Numerical Analysis for Evaluating Adhesion of Arbitrary-shaped Microstructures Using Optimization Method

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This paper discusses a method of analyzing the adhesion problem of arbitrary-shaped microstructures using FEM and an optimization. We have applied our method to square plates, and obtained realistic curved adhesion shapes. We fabricated square plates as test samples, and calculated γ_S of these samples by using our method. Adhesion criteria are also derived by numerical calculation. We then redesigned the adhesion samples by applying this method, and subsequent tests showed no adhesion of the samples.

Keywords: adhesion, finite element method, optimization method

1. INTRODUCTION

Microstructures contact their underlying substrate due to various causes, such as wet etching of sacrificial layers and actual operations. Such contact causes permanent adhesion between the microstructures and substrate and destroys the functionality of the device, and so is a serious problem in the design of microstructures.

Many authors have developed measures to prevent adhesion both theoretically and experimentally, but a design method to avoid adhesion is still necessary. C. H. Mastrangelo and C. H. Hsu investigated the adhesion problem of microstructures [1][2]. They conducted a theoretical analysis of beams and circular plates, in which the adhesion shape is assumed easily, and derived an adhesion formula for these structures and an approximation formula for square plates.

However, their analysis method is difficult to apply to arbitrary-shaped structures because of the difficulty of estimating the adhesion shape, and so a series of samples must be fabricated to calculate the surface energy γ_S.

In this paper, we present a method of calculating γ_S by using an adhesion area measured from one fabricated adhesion sample, and then analyze the adhesion problem of arbitrary-shaped structures by using this value of γ_S. A design method for preventing adhesion is also presented. We fabricated square plates of SOI wafers as test samples, and calculated γ_S from the adhesion samples. Using this value and the new design method, we then redesigned the samples to prevent sticking to the substrate.

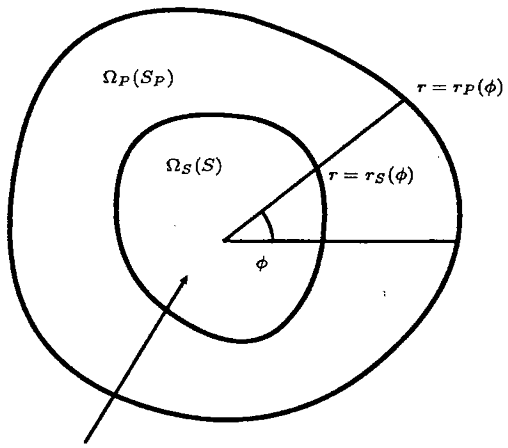


Fig. 1. Formulation of an adhesion problem of an arbitrary-shaped plate.

2. THEORY

In this section, the adhesion problem is formulated. Consider a problem as shown in Figs. 1 and 2. A suspended plate of thickness t, domain Ω_P (area S_P) is clamped to the substrate on its outer periphery as follows:

$$r = r_P(\phi) \qquad (1)$$

The plate sticks to the substrate in the central region Ω_S (area S) defined by the following curve:

$$r = r_S(\phi) \qquad (2)$$

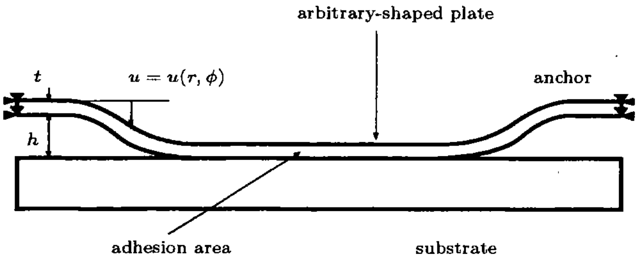


Fig. 2. Cross-section of the plate.

Adhesion area $S(0 \leq S < S_P)$ is a variable which depends on the condition of the surfaces, so we will treat this value as an independent value here.

