A study on Curvature Control of Multi-Layer Film by Sputtering

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IKAROS, the solar power sail, launched at 2010 and demonstrated that thin-film solar cells could generate the electricity. Through the demonstration, it was found that the thin-film solar cells of IKAROS were curved. If the thin-film solar cells are curved, the attitude of the spacecraft becomes unstable. Therefore, this study has focused on sputter deposition that generates the internal stress by forming thin-films. The objective of this study is curvature control of multi-layer film by sputtering with a pattern. From the experiments and simulations, the effect of sputtering on the thin-film was analyzed, and it was clarified that the cause of the non-reproducibility of shape is sputtering stress.

スパッタリング法による多層膜の形状制御に関する研究

2010 年に打ち上げられたソーラー電力セイル実証機 IKAROS は，セイルに搭載した薄膜太陽電池での発電を実証したが，同時に薄膜太陽電池が持つ曲率によりセイル自体がたわんでしまうという問題も明らかにした．曲率を持ったセイルが太陽光圧を受けることで，宇宙機自体の姿勢が不安定な状態になる．しかし，薄膜太陽電池のような薄膜多層構造物の機械的，力学的研究はあまりなされていない．そこで，本研究では，スパッタリングにより発生する内部応力に着目し，模様をつけてスパッタリングを施すことで薄膜多層構造物を任意の形状に決定する手法を提案する．

Key Words: Sputtering, Curvature Control, Membrane Structures, Multi-layer, Internal Stress.

Nomenclature

E:	:	Young’s modulus, Pa
I:	:	moment of inertia of area, m^4
x:	:	length of in-plane x-axis direction of sputtered layer, m
z:	:	length of in-plane z-axis direction of sputtered layer, m
σ_{sp}:	:	sputtering stress, Pa
A:	:	area of sputtered layer, m^2
t:	:	thickness of sputtered layer, nm
a:	:	length of in-plane x-axis direction of substrate, m
b:	:	length of in-plane z-axis direction of substrate, m

1. Introduction

In recent years, thin-film multi-layer structures have been used in various fields and products such as semiconductors and thin-film solar cells. Inside the multi-layer film, stresses are generated. These stresses are generated due to film deformation and difference in thermal expansion coefficient of each film. Due to these stresses, the multi-layer film has curvature. This curvature can be a major obstacle to using products, such as peeling of multi-layer films.

The above problem also occurred in IKAROS,1) a solar power sail demonstrator launched in 2010. IKAROS succeeded in the world's first solar-sailing between planets. As a result, it was confirmed that the power generation by thin-film solar cells attached to the sail and the attitude of IKAROS became unstable at the same time receiving solar light pressure.2) This problem is probable that the curvature of the thin-film solar cell mounted on the sail warped the sail and the disturbance was caused by the deformed sail receiving solar light pressure.3) In addition, JAXA is currently studying Jupiter Trojans asteroid search using solar power sail explorer OKEANOS.4) This OKEANOS is equipped with a thin-film solar cell on the entire sail and generates thrust by the ion engine by generating high power. In the spacecraft having such a structure, the curvature of the thin-film solar cell gives a greater disturbance. Therefore, it is indispensable to control the curvature and further the shape of the multi-layer film for handling the multi-layer film. Therefore, a method that internal stress is generated in a thin-film multi-layered structure such as a thin-film solar cell by sputtering and the curvature of the multi-layer film is canceled by this internal stress is proposed by Shirasawa, Nakamura et al..5,6) However, in these studies, curvature control was limited to one-dimensional simple analysis. Therefore, in this study, we proposed a method of control the shape of the thin-film by sputtering by two-dimensional FEM analysis under various conditions on the phenomenon found by the experiment.

