Simulation of Cracking Patterns in Sprayed Coating under Equi-Biaxial Tension*

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In order to characterize the “Repeating-division type” and the “Island delamination type” cracking patterns which are often observed in a brittle coating on a ductile substrate under increasing biaxial tensile stress, computer simulations of the cracking processes were performed for the cermet or the ceramic coating which was thermally sprayed on the substrate of a low carbon steel. The simulation was carried out using the Monte Carlo method and the analytical equations which express the relationships among crack size, tensile stress, strain, thickness and material constants of the coating and substrate. In the simulation, many cracks which have been nucleated randomly on the coating grow to either of the above cracking patterns depending on the relative strength of the coating and interface. The simulated cracking patterns agree well with those observed in bulge experiments.

Key Words: Crack Propagation, Ceramics, Fracture Mechanics, Computer Simulation, Equi-biaxial Tension, Repeating-division Type Cracking, Island-delamination Type Cracking, Thermally Sprayed Coating

1. Introduction

Various kinds of surface coating methods such as thermal spraying, PVD and CVD have been applied to provide the heat-, wear- and corrosion-resistance to machine parts and structures. In some cases, however, the coating can be cracked and delaminated under stress- or heat-cycles and overloading, thus the characterization of cracking and delamination behavior is essential to maintain the reliability of coated structures. In actual structures where the shape and the stress state are complicated, the cracking patterns are also complex and much different from those under uniaxial tension.

The present authors⁽¹⁾⁻⁽⁴⁾ have already carried out

equi biaxial tension tests of thermally sprayed coating on a low carbon steel substrate to analyze the cracking patterns. The results showed that the patterns are classified into two types depending on the relative strength of the coating and the interface, and that the interval of cracks or the diameter of the cracked area is estimated theoretically as a function of tensile stress, strength of coating, shear strength of the interface and material constants of the coating and substrate. For example, WC (88 mass%)-Co (12 mass%) cermet coating with high relative interfacial strength is repeatedly divided with an increase in equi-biaxial tensile stress to produce the “repeating-division type” cracking shown in Fig. 1(a). On the other hand, in Al₂O₃ (60 mass%)-TiO₂ (40 mass%) ceramic coating with low relative interfacial strength, the nucleation of many island-shaped cracks and delamination occur simultaneously at a certain tensile stress, i.e., the “island-delamination type” cracking pattern appears as is shown in Fig. 1(b). If simulations of the cracking patterns in sprayed coatings are possible, they will be very effective to estimate the strength of the coating and interface, to predict where and when the cracking or delamination occurs in

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Fig. 1 (a) "Repeating-division type" cracking observed in WC-Co cermet coating (thickness $B_1=0.28$ mm, nominal tensile stress of substrate $\sigma=392$ MPa) and (b) "Island-delamination type" cracking observed in $\text{Al}_2\text{O}_3\text{-TiO}_2$ ceramic coating ($B_1=0.4$ mm, $\sigma=282$ MPa) in bulge tests

coated structures, and to develop methods to restrain cracking of the coating.

Although some Monte Carlo simulations⁽⁵⁾⁻⁽⁷⁾ of cracking patterns have been carried out, they cannot be used for characterizing the cracking patterns in coatings on actual structures quantitatively because the material constants and fracture mechanics parameters of the coating, substrate and interface are not directly included in the models. Moreover, the simulated crack patterns are a little different from the actually observed ones because of the lack of theoretical consideration especially on the interface. In the present research, as a preliminary stage for the simulations of the cracking process in a coating under complex stresses, the cracking patterns under equibiaxial tension are simulated by combining the Monte Carlo method and the analytical equations which have

Fig. 2 Flowchart of simulation

Fig. 3 Modeling of coating and substrate

been derived by the present authors⁽²⁾⁽⁴⁾.