The plate deflection $u = u(r, \phi)$ satisfies the following boundary conditions:

$$\begin{array}{ll} u(r,\phi)|_{r=r_P(\phi)} = 0, & \nabla u \cdot \mathbf{n}|_{r=r_P(\phi)} = 0, \\ u(r,\phi)|_{r=r_S(\phi)} = h, & \nabla u \cdot \mathbf{n}|_{r=r_S(\phi)} = 0, \end{array} \quad \cdots (3)$$

where h is the gap between the plate and the substrate, and $\mathbf{n}$ is a unit outward normal vector on the boundary. The total energy of the system U_T is

$$U_T = U_E + U_{SC}, \cdots\cdots\cdots\cdots (4)$$

where U_E is the elastic energy of the deflected plate, and U_{SC} is the adhesion energy of the solid-solid contact. U_{SC} is expressed as follows:

$$U_{SC} = -\gamma_S S, \cdots\cdots\cdots\cdots (5)$$

where γ_S is the interfacial adhesion energy per unit area. The actual adhesion shape minimizes the value of U_T, therefore, the solution is the shape which minimizes Eq. (4).

2.1 Elastic energy In this section, the method of calculating the elastic energy of the adhesion plate is described. First, we consider a searching problem of the adhesion shape. Let S_{me} be an adhesion area measured from an adhesion sample. S_{me} is obviously a constant value, and γ_S is also a constant due to the characteristics of process conditions and materials. The actual adhesion shape Ω_{me} (the area of the region Ω_{me} equals S_{me}) minimizes the total energy U_T.

$$\begin{aligned} \min_{\Omega_{me} \in \Omega_P} \{U_T\} &= \min_{\Omega_{me} \in \Omega_P} \{U_E - \gamma_S S_{me}\} \\ &= \min_{\Omega_{me} \in \Omega_P} \{U_E\} + \text{const.} \cdots\cdots (6) \end{aligned}$$

Hence, a shape which minimizes U_T and a shape which minimizes U_E are the same shape under the condition of the measured value $S = S_{me}(0 \leq S_{me} < S_P)$. That is, the adhesion shape is calculated by minimizing the elastic energy U_E under the condition of $S = S_{me}$ being a fixed value.

This fixed area S_{me} depends on the condition of the surfaces. In other words, any adhesion area could be made under certain process conditions or adhesion energy γ_S. Therefore, the relationship between the adhesion area S and the elastic energy U_E is calculated by minimizing the elastic energy U_E under the condition of several fixed values of S. It is difficult to calculate a continuous relationship between U_E and S, but it is possible to calculate a discrete relationship by this method.

2.2 Surface energy In this section, the surface energy γ_S is calculated from the elastic energy U_E. We consider the area differential of the total energy Eq. (4) at $S = S_{me}$.

$$\left.\frac{\partial U_T}{\partial S}\right|_{S=S_{me}} = \left.\frac{\partial U_E}{\partial S}\right|_{S=S_{me}} - \gamma_S. \cdots\cdots\cdots (7)$$

The total energy U_T already takes the minimum value under the condition of $S = S_{me}$ because the condition of $S = S_{me}$ is the actual situation in this problem, therefore $\partial U_T / \partial S$ is zero, and

$$\gamma_S = \left.\frac{\partial U_E}{\partial S}\right|_{S=S_{me}} . \cdots\cdots\cdots\cdots (8)$$

The relationship between S and U_E is discrete when using the method described in the next section, so the differentiation of Eq. (8) is implemented by numerical differentiation.

2.3 Search for adhesion shape The search for an adhesion shape is a kind of optimization problem, and is divided into two portions. One is the search problem to minimize the total energy U_T, and this problem is used merely for searching for the adhesion shape. The other is used to obtain the relationship between the elastic energy U_E and the adhesion area S.