2. Cause of internal stress generated by sputtering method

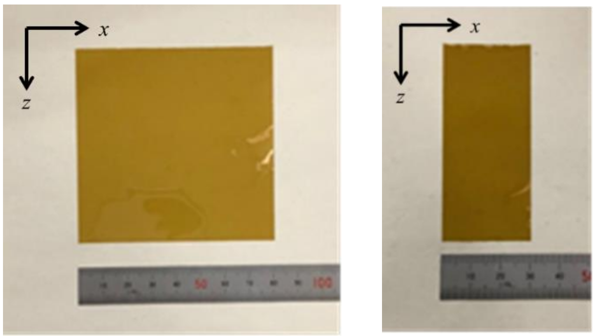
The internal stress generated by the sputtering method (hereinafter referred to as sputtering stress in this paper) is determined by the energy of the sputtered particles and the substrate temperature7) and these conditions can be controlled by several parameters. If the film formation pressure is low and the particle energy is large, the non-equilibrium of the thin-film deposition process becomes large, that is, because of its large energy, a thin-film can be formed even with an unnatural atomic arrangement, so that strain occurs in the thin-film, Stress is generated. At this time, if the substrate temperature is high, the particles can move to the more stable atomic arrangement on the thin-film or the inside, so the internal stress is alleviated. In the sputtering thin-film, the deposition pressure and the substrate temperature are important parameters for determining the internal stress, but in the sputtering method, which is the greatest advantage that film formation is possible at a low substrate temperature, raising the substrate temperature is not a good idea. Also, since an increase in particle energy also affects the deposition rate, low pressure is preferred in the industry. That is, it is a big problem in the sputtering method that the internal stress is larger for an industrially superior thin-film. However, studies on the electrical, magnetic and optical properties of thin-film materials have been extensively conducted, despite the accumulation of many useful data,8) their mechanical properties are not many studies. Although there are studies9-15) describing the relationship between sputtering conditions and internal stress, no research has yet been done to actively utilize its internal stress. This research is very useful in that this sputtering stress can be utilized. Although the thermal stress in the space environment is estimated to be several tens of MPa even though it is estimated to a large extent, since the sputtering stress is on the order of several hundreds to a thousand MPa, the influence by thermal stress can be ignored in this study.

3. Experiment of sputtering

In this experiment, the influence of sputtering for thin-film was qualitatively confirmed by confirming the film shape when film was formed on a rectangular substrate of 80 × 80 mm^2 square and 30 × 70 mm^2. Figure 3 shows a sample before film formation.

In this experiment, a DC magnetron sputtering apparatus owned by Geomatec Corporation was used. In this study, ZnO (zinc oxide) was used as a target material, but in this experiment, since ZnO is an insulator, G_2O_3 with a mass ratio of 1% was added to ZnO and used. Ube Industries UPILEX 25s which is a polyimide film with a thickness of 25 μm was used for the substrate. The target thickness of the sputtered layer was 300 nm.

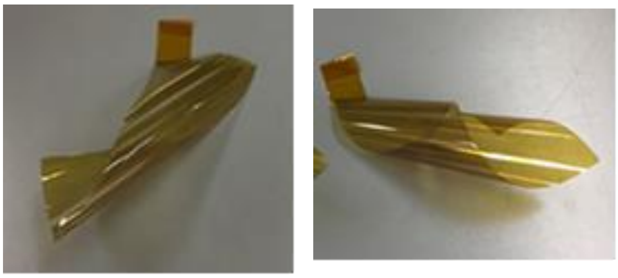
Figure 4 shows the results of sputtering experiments. Both (a) square specimen and (b) rectangular specimen were deformed by internal stress. Also, for both samples, the shape after deformation had no reproducibility and it bent in various directions. These shape changes can be confirmed that there was certain stable deformation for each substrate, but it was not only that it deformed in a certain fixed direction, but when a small external force was applied, it deflected in a direction different from the stable direction and stands still. From this, it can be seen that the sputtered film has a plurality of unstable equilibrium points. This is because there is shear stress component in the sputtering stress and there is no reproducibility in the principal directions even if the value of the main stress has reproducibility. That is, the internal stress state of the sputtered layer changes each time the film is formed.



(a) 80×80 mm^2 square. (b)70×30 mm^2 rectangular.

Fig. 3. The sample before sputtering.

(a) 80×80 mm^2 square.



(b) 70×30 mm^2 rectangular.

Fig. 4. The result of sputtering experiment.

