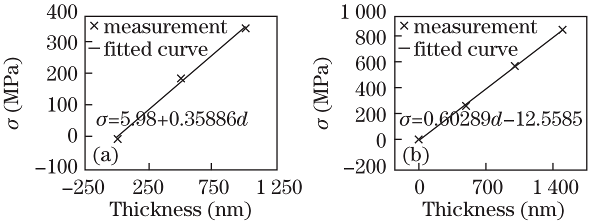


Fig. 3. Residual stress-thickness liner correlation model. (a) Ta_2O_5 single layer; (b) SiO_2 single layer.

AR coating can act as back side coating to balance the residual stress from the front side and decrease the deformation of the component.

For the AR coating S|(2L)^x(0.73H0.59L)|A at 1 319 nm, Fig. 5 shows the calculated spectrum the AR coating with different x. Table 4 gives the calculated residual stress of these AR coatings. The calculated residual stress is the plus of two parts: stress introduced by (2L)^x and the stress introduced by (0.73H0.59L). The residual stress of the whole system can be summarized by

$$\sigma = (0.60289 \times 0.28x - 12.56 + 861.7\mathrm{e}^{-1.397x} + 185.2\mathrm{e}^{-0.1236x})\ \mathrm{MPa}. \qquad (2)$$

In conclusion, we study the correlation of the residual stress and thickness for Ta_2O_5 and SiO_2 single layers. Liner model for the two variables are built for Ta_2O_5 single layer within 1 000 nm and for SiO_2 within 2 000 nm. Due to SiO_2 single layer having a wide range of stress-thickness linear correlation and introducing large compress stress, S|(2L)^x(mHnL)|A AR coating are chosen to act as residual stress introducer. The affection of last two layers becomes smaller with x increasing. In 1 319 nm, we design a series of AR coating which can introduce residual stress approximately from 560 to 900 MPa, which is can be used as back side coating to balance the stress of the front side coating.

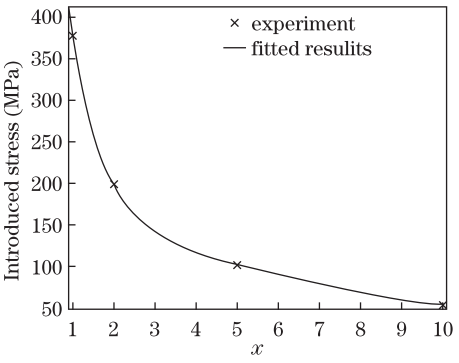


Fig. 4. Correlation between the residual stress introduced by the last two layer and the value of x.

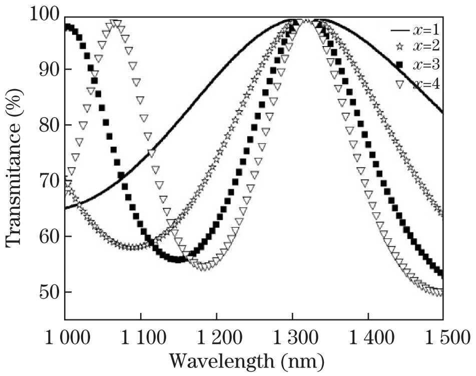


Fig. 5. Spectrum curve of the AR coatings at 1 319 nm.

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