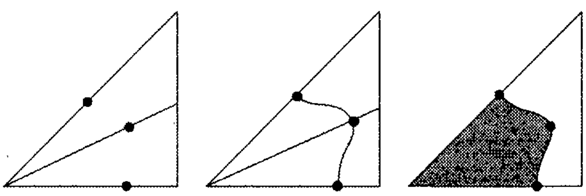
The minimization problem of U_T is defined as follows. U_T is an objective function and the adhesion shape is a design function. It is assumed that the adhesion energy per unit area γ_S is obtained experimentally or by another way. The problem of obtaining the U_E is defined as follows. U_E is an objective function, the adhesion shape is a design function, and the measured adhesion area S_{me} is a state variable. It is assumed that the adhesion area S_{me} is obtained experimentally.

These two problems have the same algorithm, so we describe the method of solving the minimization problem of U_T. Although in this paper we consider a square plate, other shapes can also be considering using the same method. A suspended square plate of width w and thickness t is considered and a 1/8 model is used in the calculation.

The algorithm is as follows:

1. An adhesion point which minimizes the elastic energy U_E of the system is defined on the plate. Boundary conditions are given by Eqs. (3). When the adhesion problem is that of a regular polygon, this operation is omitted because the adhesion point is obviously defined as the center of the object.

2. Several segments are defined on the plate and several search points are placed in the n-th piece on these



(a) Definition of the search points. (b) Spline function. (c) Adhesion shape and area.

Fig. 3. Definition of the spline function ($n = 3$).

segments as shown in Fig. 3(a):

$$P_1(r_1, \phi_1), P_2(r_2, \phi_2), \ldots, P_n(r_n, \phi_n), \cdots\cdots \quad (9)$$

where $r_1, r_2, \ldots, r_n, \phi_1, \phi_2, \ldots, \phi_n$ are unknown parameters.

3. A segmented spline function through a series of search points Eq. (9) is calculated as shown in Fig. 3(b):

$$r = r_s(P_1, P_2, \ldots, P_n; s), \cdots\cdots \quad (10)$$

where s is the parameter of the curve. The plate deflection u and the elastic energy U_E are calculated by FEM under the boundary conditions of Eq. (3) with Eq. (10). The slope of the deflection curve on the boundary also satisfies the symmetrical boundary conditions. The adhesion area is calculated by Eq. (10). We assume that γ_S is obtained experimentally or calculated by the method described in section 2.2. Therefore the total energy of the system U_T is calculated by using these values and Eqs. (4) and (5).

4. To minimize the total energy U_T, a series of points of Eq. (9) is changed by the optimization method (first order optimization method [3]) included in the ANSYS.

5. Iterate the calculations 2 to 4 until the total energy U_T is minimized.

In this paper we use $n = 3$. The numerical calculation (calculating the elastic energy U_E and optimization method) is implemented within the ANSYS.

2.4 Criteria of adhesion In this section, we outline the comparative and judging method that is needed for designing microstructures. The elastic energy of the arbitrary-shaped plate as shown in Figs. 1 and 2 is:

$$U_E = \frac{1}{2}\frac{Dh^2}{S_P}\int_{\Omega_P-\Omega_S}(\nabla^2\tilde{u})^2 dS = \frac{1}{2}U_0\int_{\Omega_P-\Omega_S}(\nabla^2\tilde{u})^2 dS, \cdots\cdots \quad (11)$$

where ∇^2 is a Laplacian operator, $D = Et^3/12(1-\nu^2)$ is the flexural rigidity of the plate, $\tilde{u} = u/h$ is a dimensionless deflection function, and

$$U_0 = \frac{Dh^2}{S_P} \cdots\cdots \quad (12)$$

is a value which has the unit of energy. The dimensionless representation of Eq. (4) is given as follows:

$$\widetilde{U_T} = \widetilde{U_E}(\xi) - \widetilde{\gamma_S}\xi, \cdots\cdots \quad (13)$$

where $\widetilde{U_T} = U_T/U_0$, $\widetilde{U_E} = U_E/U_0$, $\xi = S/S_P$, and

$$\widetilde{\gamma_S} = \frac{\gamma_S}{U_0/S_P}. \cdots\cdots \quad (14)$$

The form of the function $\widetilde{U_E}$ is determined by the morphology of the system, and is also independent of S_P, t, and h.