4. Analysis of isotropic stress

4.1. Summary of analysis

As mentioned in Chapter 2, thermal stress and sputtering stress occur in the sputtered sample, but we analyzed sputtering stress which is dominant in this study. Also, as mentioned in Chapter 3, there is no reproducibility in the stress state of sputtering stress. So, there is a possibility that the shear stress component does not exist in the sputtering stress, namely, an isotropic stress state may occur. In order to understand phenomena in each, in this study, analysis of the thin-film shape was carried out separately into two kinds, in the case of isotropic stress state and the case where shear stress exists.

In this research, we analyzed using Abaqus which is one of general-purpose FEM software. A shell element was used for the element. The physical property values of the substrate and the target material used in the experiment were used as the physical property value.

4.2. Case of full surface sputtering

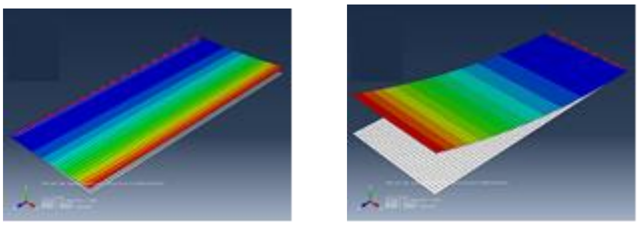
In this section, the shape when isotropic stress was applied to a bi-layered film sputtered over the entire rectangular substrate was confirmed. Here, the entire surface refers to the entire surface on one side of the substrate. Of the two-layer film of 70 × 30 mm^2, an isotropic stress simulating sputtering stress was applied to the sputtered layer, and the changed film shape was considered. We set the boundary condition to three types of fixed boundary condition, short side fixed, long side fixed and vertex fixed type, and confirmed the difference in film shape by the fixed types. The analysis results are shown in Fig. 5. The contour represents the displacement in the *y* direction (out-of-plane direction), indicating that the displacement is larger as it approaches red. Also, the film before deformation is shown in white. The dotted line or dot in red in the figure indicates a fixed portion. Table 1 shows the strain energy after deformation under each boundary condition.

From Fig. 5, it is found that when the long side is fixed, the short side was bent and when the short side was fixed, the long side was bent. That is, the sides perpendicular to the fixed sides were bent. Also, even when the apex was fixed, the long side bent. From Table 1, it can be seen that the strain energy was almost the same value at any boundary condition. From this, it can be said that there is a possibility that the vertex fixing may bend to either the long side or the short side depending on initial conditions such as fixing method.

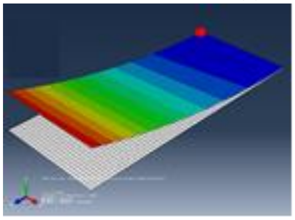
4.3. Case of partial sputtering

In this section, using the same substrate as used in Section 4.2, we qualitatively analyzed the influence of isotropic inner stress on film shape when sputtering a part of the substrate.

We considered a sputtering with a width of *z* = 10, 20 mm in length and fixing the lateral to *x* = 30 mm as shown in Fig. 6 on the 70 × 30 mm^2 substrate used in Section 4.2. The boundary condition is fixed at one vertex.



(a) Long side fixed.　(b) Short side fixed.



(c) Vertex fixed.

Fig. 5. The displacement in the y direction of bi-layered film when isotropic stress was applied.

Table. 1. Strain energies at the time of membrane deformation at each sputter shape and boundary condition. (μJ)

	(a) Long side fixed	(b) Short side fixed	(c) Vertex fixed
Entire surface sputtering	1.59411	1.57892	1.57649
Sputtered area 20 × 30 mm^2	15.3070	16.3431	15.3069