2. Simulation Method

2.1 Flow of simulation

Figure 2 shows the flowchart of simulation. First, in the model of coating and substrate shown in Fig. 3, the geometrical dimensions and material parameters, thickness, elastic constants, Poisson's

ratios of coating and substrate, plastic constant and yield strength of substrate, are input to the lattices of the coating. These parameters are the same at every position, while tensile strength or surface energy of the coating and interfacial strength or interfacial energy are randomly distributed to the lattices. Second, after calculating the stresses in the coating and substrate under a given equi-biaxial nominal tensile stress σ on the substrate, whether a crack starts or not in a lattice is determined, i.e., if the stress in a lattice σ_i reaches a critical strength of the lattice σ_{ci} the crack nucleation occurs in the lattice of the coating. Third, the type of cracking pattern (repeating-division type or island-delamination type) is discriminated according to the relative strength of the coating and the interface. Finally, crack propagation, crack connection and delamination processes are simulated on the basis of analytical results^{(2),(4)}.

2.2 Strength distribution in coating and along interface

Random values of coating strength $\sigma_{ci}(i, j)$ ($0 \leq i < 100, 0 \leq j < 100$) are distributed to the lattices at the i -th row and j -th column in Fig. 3 by the next equation.

$$\sigma_{ci}(i, j) = \sigma_{c1min} + (\sigma_{c1max} - \sigma_{c1min}) \cdot \frac{\sum_{k=1}^N R(k)}{N \times (M-1)} \quad (1)$$

Here, $R(k) = \text{random}(M)$ is a routine which produces a random integer from 0 to $(M-1)$, and N is the number of execution of the routine. The $\sigma_{ci}(i, j)$ change depending on the integers $M(>2)$ and (>2) and the $\sigma_{ci}(i, j)$ are given by a normal distribution between a minimum strength σ_{c1min} and a maximum strength σ_{c1max} . Using the same method, the interfacial strengths $\tau_{ci}(i, j)$ between τ_{c1min} and τ_{c1max} with a normal distribution are also distributed randomly to the lattices.

2.3 Stress in coating and substrate before crack initiation

The tensile stresses in the coating and substrate, σ_1 and σ_2 , are assumed to be uniform before crack initiation, and they are calculated by the following equations⁽²⁾.

$$\begin{aligned} \sigma_1 &= \frac{(1-\nu_2)}{(1-\nu_1)} \cdot \frac{E_1}{E_p} \left\{ \sigma - \left(1 - \frac{E_p}{E_e} \right) \sigma_{ys} \right\} / \\ &\quad \left\{ 1 + \frac{B_1}{B_2} \cdot \frac{(1-\nu_2)}{(1-\nu_1)} \cdot \frac{E_1}{E_p} \right\} \\ \sigma_2 &= \left\{ \sigma + \frac{(1-\nu_2)}{(1-\nu_1)} \cdot \frac{B_1}{B_2} \cdot \frac{E_1}{E_p} \left(1 - \frac{E_p}{E_e} \right) \sigma_{ys} \right\} / \\ &\quad \left\{ 1 + \frac{B_1}{B_2} \cdot \frac{(1-\nu_2)}{(1-\nu_1)} \cdot \frac{E_1}{E_p} \right\} \quad (2) \end{aligned}$$

Here, B_1 and B_2 are thicknesses of the coating and substrate, σ is applied nominal tensile stress, E_1 and ν_1 are elastic modulus and Poisson's ratio of coating,

Fig. 4 Crack initiation and propagation

and, E_e , E_p , σ_{ys} and ν_2 are elastic modulus, plastic modulus, yield strength and Poisson's ratio of the substrate, respectively, where the deformation behavior of the substrate is assumed to be that of a linear-hardening material.

2.4 Crack initiation and propagation

With increasing equi-biaxial tensile stress σ , when the stress in coating σ_1 calculated by Eq.(2) reaches the smallest strength of coating at a lattice S shown in Fig. 4(a), a crack originates at the point. In the magnification of the circular area around S shown in Fig. 4(b), the nucleated crack propagates in one of eight possible directions in which the strength is the smallest (e.g. the direction to lattice 1) to form a crack SA. Because the stress concentration at crack tips A and S is large, while the stresses of lattices which locate in the perpendicular direction to SA (2 and 4) are released, the next possible growth direction of the crack SA is either 1', 2', 4' from point A or 5, 7, 8 from point S. The crack SA can propagate to one of the six lattices at which the strength is the minimum. However, stress intensity factor at a crack tip varies with the crack propagation direction, e.g., the stress intensity factor when a through-thickness crack propagates in the direction of $\theta = 45^\circ$ is about 70% smaller than that when the crack propagates straight ($\theta = 0$)⁽⁸⁾. In the present simulation, therefore, if the ratio of the strength of each lattice in the direction of $\theta = 45^\circ$ to the strength of lattice in the direction of $\theta = 0$ is smaller than 0.7, the crack propagates in the direction of $\theta = 45^\circ$, while if the ratio is larger than 0.7, the crack propagates straight ($\theta = 0$). With an increase in σ , the above process is repeated, and a zigzag crack will be formed as is shown in Fig. 4(a).