If the continuous relationship between the elastic energy U_E and the adhesion area ξ is able to be calculated analytically, it is easy to derive adhesion criteria. However, the continuous relationship between them is difficult to calculate analytically. Therefore, we numerically calculate a discrete relationship between them and derive the adhesion criteria from the discrete relation.

When ξ is a fixed value ξ' $(0 \le \xi' < 1)$, the corresponding adhesion energy $\widetilde{\gamma_S}$ is also a fixed value $\widetilde{\gamma_S}'(= \text{const.})$. Thus, we obtain

$$\min_{\Omega' \in \Omega_P}\left\{\widetilde{U_T}\right\} = \min_{\Omega' \in \Omega_P}\left\{\widetilde{U_E} - \widetilde{\gamma_S}'\xi'\right\} = \min_{\Omega' \in \Omega_P}\left\{\widetilde{U_E}\right\} + \text{const.}, \cdots\cdots \quad (15)$$

where Ω' is an adhesion shape, the area of which has the fixed value ξ'. If we find a shape that minimizes $\widetilde{U_E}$ under the constant area ξ', the relationship between $\widetilde{U_E}$ and ξ' is obtained. The method described in section 2.3 is used to search for the adhesion shape Ω'. This discussion does not depend on a specific value of ξ', so the relationships between ξ' and $\widetilde{U_E}$ are obtained by calculating several values of ξ' in $0 \le \xi' < 1$.

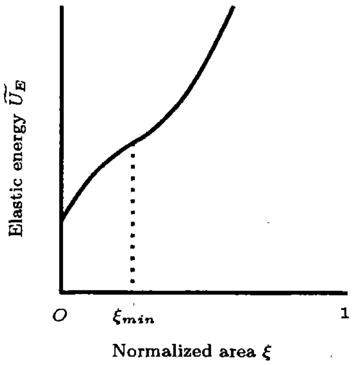
Consequently, we regard the several values of ξ' as the values of the independent variable ξ again, and so obtain a discrete relationship between the elastic energy $\widetilde{U_E}$ and the adhesion area ξ is obtained.

Therefore, we can calculate $\widetilde{\gamma_S}$ by the dimensionless expression of Eq. (8).

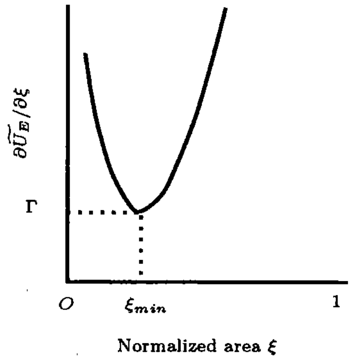
$$\widetilde{\gamma_S} = \left.\frac{\partial\widetilde{U_E}}{\partial\xi}\right|_{\xi=\xi_{me}} \cdots\cdots \quad (16)$$

where $\xi_{me} = S_{me}/S_P$ $(0 \le \xi_{me} < 1)$. Equation (16) is implemented by a numerical differentiation because the relationship between $\widetilde{U_E}$ and ξ calculated above is discrete.

On the other hand, Figure 4 shows a typical curve of $\widetilde{U_E}$ and a typical curve of $\partial\widetilde{U_E}/\partial\xi$. $\partial\widetilde{U_E}/\partial\xi$ has a minimum value. Let Γ be the minimum value of $\partial\widetilde{U_E}/\partial\xi$ as follows:



(a) Typical relationship between adhesion area and elastic energy. ξ_{min} is the value which minimizes $\partial\widetilde{U_E}/\partial\xi$.



(b) Typical relationship between adhesion area and area differential of elastic energy. ξ_{min} is the value which minimizes $\partial\widetilde{U_E}/\partial\xi$.

