Identification analysis of order of singularity near vertex on interface in three-dimensional bonded structures

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Abstract
In this paper, an identification procedure for the order of singularity near the interface edge of bonded structures is shown based on the finite element method using singular elements and the adjoint variable method in three dimensions. In this study, the three-dimensional Akin’s singular element is introduced for discretization of the governing equation, and the formulation for the parameter identification analysis is carried out based on the adjoint variable method. A simple rectangular bonded structure model is employed in numerical analysis, and several numerical experiments are performed.

Keywords parameter identification, adjoint variable method, Akin’s singular element, order of singularity, bonded structures

1. Introduction
In recent years, considerable researches have been carried out to clarify the stress singularity near the interface edge of bonded structures, e.g., researches on stress singularity under thermal stress loading [1] and comparison of the intensity of the stress singularity between bonded plates and tubes [2]. These studies have centered on the influence of the material properties and the shape of the bonded edge for bonded strength by the order of singularity and the intensity of stress singularity. In the strength evaluation, the order of singularity is first obtained, and the intensity of stress singularity is obtained by the least squares approximation for the computed stress distribution. On the other hand, the intensity of stress singularity is obtained by stress analysis using volume force distributed on a fictitious boundary in the region of the stress singularity. This method has been applied to a V-notched model [1], material with an inclusion model [3], and an interface crack model [4]. With this method, it is also necessary to obtain the order of singularity before calculating the intensity of the stress singularity.

In a two-dimensional model, the order of a singularity using the Bogy’s characteristic equation [5], and the calculation method of the order of singularity is based on the Stroh formalism [6]. In a three-dimensional model, the order of singularity is obtained by eigen analysis based on the finite element method [7]. However, these methodologies are tools for the strength evaluation prior to the design of bonded structures, so it is difficult to apply these methodologies at actual sites. Therefore, an identification procedure for the order of singularity using these measurement values is proposed in this paper. The adjoint variable method [8] and the direct differentiation method [9] are frequently employed in parameter identification problems. However, it is necessary to include the target parameter explicitly in the governing equation, and it is difficult to formulate this identification problem due to implicit inclusion of the order of singularity in the governing equation. Hence, in this study, the finite element method using singularity elements including the order of singularity is applied to the stress analysis [10]. For a singular element, the order of singularity is included in the interpolation function in the finite element method. It appears possible to formulate the identification analysis of the order of singularity due to explicit inclusion of the parameter in the governing equation. In this study, identification analysis based on the adjoint variable method was carried out on a three-dimensional tensile test model. The displacements measured on the specimen surface are employed in the identification analysis. Several results of numerical experiments are shown in this paper.

2. Stress analysis using singular element

2.1 Akin’s singular element
The shape function $N_i(i = 1, 2, 3, 4)$ of the linear tetrahedron element in the FEM is written as (1)–(4) using the coordinate system $\xi, \eta, \alpha$.

$N_1 = 1 - \xi - \eta$  \hspace{1cm} (1)
$N_2 = \xi$  \hspace{1cm} (2)
$N_3 = \eta$  \hspace{1cm} (3)
$N_4 = \alpha$.  \hspace{1cm} (4)
Akin’s singular element in three dimensions is represented as (5)-(8) [11].

\[ SN_1 = 1 - \frac{1 - N_1(\xi, \eta, \alpha)}{R(\xi, \eta, \alpha)}, \quad (5) \]
\[ SN_2 = 1 - \frac{1 - N_2(\xi, \eta, \alpha)}{R(\xi, \eta, \alpha)}, \quad (6) \]
\[ SN_3 = 1 - \frac{1 - N_3(\xi, \eta, \alpha)}{R(\xi, \eta, \alpha)}, \quad (7) \]
\[ SN_4 = 1 - \frac{1 - N_4(\xi, \eta, \alpha)}{R(\xi, \eta, \alpha)}, \quad (8) \]

where \( SN_i (i = 1, 2, 3, 4) \) indicate the shape function in Akin’s singular element. The function \( R(\xi, \eta, \alpha) \) is represented by (9).

\[ R(\xi, \eta) = (1 - N_1)^\lambda (\xi + \eta + \alpha)^\lambda, \quad (9) \]

where \( \lambda \) indicates the order of singularity, and the stress distribution around singular point is expressed by using the parameter \( \lambda \) such as \( \sigma_{ij} \propto r^{-\lambda} \). The variables \( \sigma_{ij} \) and \( r \) are the stress component and the distance from the singular point, respectively. It is known that the accuracy of the stress analysis in the singularity field increases, if the Akin’s singular element is employed [10].

