DEM simulation of Crack propagation in brittle coatings

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ABSTRACT

Coatings are used in different industries in order to improve the surface properties in components and instruments. In some situations, such as improving the wear resistance of an instrument, brittle coatings have been considered. Dominant failure mode in these structures is crack initiation and propagation. So, investigating the fracture behavior of these structures is in great importance. In this paper, discrete element method is used to simulate the crack initiation and propagation in coating/substrate structures. This method has a great ability to predict damage initiation and propagation in structures. For this purpose, a discrete element solver code is written by authors. Brittle elastic behavior is considered in coating and substrate and the effect of elastic mismatch in constituents of structure and the coating thickness in damage initiation and propagation were investigated. The results showed that in structures in which coating stiffness is less than substrate stiffness, in the case of low thickness of coating, damage appears as crack initiation and propagation into the substrate but, by increasing the coating thickness, crack grows into or parallel to interface. In structures in which the coating stiffness is greater than substrate stiffness, no matter to the coating thickness, crack grows to the substrate.

KEYWORDS

Coating/substrate structures, Brittle coating, Discrete element method, Damage propagation

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1. Introduction

Coatings are used in many industries to improve surface properties. Crack creation in coatings may cause catastrophic issues in the whole of the structure. Therefore, the prediction of damage initiation and the evolution pattern have great importance.

In brittle coatings, damages appear due to tensile stresses at the surface and propagate through the thickness. At this state, depending on the mechanical properties of different constituents, cracks may cease at the interface of coating and substrate, propagate through the interface or propagate on the substrate [1].

Three and four point bending tests on coating/substrate structures are common methods to investigate cracking under tensile stress in these structures [2]. Bending tests have been performed in order to fracture toughness calculation at coating or interface (e.g. [3]) or to clarify the damage growth pattern (e.g. [4]). In addition to experimental observations, finite element simulations on crack evolution patterns have been performed [2,5].

Unlike the previous numerical simulations which used FEM, discrete element method (DEM) is used in the present paper in order to capture the local damages in the brittle coating/substrate structures due to three-point bending. DEM considers discrete nature for bulk material. In this method, the domain is discretized with a set of rigid disks (in 2D) and spheres (in 3D) which have interaction with themselves. Macroscopic behavior of the material arises from the interaction of particles at microscale. These particles can be bonded together to simulate the continuous solid material [6]. In this situation, micro-cracks create when the bonds break. DEM has been used by Ghasemi and Falahatgar to simulate delamination due to thermal loading [7] and damages due to three-point bending by the use of cohesive contact model [8] in brittle coating/substrate structures.

In this paper, DEM is used to simulate damage initiation and propagation in brittle coating/substrate systems under three-point bending by the use of elastic-perfectly brittle bond model. DEM solver code is written in FORTRAN programming language by the authors and validation is performed by comparing the DEM simulation results with experimental ones, qualitatively and quantitatively. Parametric study was performed and the effects of elastic parameters mismatch between coating and substrate and coating thickness on damage initiation and propagation is investigated.

2. Discrete element method

As noticed before, in this method, the interaction of particles, define the macroscopic behavior of the bulk material. The translational and rotational motion of particles is governed by Newton and Euler’s equation (rigid body dynamic). Explicit time integration of these equations leads to new position of each particle.

\[ u_{i}^{n+1} = u_{i}^{n} - 2u_{i}^{n} + \frac{F_{i}}{m} \Delta t^{2} \]

\[ \theta_{i}^{n+1} = \theta_{i}^{n} - 2\theta_{i}^{n} + \frac{T_{i}}{I_{i}} \Delta t^{2} \]

In these equations, \( F_{i} \) and \( T_{i} \) are the resultant forces and moments acting on each particle and are calculated by elastic-perfectly brittle force-displacement relations of each bond [9,10]. In addition, \( m_{i} \) and \( I_{i} \) are the mass and moment of inertia of particle, \( u_{i} \) is the translational displacement, \( \theta_{i} \) is the rotational displacement, and \( \Delta t \) is the stable time step.

In this paper, in the coating and substrate, bond breakage happens when the stresses reach the material tensile strength. This criterion is explained by Tavarez and Plesh [10]. At the interface, due to mixed mode fracture, bond breakage criterion considers both the normal and shear stresses.

3. Results and discussion

Validation is performed with experimental results [4], qualitatively and quantitatively. Table 1 gives the material properties and dimensions. Figure 1 compares damage evolution, qualitatively and load-displacement curves, quantitatively.

<table>
<thead>
<tr>
<th>Table 1. Mechanical properties and dimensions [4]</th>
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<tbody>
<tr>
<td>100 GPa</td>
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<td>200 GPa</td>
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<tr>
<td>200 MPa</td>
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<tr>
<td>350 MPa</td>
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<td>3 mm</td>
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In the remainder of the paper, two different coefficient of elastic mismatch (\( \alpha \)) which is introduced in [11] and two coating thickness ratios (\( h_{c}/h_{s}=0.15 \) and \( h_{c}/h_{s}=0.4 \)) are considered to define the effects of elastic mismatch and coating thickness. In these results, material strength is considered as \( E/1000 \) (\( E \) is the
Young’s modulus of the constituents). In addition, mechanical properties of interface are the average properties of coating and substrate. Figure 2 shows the damage evolution for all cases.

Figure 1. (a) Experimental observation with 500 µm coating thickness [4] (b) DEM simulation result and (c) load-displacement curves

Figure 2. Damage evolution in (a) $\alpha=0.7$ and (b) $\alpha=0$ with two different coating thicknesses

4. Conclusions

Damage evolution is simulated in brittle coating/substrate structure to clarify the effects of elastic mismatch and coating thickness. The results show that, when there is high difference in mechanical properties of coating and substrate, for thick coatings, damage propagates at the interface but for thin coatings, damage propagation appears at substrate. By reduction their differences, no matter the coating thickness, damage propagates to the substrate.

5. References