Fig. 4. Typical curve of the elastic energy and the area differential of the elastic energy.

$$\Gamma = \min_{0\leq\xi<1}\left\{\frac{\partial\widetilde{U_E}}{\partial\xi}\right\} \cdots\cdots (17)$$

If an experimental value of $\widetilde{\gamma_S}$ is less than Γ, there is no value of ξ_{me} that is defined by Eq. (16). In other words, there is no solution under the boundary conditions of Eq. (3). This means that the plate does not stick to the substrate. Thus, we can judge whether adhesion occurs or not as follows:

$$\widetilde{\gamma_S} \geq \Gamma \quad (\frac{\Gamma}{\widetilde{\gamma_S}} \leq 1) \quad \text{Stick,} \cdots\cdots (18)$$

$$\widetilde{\gamma_S} < \Gamma \quad (\frac{\Gamma}{\widetilde{\gamma_S}} > 1) \quad \text{Peel.} \cdots\cdots (19)$$

The adhesion problem is thus a comparison of Γ with $\widetilde{\gamma_S}$. C. H. Mastrangelo and C. H. Hsu defined the ratio of Γ and $\widetilde{\gamma_S}$ using a different method [1], and they called this value N_P.

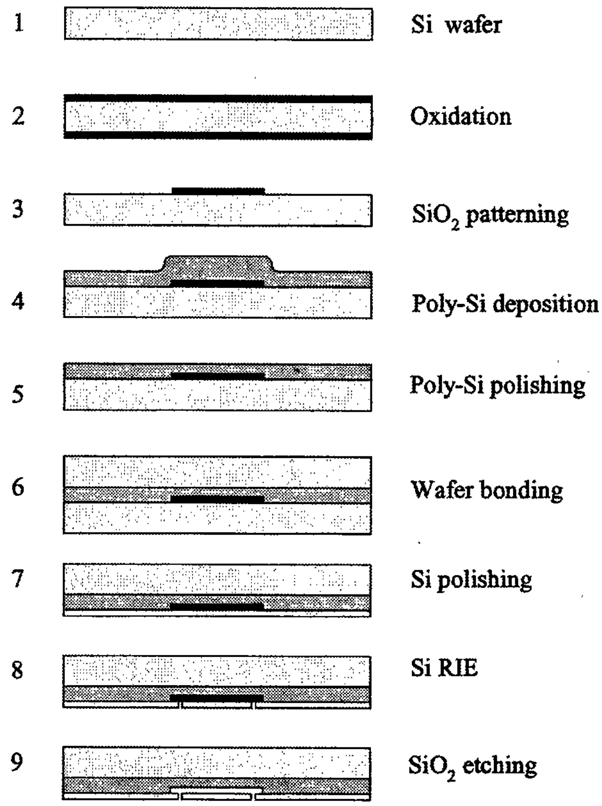


Fig. 5. Fabrication process of the test samples.

3. CALCULATION AND EXPERIMENT

To compare the theoretical results with the experimental ones, we fabricated square plates from SOI wafers as test samples. The fabrication process is shown in Fig. 5, and the cross-section of the sample is shown in Fig. 6.

3.1 Calculation of γ_S In this section, the value of γ_S is calculated from an adhesion sample fabricated as shown in Fig 5. The conditions of the sample are shown in Table 1.

Table 1. Conditions of the square plate

Width w	2000 μm
Thickness t	3.4 μm
Gap h	2 μm
Initial stress σ_R	0 GPa
Young's modulus E	145 GPa
Poisson's ratio ν	0.27

The adhesion area was measured from an infrared microscope photograph. The normalized adhesion area is $\xi_{me} = 0.39$. Figure 7(a)is an infrared microscope photograph of the adhesion sample. The dimensionless elastic energy $\widetilde{U_E}$ is calculated by FEM. Linear shell elements are used in this calculation and the number of elements is about 900. The first-order optimization