It is difficult to obtain the stress or stress intensity factor at a crack tip in the coating analytically because they depend on the crack length and shape, distance to adjacent cracks or to boundaries of the coating, and deformation characteristics of the substrate. Moreover, the numerical calculation of the stress intensity factor by the FEM method also needs a large amount of computation due to the same

Fig. 5 An idealized model of "repeating division type" cracking of coating

reasons. Consequently, the stress intensity factor is not calculated in the present simulation, but the stress of coating σ_1 calculated by Eq. (2) is directly compared with the strength of each coating lattice to determine the crack propagation direction.

2.5 Discrimination of cracking patterns

According to the previous research⁽⁴⁾, if the ratio of tensile strength of coating σ_{c1} to interfacial shear strength τ_c^i is small and satisfies the following inequality equation, the "repeating-division type" crack occurs. On the contrary, if the ratio of σ_{c1} to τ_c^i is large and does not satisfy the equation, the "island-delamination type" cracks are formed.

$$\frac{\sigma_{c1}}{\tau_c^i} < \frac{1}{\sqrt{2}aB_1(\sqrt{1-\nu_1^2}-\nu_1\sqrt{1-\nu_1})}, \quad (3)$$

$$\alpha \equiv \{2G_{2p}/(E_1B_1z_0)\}^{1/2}$$

Here, $G_{2p} = E_p/2(1+\nu_2)$ is plastic shear modulus of substrate, and z_0 is the distance from the interface to a position in the substrate from which the effect of constraint due to coating completely fades away (as is described in Section 2.6). Thus, the type of cracking pattern is discriminated only by inputting the material constants into Eq. (3).

Fig. 6 Stress distribution in the coating and substrate

2.6 Simulation of "repeating-division type" cracking pattern

Figure 5(a) represents an idealized model of the repeating-division process of coating. The initial square-shaped coating is divided into two areas by a crack of length a_1 . With increasing tensile stress, both areas are divided into eight areas by cracks of length $a_1/2$. By the repetition of the process, the division areas of the coating become smaller and smaller. In order to calculate the tensile or shear stress in the coating or along the interface, a unit square of divided coating is considered as is shown in Fig. 5(b). The lengths of the two sides are L_x and L_y , and the coordinate origin is located at the center of the square. Two-dimensional stress distribution in the coating and substrate is shown in Fig. 6, where the tensile stress in the x and y directions in the coating, σ_{x1} and σ_{y1} , are assumed to be uniform in the z direction and the shear stresses τ_{zx1} and τ_{zy1} do not exist. In the substrate within $0 < z \leq z_0$, the tensile stress σ_{x2} and the shear stress τ_{zx2} vary with z , while $\sigma_{x2} = \sigma_2$ and $\tau_{zx2} = 0$ hold at the position beyond $z > z_0$. The average of σ_{x2} ($0 \leq z \leq z_0$) is denoted as σ_{x2}^0 .