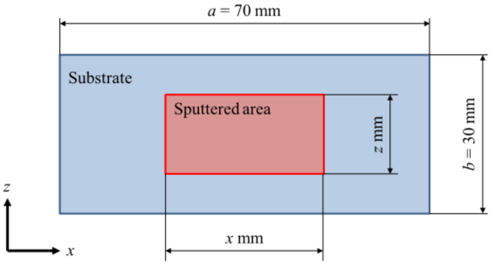
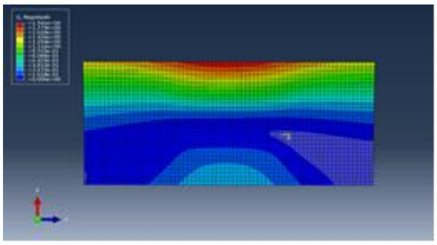
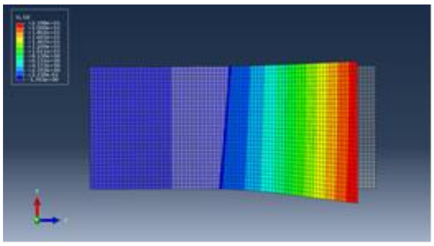


Fig. 6. The figure of analysis target.



(a) *z* = 10 mm.



(b) *z* = 20 mm.

Fig. 7. The displacements in the *y* direction when *x* = 30 mm fixed.

Figure 7 shows the analysis results. The thin-films before deformation are simultaneously displayed in gray. As can be seen from Fig. 7, the short side bent when *z* = 10 mm, and the long side bent when *z* = 20 mm. This change in the deflection direction can be explained by the ratio of the driving force for deforming the membrane and the flexural rigidity. If the one-dimensional stresses are generated in the depth direction when viewed from the short side of the substrate and when viewed from the long side, we consider the bending rigidity which is the resistance force against deformation for each side and the driving force trying to deform the membrane. The flexural rigidity is expressed by the product *EI* of the Young's modulus *E* of the substrate and the geometrical moment of inertia *I*. Here, since the thickness of the sputtered layer is sufficiently small with respect to the substrate, the flexural rigidity of the sputtered layer is negligible. The driving force to deform the membrane is represented by the product $\sigma_{sp}A$ of the sputtering stress σ_{sp} and the cross-sectional area *A* of the sputtered area. When comparing ratio of the flexural rigidity in driving force as shown below,

$$\frac{EI}{\sigma_{\mathrm{sp}}A}, \tag{1}$$

for the long side and the short side respectively, the Young's modulus, the sputtering stress, and the thickness of substrate t are equal to each other, so finally it can be came to comparison between the ratio of the width a of the substrate in the x direction to the width x of sputtered area as shown Eq. (2) and the ratio of the width b of the substrate in the z direction to the width z of sputtered area as shown Eq. (3).

$$\frac{x}{a}. \tag{2}$$

$$\frac{z}{b}. \tag{3}$$

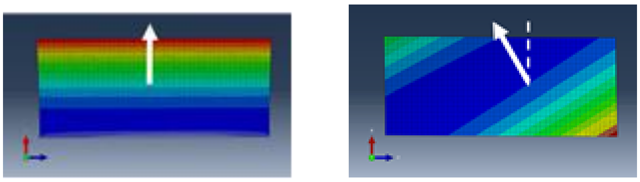
When comparing them, the smaller value means that the rigidity with respect to the driving force is lower, and this side is more likely to be deflected.

5. Analysis of inner stress with share stress

5.1. Case of full surface sputtering

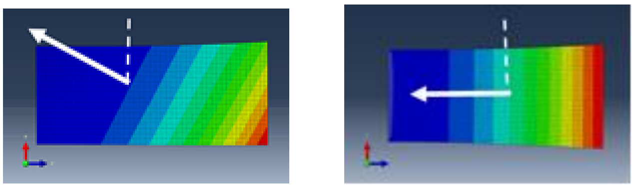
In this section, we showed analysis of the shape when shear stress exists in sputtering stress. Since the shear component is present in the sputtering stress and there is no reproducibility in the stress state, it was shown that reproducibility is not seen in the shape of the film because the principal directions is changed each time the film is formed. In this section, in order to verify this fact, initial stress that simulates sputtering stress was given to the thin-film (two-layer film) sputtered on the whole surface, and the change in the shape of the thin-film when changing the principal directions was confirmed. Boundary condition was one vertex perfectly fixed. Analysis model was the same model as in Section 4.2. The principal direction of stress generated in the sputtered layer was changed by 30 deg between 0 and 90 deg. Here, the direction of the white arrow shown in Fig. 8 is defined as the principal directions and white arrow shown in Fig. 8(a) is defined as the principal directions 0 deg.