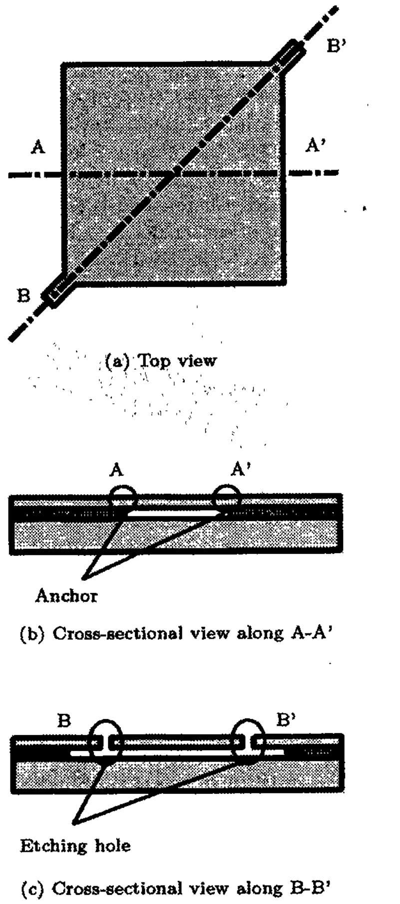


Fig. 6. Cross-section of the square sample. (a)Top view of the square plate. See Fig. 7(a), 7(b), (b)Cross-sectional view along A-A', (c)Cross-sectional view along B-B'.

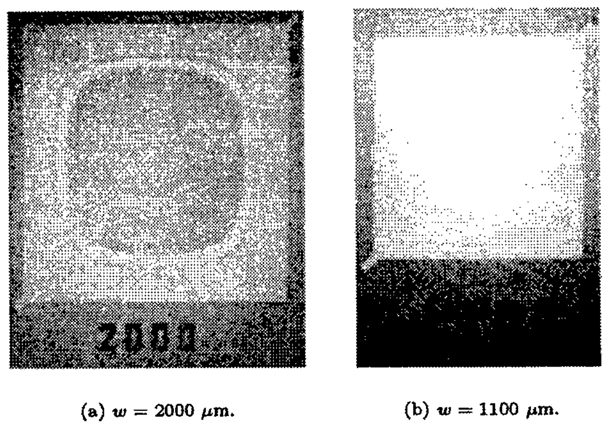


Fig. 7. Infrared microscope photograph of the adhesion and peeling samples. (a) Adhesion sample ($w = 2000\ \mu$m), (b) Peeling sample ($w = 1100\ \mu$m).

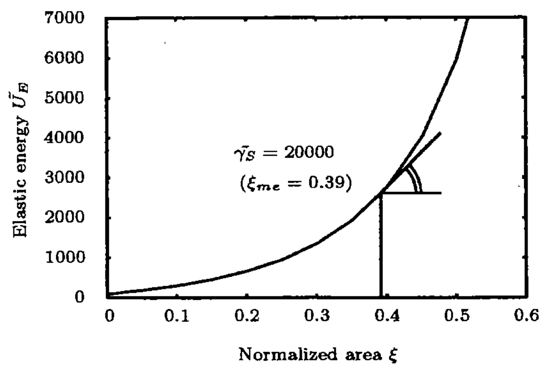


Fig. 8. Relationship between adhesion area and elastic energy ($w = 2000\ \mu$m, $\xi_{me} = 0.39$).

method which is built into the application functionality [3] is used as the optimization method. The relationship between ξ and $\widetilde{U_E}$ is shown in Fig. 8. The area differential coefficient of $\widetilde{U_E}$ at $\xi_{me} = 0.39$ is

$$\widetilde{\gamma_S} \simeq 20000. \qquad (20)$$

This value is equal to 2.6 mJ/m^2 by Eq. (14). The γ_S calculated from Mastrangelo's approximation formula of square plates [1] is 2.2 mJ/m^2. The error of these values is 30%. The difference is due to the fact that C. H. Mastrangelo and C. H. Hsu assumed that the adhesion shape is of the same shape as the outer boundary.