2.2 Derivation of finite element equation

The weighted residual equation for the governing equation of the elastic body deformation is shown in (10).

\[ \int_{\Omega_e} \{ u_e^* \}^T [B_{e(\lambda)}]^T [D_e][B_{e(\lambda)}] \{ u_e \} \, d\Omega \]
\[ = \int_{\Gamma_e} \{ u_e^* \}^T \{ f_e \} \, d\Gamma, \quad (10) \]

where \( \{ u_e^* \} \) and \( [B_{e(\lambda)}] \) indicate the weighting function vector and the matrix expressed by differentiation of the shape function with respect to \( x, y \) and \( z \). Finally, the finite element equation superposed in the whole domain is written as (11).

\[ [K_{(\lambda)}] \{ u \} = \{ f \}. \quad (11) \]

In (11), \( [K_{(\lambda)}] \), \( \{ u \} \) and \( \{ f \} \) indicate the stiffness matrix, the displacement vector and the external and the reaction force vector. Akin’s singular element is included in the stiffness matrix \( [K_{(\lambda)}] \), and is represented as (12). Akin’s singular element is employed for elements including the singular point as shown in Fig. 1.

\[ [K_{(\lambda)}] = \sum_{e=1}^{mx} \int_{\Omega_e} [B_{e(\lambda)}]^T [D_e][B_{e(\lambda)}] \, d\Omega, \quad (12) \]

where the matrices \( [B_{e(\lambda)}] \) and \( [D_e] \) represent the matrix expressed by the differential operator and the elastic matrix. The parameter \( mx \) indicates the total number of elements. The order of singularity \( \lambda \) is included in the matrix \( [B_{e(\lambda)}] \).

3. Identification of order of singularity

In this paper, we consider an identification method of the order of singularity using displacement values. First of all, the performance function is represented by the square sum of the residual between the computed displacement \( \{ u \} \) and the observed displacement \( \{ u_{obs} \} \): it is defined as (13).

\[ J = \frac{1}{2} \left( \{ u \} - \{ u_{obs} \} \right)^T [Q] \left( \{ u \} - \{ u_{obs} \} \right) \]
\[ + \left( \{ P \}^T \left( [K_{(\lambda)}] \{ u \} - \{ f \} \right) \right). \quad (13) \]

Considering the stationary condition of the Lagrange function \( \delta J = 0 \), the adjoint variable equation shown in (15) is then obtained.

\[ \int_{\Omega_e} \{ u_e^* \}^T \{ P \} + \{ Q \}^T (\{ u \} - \{ u_{obs} \}) \, d\Omega = 0. \quad (14) \]

The gradient of the Lagrange function \( J^* \) with respect to the order of singularity \( \{ \lambda \} \) is also derived as (16).

\[ \frac{\partial J^*}{\partial \{ \lambda \}} = \left( \{ P \}^T \frac{\partial [K_{(\lambda)}]}{\partial \lambda} \right) \{ u \}. \quad (16) \]

The updated equation of the order of singularity, \( \{ \lambda \} \) based on the steepest descent method, is written as (17).

\[ \{ \lambda \}^{(l+1)} = \{ \lambda \}^{(l)} - \gamma \frac{\partial J^*}{\partial \{ \lambda \}} \]

where \( l \) and \( \gamma \) respectively indicate the number of iterations and step length. The iterative computation is continued until the value of \( \frac{\partial J^*}{\partial \{ \lambda \}} \) falls below the convergence criterion \( \epsilon \). The computational flow of the identification analysis of the order of singularity is shown below.
Table 1. Material properties.

| Case  | Material | Young’s modulus, GPa | Poisson ratio |
|-------|----------|----------------------|--------------|
| Case-A | Si       | 166.0                | 0.26         |
|       | Re       | 2.74                 | 0.38         |
| Case-B | Fe       | 216.0                | 0.30         |
|       | Al       | 69.09                | 0.33         |

(1) The initial order of the singularity \( \lambda^{(1)} \) and convergence criterion \( \epsilon \) are input.