The analysis result is shown in Fig. 8. As shown in the figure, the thin-film is bent along a straight line perpendicular to the principal directions. From the above, it can be inferred that the reason for the non-reproducibility in the shape shown in Chapter 3 is share stress of sputtering stress. Since the stress state of the sputtering stress cannot be controlled, it is difficult to estimate the deflection direction of the film in the entire surface sputtering.



(a) Principal direction of 0 deg.

(b) 30 deg.



(c) 60 deg.

(d) 90 deg.

Fig. 8. The shapes of entire sputtered bi-layer films at each principal direction

5.2. Case of partial sputtering

As described in Section 5.1, it is difficult to estimate the deflection shape of the film when sputtering is performed on the entire surface. Also, as shown in Section 3.1, the stress state of sputtering stress is not reproducible. Therefore, the non-reproducibility of the stress state of the sputtering stress is a problem to be solved in thin-film shape control, and it is necessary to consider countermeasures that are not influenced by the randomness in the principal directions. Therefore, we considered sputtering only a part of the substrate.

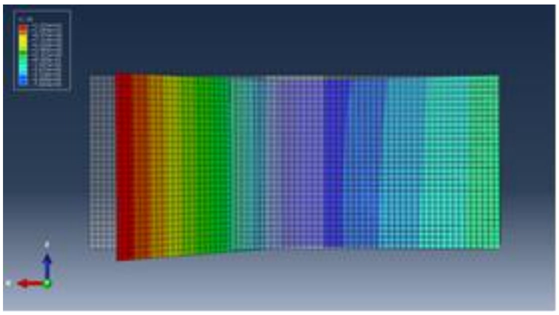
A rectangular sputtered thin-film was modeled on a 70 × 30 mm^2 square rectangular substrate as shown in Fig. 6, and the change in shape when changing the width of this sputtered area was examined. We considered a case where the width of the sputtered area was fixed at $z = 30$ mm and width x was changed, and width z was changed while fixing x at 70 mm. The same physical property values as those used in the analysis in Chapter 4 were used and the internal stress simulating the sputtering stress was given to the sputtered layer. The angle between the principal directions and the x axis in the plane is 30 deg. Also, for the boundary condition, one vertex was perfectly fixed, and the y direction displacement of one different point is fixed.

As an example of the analysis results, the analysis results in the sputtered area size 10 × 30 mm^2 and 50 × 30 mm^2 are shown in Fig. 9. The figure is a view of the membrane looking down from the out-of-plane y-axis. Furthermore, Fig. 10 shows the relationship between the deflection direction angle and the width of the sputtered area under each analysis condition. The deflection direction angle was defined as 0 deg when the isotropic stress is applied to each sputtered area, (e.g. since the long side is bent when sputter size is 10 × 30 mm^2 ,in this case, the z-axis direction is 0 deg), and the angle from this is defined as the deflection direction angle.

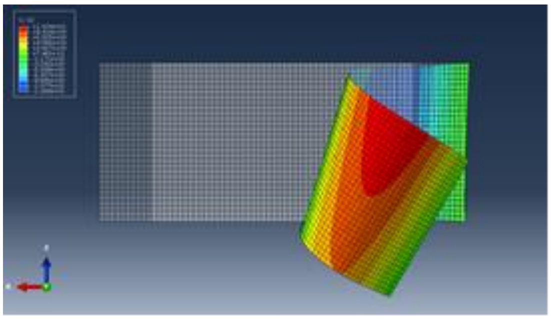
Comparing Fig. 9 with Fig. 8(b), the more width of sputtered area is attenuated, the more the deflection direction angles of Fig. 9, in which the region was narrowed down and sputtered, are smaller than the angle of Fig. 8 (b) which gives the same principal directions 30 deg. Also, from Fig.10, the deflection direction angles become smaller by reducing the width of the sputtered area. From these, it can be said that even if the stress state of the sputtering stress cannot be controlled, the film can be deflected in a desired direction by sputtering while narrowing down the region.