According to the stress analysis by the present authors⁽⁴⁾, the tensile stresses in the x and y directions in the coating, σ_{x1} and σ_{y1} , are expressed by the following equations.

$$\sigma_{x1}(x, y) = \frac{E_1 \varepsilon_2}{1-\nu_1} \left\{ 1 + \frac{\nu_1 \cdot \cosh(\sqrt{1-\nu_1} \cdot \alpha x) \cdot \cosh(\sqrt{1-\nu_1} \cdot \alpha y)}{\cosh(\sqrt{1-\nu_1} \cdot \alpha L_x/2) \cdot \cosh(\sqrt{1-\nu_1} \cdot \alpha L_y/2)} \right. \\ \left. - \frac{\cosh(\sqrt{1-\nu_1^2} \cdot \alpha x)}{\cosh(\sqrt{1-\nu_1^2} \cdot \alpha L_x/2)} - \frac{\nu_1 \cdot \cosh(\sqrt{1-\nu_1^2} \cdot \alpha y)}{\cosh(\sqrt{1-\nu_1^2} \cdot \alpha L_y/2)} \right\} \\ \sigma_{y1}(x, y) = \sigma_{x1}(x \rightarrow y, y \rightarrow x) \quad (4)$$

Moreover the shear stresses in the x and y directions at interface between the coating and substrate, τ_{zx}^i and τ_{zy}^i , are given by

$$\tau_{zx}^i(x, y) = -\frac{E_1 \varepsilon_2 B_1 \alpha}{1-\nu_1} \left\{ \frac{\nu_1 \sqrt{1-\nu_1} \cdot \sinh(\sqrt{1-\nu_1} \cdot \alpha x) \cdot \cosh(\sqrt{1-\nu_1} \cdot \alpha y)}{\cosh(\sqrt{1-\nu_1} \cdot \alpha L_x/2) \cosh(\sqrt{1-\nu_1} \cdot \alpha L_y/2)} \right. \\ \left. - \frac{\sqrt{1-\nu_1^2} \cdot \sinh(\sqrt{1-\nu_1^2} \cdot \alpha x)}{\cosh(\sqrt{1-\nu_1^2} \cdot \alpha L_x/2)} \right\} \\ \tau_{zy}^i(x, y) = \tau_{zx}^i(x \rightarrow y, y \rightarrow x) \quad (5)$$

where ε_2 is the strain of the substrate in the x or y direction, and the relationship between ε_2 and σ_2 is given by $\varepsilon_2 = (1-\nu_2)\{\sigma_{ys}/E_e + (\sigma_2 - \sigma_{ys})/E_p\}$ when the plastic deformation of the substrate occurs.

The actual method to calculate the stress in the coating is schematically shown in Fig. 7. Consider a case

Fig. 7 Actual repeating-division process in coating

that a curvilinear crack esf runs from a point s in a divided coating area $abcd$, and two cracks gh and kj propagate in the areas with an increase in equi-biaxial tensile stress. The stress distribution in the divided areas is complicated because the shapes of the coating areas are irregular. For simplicity, the stresses in the x and y directions in the areas, σ_{x1} and σ_{y1} , are still calculated using Eq.(4), where L_x and L_y in the equation are taken as the length of each side of an equivalent square, i.e., L_x and L_y are approximated to the averages of two sides of the circumscribed and inscribed squares to the irregular area $hbfg$. It is assumed that the stress between the circumscribed and inscribed squares is zero. Thus, a new crack originates and propagates from a lattice in the region in the similar way as described in Section 2.4.

With the progress of repeating divisions of coating, when the interfacial shear stress at a crack tip τ_{zx}^i or τ_{zy}^i reaches a critical shear strength τ_c^i at a lattice, the division stops and the delamination of the coating including the lattice occurs.

2.7 Simulation of "island-delamination type" cracking pattern

If the equi-biaxial tensile stress σ increases and the tensile stresses in lattices reach certain values which are randomly distributed, short linear or zigzag cracks start here and there in the coating. At the same time, the cracks bifurcate and connect with each other to form island-shaped cracks as shown in Fig. 1 (b). If the islands are approximated by disks or hexagons, the average diameter of the disks or average length of diagonal lines of the hexagons, $2a_0$, can be calculated as follows⁽²⁾ using Griffith theory ;

$$2a_0 = 2\gamma_c B_1 \left/ \left\{ \frac{(1-\nu_1)B_1}{E_1} \sigma_{d1}^2 + \frac{(1-\nu_2)B_2}{E_p} (\sigma_d - \sigma_{d2})^2 - 2\gamma_{12} \right\} \right. \quad (6)$$

Fig. 8 Model of "island-delamination type" cracking in coating

where, σ_{d1} , σ_{d2} and σ_d are the tensile stresses at delamination in the coating, substrate with coating and substrate without coating, respectively, γ_c and γ_{12} are the surface energy of the coating per unit area and the interfacial energy per unit area between the coating and substrate.