(2) The displacement vector \( \{u\} \) is computed using the finite element equation, i.e., the superposition equation of (10), using Akin’s singular element.

(3) The computation is ended if the gradient of the Lagrange function with respect to the order of singularity \( \lambda^{(l)} \) is less than the convergence criterion \( \epsilon \). Otherwise, go to step 4.

(4) The adjoint variable vector \( \{P\} \) is computed using the adjoint equation, (15).

(5) The gradient of the Lagrange function is computed with respect to the order of singularity \( \lambda^{(l)} \), (16).

(6) The order of singularity \( \lambda^{(l)} \) is updated by (17). Return to step 2.

4. Numerical experiments

The results of numerical experiments for identification analysis of order of singularity are shown in this section using three-dimensional bonded structure models. Silicon-resin(Si-Re) and mild steel-aluminum(Fe-Al) bonded structure models are employed as numerical examples, and are respectively shown in Figs. 2 and 3 including the size of the numerical model and their boundary conditions. Their material properties are shown in Table 1. The orders of the singularity at the vertex on the interface edge, \( \lambda_{\text{vertex}} \), in Si-Re and Fe-Al models are shown in Table 2. These orders of singularity are obtained by eigen analysis based on the three-dimensional finite element method [7]. Akin’s singular element is employed for elements including the singular point, i.e., the vertex on the interface edge, as shown in Fig. 1. The other computational conditions are shown in Table 3. In this study, the displacement values for \( x \), \( y \) and \( z \) directions on the upper surface are used as the observed values in the identification analysis of the order of the singularity as shown in Figs. 2 and 3.

Computational results are shown in Figs. 4–7. Figs. 4 and 5 show the variation of the gradient of the Lagrange function \( J^* \) as a function of the order of singularity \( \lambda_{\text{vertex}} \) and the variation in the order of the singularity \( \lambda_{\text{vertex}} \) in Case A (Si-Re model). Consequently, from Fig. 4, it is found that the iterative computation is correctly performed such that the stationary condition, \( \delta J^* = 0 \), is satisfied. In addition, from Fig. 5, it is seen that the order of the singularity gradually increases, finally coincides with the target value. Furthermore, Figs. 6 and 7 show the same results in Case B (Fe-Al model); similarly, the iterative computation is correctly carried out such that the stationary condition is satisfied (see Fig. 6.). From Fig. 7, it is found that the order of the singularity can be correctly identified, even if the initial value of the order of the singularity \( \lambda^{(1)} \) is greater than the target value.

5. Conclusions

In this study, an identification analysis was carried out of the order of singularity at the vertex of the interface edge of a three-dimensional bonded structure model based on the finite element method using singular elements and the adjoint variable method was carried out. In present formulation, Akin’s singular element
is adopted, and the gradient of the Lagrange function with respect to the order of singularity was derived. The steepest descent method was employed in the iterative computation for the identification analysis. In this study, silicon-resin (Si-Re) and mild steel-aluminum (Fe-Al) bonded structure models were employed as computational models. Consequently, in both models, the order of singularity for each model could be appropriately identified. The present study reveals even if the target parameter identified by the iterative computation is not explicitly included in the governing equation, the unknown parameter can be identified by adopting the parameter in the interpolation function in the finite element analysis. Although multiple orders of a singularity are generally obtained by eigen analysis, the unique order of a singularity can be identified based on the present method using the observed displacement values. This is one advantage of the present method. However, it is also necessary to consider cases in which the stress field is expressed as multiple orders of singularity. The present method can also be extended to identification analysis of multiple orders of a singularity such that the computed stress field is agreement with the practical stress field by using the observed displacement value. This area holds potential for future investigations.

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