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 $\gamma_S$ 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. Heu investigated the adhesion problem of microstructures\(^7\). 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 $\gamma_S$.

In this paper, we present a method of calculating $\gamma_S$ 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 $\gamma_S$. A design method for preventing adhesion is also presented. We fabricated square plates of SOI wafers as test samples, and calculated $\gamma_S$ from the adhesion samples. Using this value and the new design method, we then redesigned the samples to prevent sticking to the substrate.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{Formulation of an adhesion problem of an arbitrary-shaped plate.}
\end{figure}

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 $\Omega_p$ (area $S_p$) is clamped to the substrate on its outer periphery as follows:

$$r = r_p(\phi). \quad (1)$$

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

$$r = r_s(\phi). \quad (2)$$
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:

\[
\begin{align*}
    u(r, \phi)|_{r=r_P(\phi)} &= 0, & \nabla u \cdot \mathbf{n}|_{r=r_P(\phi)} &= 0, \\
    u(r, \phi)|_{r=r_S(\phi)} &= h, & \nabla u \cdot \mathbf{n}|_{r=r_S(\phi)} &= 0,
\end{align*}
\]

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

\[
U_T = U_E + U_{SC}, \tag{4}
\]

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:

\[
U_{SC} = -\gamma_S S, \tag{5}
\]

where \( \gamma_S \) 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 \( \Omega_{me} \) be an adhesion area measured from an adhesion sample. \( \Omega_{me} \) is obviously a constant value, and \( \gamma_S \) is also a constant due to the characteristics of process conditions and materials. The actual adhesion shape \( \Omega_{me} \) (the area of the region \( \Omega_{me} \) equals \( S_{me} \)) minimizes the total energy \( U_T \).

\[
\min_{\Omega_{me} \subset \Omega_P} \{ U_T \} = \min_{\Omega_{me} \subset \Omega_P} \{ U_E - \gamma_S S_{me} \} = \min_{\Omega_{me} \subset \Omega_P} \{ U_E \} + \text{const.} \tag{6}
\]

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 \( \gamma_S \). 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 \( \gamma_S \) is calculated from the elastic energy \( U_E \). We consider the area differential of the total energy Eq. (4) at \( S = S_{me} \).

\[
\left. \frac{\partial U_T}{\partial S} \right|_{S=S_{me}} = \left. \frac{\partial U_E}{\partial S} \right|_{S=S_{me}} - \gamma_S. \tag{7}
\]

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

\[
\gamma_S = \left. \frac{\partial U_E}{\partial S} \right|_{S=S_{me}}. \tag{8}
\]

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 \( \gamma_S \) 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 considered 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

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segments as shown in Fig. 3(a):

\[ P_1(r_1, \phi_1), P_2(r_2, \phi_2), \ldots, P_n(r_n, \phi_n), \ldots \]  

(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):

\[ r = r_s(P_1, P_2, \ldots, P_n; s), \ldots \]  

(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 \( \gamma_S \) 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 (8)) 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:

\[ U_E = \frac{1}{2} \int_{\Omega} \left( \nabla^2 \bar{u} \right)^2 dS \]

\[ \quad = \frac{1}{2} U_0 \int_{\Omega_p \cap \Omega_{\xi}} \left( \nabla^2 \bar{u} \right)^2 dS \]  

(11)

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

\[ U_0 = \frac{Dh^2}{S_p} \]  

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

\[ \tilde{U}_T = \tilde{U}_E(\xi) - \gamma_S \xi \]  

(13)

where \( \tilde{U}_T = U_T / U_0, \tilde{U}_E = U_E / U_0, \xi = S/S_p \), and

\[ \gamma_S = \frac{\gamma_S}{U_0/S_p} \]  

(14)

The form of the function \( \tilde{U}_E \) 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 \( \xi \) 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 \( \xi \) is a fixed value \( \xi' \) (0 \( \leq \xi' < 1 \)), the corresponding adhesion energy \( \gamma_S \) is also a fixed value \( \gamma_S \) (const.). Thus, we obtain

\[ \min_{\xi' \in \Omega'} \left\{ \tilde{U}_E \right\} = \min_{\xi' \in \Omega'} \left\{ \tilde{U}_E - \gamma_S \xi' \right\} \]

(15)

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

Consequently, we regard the several values of \( \xi' \) as the values of the independent variable \( \xi \) again, so obtain a discrete relationship between the elastic energy \( \tilde{U}_E \) and the adhesion area \( \xi \) is obtained.