7. The patterns for shape control

In this section, we investigated sputtering patterns for shape control of thin-film structures with curvature by analysis. In Section 5.2, it was showed that when the width of the sputtered layer is shorter than that of the substrate and sputtered area is a rectangular shape, the influence of shear

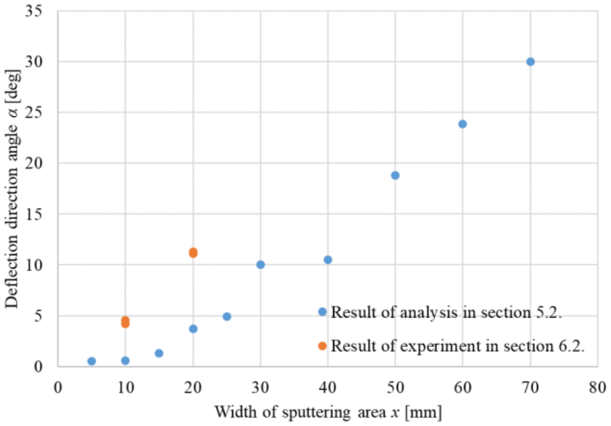


(a) In case of sputtered area 10 × 30 mm^2.

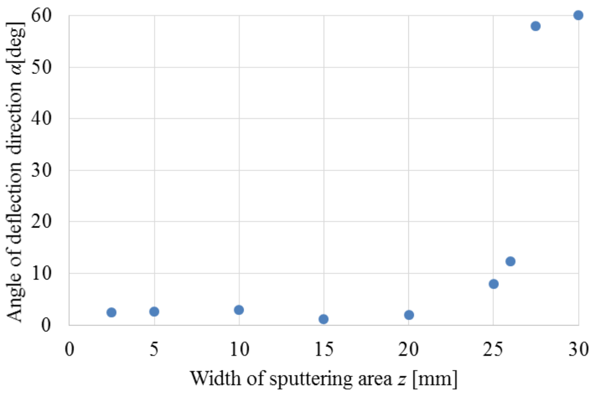


(b) In case of sputtered area 50 × 30 mm^2.

Fig. 9. The example of results of analysis.



(a) z =30 mm fixed.



(b) x = 70 mm fixed.

Fig. 10. The relationship between the deflection direction angle and the width of the sputtered area under each analysis condition.

stress is reduced, and the deflection direction is uniquely determined easily. We utilized and developed this, and shape control aimed at reducing curvature and deflection direction angle of thin-film structure with curvature.

The initial shape of the thin-film structure having the curvature and deflection direction angle is modeled by giving the initial stress whose principal directions is 30 deg to the first layer of 70 × 30 mm^2 two-layered film. The deflection direction angle at this time is 30 deg with respect to the z axis. This initial shape is shown in Fig. 11. A sputtered layer is added to the upper part of this two-layered film, and the shape of the thin-film structure when a sputtering stress having an arbitrary principal direction is given is analyzed. The sputtering stress at this time is compressive stress. Regarding the shape of the sputtered layer, we considered case where the sputtered area is 10 × 30 mm^2 in Fig. 6 and a cross shape as shown in Fig. 12.

Figure 13 shows the analysis results in the case of the sputtered area of 10 × 30 mm^2, and Fig. 14 shows the analysis result in the case where the sputtered area is cross. Comparing the initial shape with Fig. 13, both the curvature and deflection direction angles decrease. The deflection direction angle decreased from 30 deg to 9.8 deg. From this, the method of limiting the sputtered area and sputtering in a rectangular shape for reducing the deflection direction angle is also useful for thin-film structures having curvature and deflection direction angle from the beginning. From Fig. 14, it can be qualitatively confirmed that the curvature and the deflection direction angle was further suppressed as compared with the case of the rectangular sputtered area. This is because each sides of the long side and the short side is deflected by shaping two rectangles like a cruciform shape, so that the rigidity of each sides is increased so as to cancel out each other's deflection, as a result, a whole shape close to a flat shape.