In the simulation, first, such lattices are found of which the strengths are small and the distance among them is larger than $2a_0$, and they are grown to short linear cracks of length a_i ($< a_0$) in random directions as is schematically shown in Fig. 8. They are called L_1 type cracks. If the island is assumed to have an ideal hexagon shape, the number of L_1 type cracks N will be calculated by the next equation,

$$N \approx S / (6 \times a_0^2 \sin 60^\circ / 2) \quad (7)$$

where S is total area of coating. The interaction among the cracks is neglected and the propagation direction of each crack is independent at this stage.

Second, considering that the ideal bifurcation angle of cracks is $2\pi/3$ ⁽⁸⁾ and the hexagonal division pattern is stable, the initial N cracks are bifurcated at their tips with the angle of $2\pi/3$. The bifurcated cracks, L_2 type cracks, are hypothetical cracks with length equal to a_i . In fact, bifurcation angles and lengths should be determined to minimize free energy (sum of increment of surface energy and decrement of strain energy). Because the strain energy of the coating is completely released after delamination, the problem to find the most stable connection paths of the cracks can be replaced by a problem to minimize surface energy of coating, that is, to minimize the total length of all cracks. For this purpose, the tips of three bifurcated cracks are connected to form a triangle (L_3 type cracks). By connecting three tips of initial cracks (L_1 type cracks) with the center of the triangle by L_4 type cracks, the island cracks such as,

ao_1cdo_2b , o_2do_3g and $go_3eo_4mo_5h$, are obtained. There are two special cases. One is that there remain two isolated tips. In this case, the middle point of the connecting line of the two tips is considered as the merging point. Another is that there remains only one tip. In that case, the line is drawn such that the tip is connected to the nearest bifurcation point or merged point directly.

3. Simulation Results and Discussions

The simulations were carried out for the “repeating-division type” cracking pattern observed in WC-Co cermet coating and the “island-delamination type” cracking pattern in Al_2O_3 - TiO_2 ceramic coating on a

Table 1 Materials constants input for simulation of cermet coating and ceramic coating on a ductile substrate

substrate	coating	
SPCC-S	WC-Co cermet	Al_2O_3 - TiO_2 ceramic
$B_2 = 1\text{mm}$ $E_c = 205\text{GPa}$ $E_p = 2.9\text{GPa}$ $\nu_2 = 0.3$ $\sigma_{ys} = 240\text{MPa}$ $z_0 = 0.15\text{mm}$	$B_1 = 0.05, 0.14, 0.28\text{mm}$ $E_1 = 163\text{GPa}$ $\nu_1 = 0.3$ $\sigma_{cl} = 120\text{MPa}$ $\sigma_{clmin} = 80\text{MPa}$ $\sigma_{clmax} = 160\text{MPa}$ $\tau_c^i = 75\text{MPa}$ $\tau_{cmin}^i = 50\text{MPa}$ $\tau_{cmax}^i = 100\text{MPa}$	$B_1 = 0.4\text{mm}$ $E_1 = 9.1\text{GPa}$ $\nu_1 = 0.3$ $\sigma_{cl} = 55\text{MPa}$ $\sigma_{clmin} = 30\text{MPa}$ $\sigma_{clmax} = 70\text{MPa}$ $\tau_c^i = 35\text{MPa}$ $\tau_{cmin}^i = 25\text{MPa}$ $\tau_{cmax}^i = 45\text{MPa}$

low carbon steel (JIS: SPCC-S) substrate in bulge tests. Geometrical dimensions and material parameters of the coating and the substrate used for calculation are shown in Table 1^{(2),(4),(9),(10)}. Material constants of WC(88 mass%)-Co(12 mass%) cermet coating have been obtained in the previous experiments^{(4),(9)}. The average tensile strength of Al_2O_3 (60 mass%)- TiO_2 (40 mass%) ceramic coating is calculated by inputting the tensile stress at delamination ($\sigma = \sigma_d = 275\text{MPa}$) which has been obtained in the previous equi-biaxial tensile test (coating thickness $B_1 = 0.4\text{mm}$)⁽²⁾ into Eq.(2), i.e., $\sigma_{cl} = 55\text{MPa}$ is obtained. The interfacial shear strength τ_c^i is calculated from Eq.(8) by putting $x = L_x/2 = L/2$, $y = L_y/2 = L/2$ in Eq.(5).