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

\[ \gamma_S = \frac{\partial \tilde{U}_E}{\partial \xi} \bigg|_{\xi = \xi_m} \]  

(16)

where \( \xi_m = S_m / S_p \) (0 \( \leq \xi_m < 1 \)). Equation (16) is implemented by a numerical differentiation because the relationship between \( \tilde{U}_E \) and \( \xi \) calculated above is discrete.

On the other hand, Figure 4 shows a typical curve of \( \tilde{U}_E \) and a typical curve of \( \partial \tilde{U}_E / \partial \xi \). \( \partial \tilde{U}_E / \partial \xi \) has a minimum value. Let \( \Gamma \) be the minimum value of \( \partial \tilde{U}_E / \partial \xi \) as follows:
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 $\gamma_S$  
In this section, the value of $\gamma_S$ is calculated from an adhesion sample fabricated as shown in Fig 5. The conditions of the sample are shown in Table 1.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width $w$</td>
<td>2000 $\mu$m</td>
</tr>
<tr>
<td>Thickness $t$</td>
<td>3.4 $\mu$m</td>
</tr>
<tr>
<td>Gap $h$</td>
<td>2 $\mu$m</td>
</tr>
<tr>
<td>Initial stress $\sigma_I$</td>
<td>0 GPa</td>
</tr>
<tr>
<td>Young's modulus $E$</td>
<td>145 GPa</td>
</tr>
<tr>
<td>Poisson's ratio $\nu$</td>
<td>0.27</td>
</tr>
</tbody>
</table>

The adhesion area was measured from an infrared microscope photograph. The normalized adhesion area is $\xi_{ne} = 0.29$. Figure 7(a) is an infrared microscope photograph of the adhesion sample. The dimensionless elastic energy $U_{E}$ is calculated by FEM. Linear shell elements are used in this calculation and the number of elements is about 900. The first-order optimization
method which is built into the application functionality\textsuperscript{(23)} is used as the optimization method. The relationship between $\xi$ and $\bar{U}_E$ is shown in Fig. 8. The area differential coefficient of $\bar{U}_E$ at $\xi_{me} = 0.39$ is

$$\bar{\tau}_S = 200000$$

(20)

This value is equal to 2.6 mJ/m$^2$ by Eq. (14). The $\gamma_S$ calculated from Mastrangelo's approximation formula of square plates\textsuperscript{(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 $\partial \bar{U}_E / \partial S$ of square plates is

$$\Gamma \simeq 2000$$

(21)

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

$$\frac{\Gamma}{\bar{\gamma}_S} = \frac{2000}{\gamma_S / (U_0 / S_P)} = \frac{2000 \varepsilon^3 h^2}{12(1 - \nu^2) \gamma_S S_P^2} \approx \frac{170 \varepsilon^3 h^2}{(1 - \nu^2) \gamma_S w^4}$$

(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\textsuperscript{(1)}:

$$\frac{\Gamma}{\bar{\gamma}_S} = \frac{186 \varepsilon^3 h^2}{(1 - \nu^2) \gamma_S w^4}$$

(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 \( \Gamma / \gamma_0 \) of the original condition by Eqs. (20) and (21).

\[
\frac{\Gamma}{\gamma_0} = \frac{2000}{20000} = 0.1
\]

(24)

It is confirmed that \( \Gamma / \gamma_0 = 0.1 \) of the sample is less than 1, so adhesion of the sample is confirmed by Eq. (18).

The plate peels from the substrate when \( \Gamma / \gamma_0 = 1 \) from Eq. (18) and \( \Gamma / \gamma_0 \) is proportional to \( 1/w^4 \) from Eq. (22), so the critical width of the plate, \( w_{\text{peel}} \), is calculated as follows:

\[
\frac{1}{w_{\text{stick}}} : 0.1 = \frac{1}{w_{\text{peel}}} : 1
\]

(25)

where \( w_{\text{stick}} \) is the original value of the plate width (Table 1), and \( w_{\text{peel}} \) is the redesigned value of the plate width. It is necessary to make \( w_{\text{peel}} \) to be 1100 \( \mu \text{m} \) \( (\approx \sqrt[4]{0.1} \times 2000 \text{ \( \mu \text{m} \)}) \) or less by Eq. (25). The sample, the width of which is less than or equal to 1100 \( \mu \text{m} \), 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 \( \gamma_0 \) by using measured adhesion area. For the convenience of the design, we defined the dimensionless surface energy \( \gamma_0 \) 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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References


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