In this cruciform sputtered area, the curvature can be adjusted by adjusting the width of each side of sputtered area. Therefore, by adjusting the width according to the curvature, the rigidity, and the sputtering stress value of the thin-film structure as the control target, shape control with higher accuracy becomes possible. In this paper, analysis by compression stress is shown, but it was confirmed that it is possible to control the curvature and deflection direction angle similarly with tensile stress. The sputtering stress varies depending on the target material and various conditions during sputtering, such as values, tension / compression, etc.[11-15] By using this, it is possible to control the shape according to the method described in this paper, even for thin-film solar cells and the like which are restricted in sputtering surface.

8. Conclusion

In this paper, experiments and analyzes were conducted on the shape of sputtered bilayer films. Experiments showed that the shape after sputtering was not reproducible under the same conditions. We also analyzed the effect of sputtering stress on the shape of the bilayer films. For isotropic stress, it showed a different shape depending on the fixing method and showed no difference in the strain energy. In the presence of the shear stress component, it showed that the bilayer film bends along the line perpendicular to the principal directions. From this result, it was considered that sputtering stress is involved in shape non-reproducibility. The sputtering patterns capable of controlling the shape of the thin-film under an arbitrary stress state was shown. It was shown that the shape after deformation is easily uniquely determined by the rectangular sputtering shape with the width reduced relative to the width of the substrate. In addition, it was shown that by using this sputtering shape, it is possible to control the shape of thin-film structure having curvature and deflection direction angle from the beginning. Moreover, it showed that control with higher precision is possible by the shape of the cruciform shape to which this is applied.

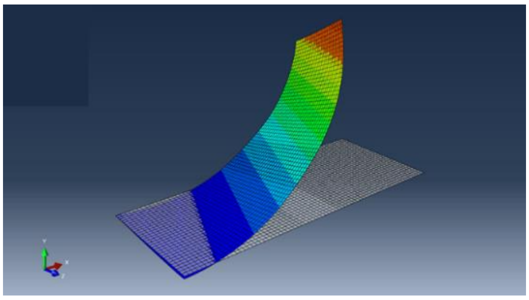


Fig. 11. The initial shape of thin-film structures with curvature.

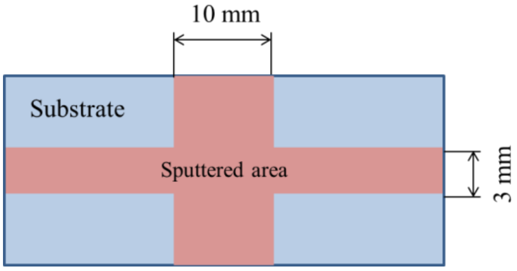


Fig. 12. The figure of cruciform sputtered area.

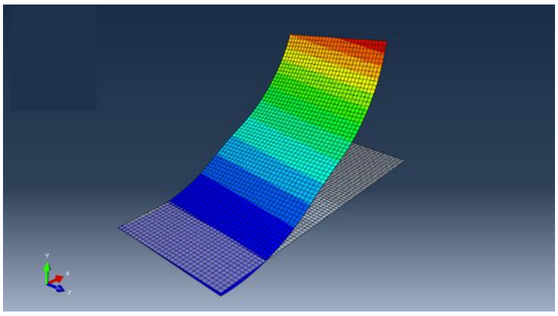


Fig.13. The result of analysis in case where sputtered area is 10×30 mm^2.

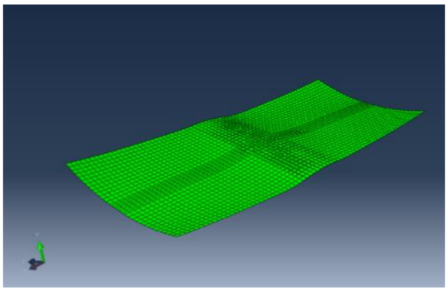


Fig. 14. The result of analysis in case where sputtered area is cruciform.

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