3.2 Adhesion criteria of square plates The minimum value of $\partial\widetilde{U_E}/\partial S$ of square plates is

$$\Gamma \simeq 2000. \qquad (21)$$

This is a minimum of the differential coefficient that is calculated from the discrete relationship between $\widetilde{U_E}$ and ξ as described in section 2.4. Hence the explicit adhesion criteria formula of square plates called N_P [1] is calculated by Eqs. (14) and (21):

$$\frac{\Gamma}{\widetilde{\gamma_S}} = \frac{2000}{\gamma_S/(U_0/S_P)} = \frac{2000Et^3h^2}{12(1-\nu^2)\gamma_S S_P^2} \approx \frac{170Et^3h^2}{(1-\nu^2)\gamma_S w^4}, \qquad (22)$$

where S_P is the area of the square ($= w^2$) and w is the width of the square plate. The meaning of this formula is described in Eqs. (18) and (19). C. H. Mastrangelo and C. H. Hsu derived this formula in a different way. They calculated that the numerical factor of Eq. (22) is 186 as follows [1]:

$$\frac{\Gamma}{\widetilde{\gamma_S}} = \frac{186Et^3h^2}{(1-\nu^2)\gamma_S w^4}. \qquad (23)$$

They assumed the adhesion shape as a square. The error of two numerical factors is derived from the degree of approximation to calculate the adhesion shape. Equation (22) is obtained by searching for the adhesion shape numerically, so the numerical factor of Eq. (22) is more precise than that of Eq. (23).

3.3 Example of design In this section, we redesign a dimension of the adhesion sample in Sec. 3.1.

The width w is redesigned to prevent adhesion to the substrate, and the thickness t and gap h remain the same. We calculate $\Gamma/\widetilde{\gamma_S}$ of the original condition by Eqs. (20) and (21).

$$\frac{\Gamma}{\widetilde{\gamma_S}} = \frac{2000}{20000} = 0.1. \cdots\cdots\cdots\cdots\cdots\cdots (24)$$

It is confirmed that $\Gamma/\widetilde{\gamma_S}(= 0.1)$ of the sample is less than 1, so adhesion of the sample is confirmed by Eq. (18).

The plate peels from the substrate when $\Gamma/\widetilde{\gamma_S} = 1$ from Eq. (18) and $\Gamma/\widetilde{\gamma_S}$ is proportional to $1/w^4$ from Eq. (22), so the critical width of the plate, w_{peel}, is calculated as follows:

$$\frac{1}{w_{stick}^4} : 0.1 = \frac{1}{w_{peel}^4} : 1, \cdots\cdots\cdots\cdots\cdots\cdots (25)$$

where w_{stick} is the original value of the plate width (Table. 1), and w_{peel} is the redesigned value of the plate width. It is necessary to make w_{peel} to be 1100 μm ($\simeq \sqrt[4]{0.1} \times 2000$ μm) or less by Eq. (25). The sample, the width of which is less than or equal to 1100 μm, does not adhere to the substrate as shown in Fig. 7(b).

4. CONCLUSION

A method of analyzing the adhesion of arbitrary-shaped microstructures by using an optimization method and FEM was proposed. We applied this method to square plates, and obtained a more realistic curved adhesion shape. We also proposed a numerical calculation of surface energy γ_S by using measured adhesion area. For the convenience of the design, we defined the dimensionless surface energy $\widetilde{\gamma_S}$ in order to compare different shapes, and redesigned the dimension of the square plate that adhered in the experiment to prevent sticking to the substrate.

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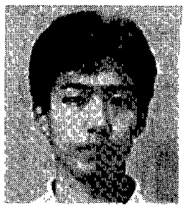

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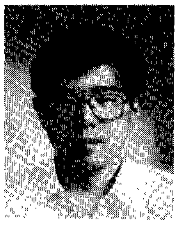

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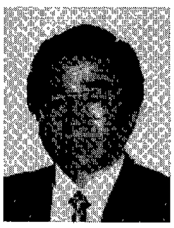

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