$$\tau_c^i = \frac{\sqrt{2aE_1\varepsilon_2B_1}}{1-\nu_1} \{ \sqrt{1-\nu_1^2} \cdot \tanh(\sqrt{1-\nu_1^2} \cdot aL/2) - \nu_1 \sqrt{1-\nu_1} \cdot \tanh(\sqrt{1-\nu_1} \cdot aL/2) \} \quad (8)$$

Because $L \div 2a_0 = 1.2\text{mm}$ ⁽²⁾ was observed at delamination, $\tau_c^i = 35\text{MPa}$ is obtained.

Parameters of the WC-Co cermet coating satisfy Eq.(3), so the “repeating-division type” cracking occurs. The simulated pattern is shown in Fig. 9. With increasing nominal stress, the coating is divided repeatedly into very small areas and the delamination occurs in some areas (white areas). The pattern of

Fig. 9 Simulated patterns of “repeating-division type” cracking for WC-Co cermet coating ($B_1 = 0.28\text{mm}$)

Fig. 10 Comparison of the simulated relation between stress of substrate and crack interval with that of the experiment

Fig. 11 Simulated pattern of "repeating-division type" cracking for cermet coating ($B_1=0.28$ mm, $\sigma_{c1min}=30$ MPa, $\sigma_{c1max}=180$ MPa, $\sigma=392$ MPa)

Fig. 9(d) agrees relatively well with that experimentally observed in the bulge test shown in Fig. 1(a). Figure 10 is of a previous experimental result⁽⁴⁾ which shows the relationships between tensile stress and average distance between cracks obtained from the bulge test of disk specimens with WC-Co cermet coating. This figure also shows the average distance between cracks obtained by the present simulation where the values of σ_c and τ_c^i are assumed to be constant irrespective of coating thickness. The experimental curves agree relatively well with the calculation curves, so the simulated division processes of coating approximately express those observed in the bulge test.

In a trial simulation when the strengths of coating lattices σ_{c1} were varied in a wider range between

Fig. 12 Simulated patterns of "island-delamination type" cracking for Al_2O_3 - TiO_2 ceramic coating ($B_1=0.4$ mm, $\sigma=282$ MPa)

$\sigma_{c1min}=30$ MPa and $\sigma_{c1max}=180$ MPa, the pattern became more zigzag as is shown in Fig. 11 than that in Fig. 9(d). It may be possible to estimate the scatter of coating strength from the shape of the division pattern.

Parameters of Al_2O_3 - TiO_2 ceramic coating do not satisfy Eq.(3), so the "island-delamination type" cracking takes place. Because the actual process from initiation of cracks to perfect construction of islands is completed in a very short time, it is difficult to discriminate the crack initiation, bifurcation and connection distinctly. However, the three execution

(repeating calculation) stages are picked from the simulation as is shown in Fig. 12. The sizes of simulated islands in Fig. 12(c) vary in a wider range than the observed sizes in Fig. 1(b). The reason for the discrepancy will be that the growth of initial cracks is assumed to be random and the interactions among them are not considered in the present simulation.

Thus, the actual cracking patterns observed in the WC-Co cermet coating and the $\text{Al}_2\text{O}_3\text{-TiO}_2$ ceramic coating can be reproduced relatively well by the present simulation. The simulation method can be expanded to predict the cracking patterns in actual machine parts or structures with various shapes which receive complex bi-axial stresses.

4. Conclusion

The "repeating-division type" cracking pattern observed in WC-Co cermet coating and the "island-delamination type" cracking pattern in $\text{Al}_2\text{O}_3\text{-TiO}_2$ ceramic coating are simulated by combining the Monte Carlo method with the stress analysis or energy analysis introduced by the present authors. The actual cracking patterns observed in the bulge tests of the coatings are reproduced relatively well by the present simulations.

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