



## Discrete Element Method 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 of great importance. In this paper, the 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 the low thickness of the coating, damage appears as crack initiation and propagation into the substrate but, by increasing the coating thickness, the crack grows into or parallel to the interface. In structures in which the coating stiffness is greater than substrate stiffness, no matter to the coating thickness, the crack grows to the substrate.

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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 [3] or to clarify the damage growth pattern [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 Finite Element Method (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 the 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. The macroscopic behavior of the material arises from the interaction of particles at the 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 [7, 8] to simulate delamination due to thermal loading and damages due to three-point bending by the use of cohesive contact model 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 the 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. A parametric study was performed and the effects of elastic parameters mismatch between coating and substrate and coating thickness on damage initiation and propagation are investigated.

## 2. DISCRETE ELEMENT METHOD

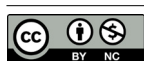
As noticed before, in this method, the interaction of particles, define the macroscopic behavior of the bulk material. The translational and rotational motion of particles is governed by Newton and Euler's equation (rigid body dynamic). Explicit time integration of these equations leads to the new position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

$$u_i^{n+1} = u_i^{n-1} - 2u_i^n + \frac{F_i}{m_i} \Delta t^2 \quad (1)$$

$$\theta_i^{n+1} = \theta_i^{n-1} - 2\theta_i^n + \frac{T_i}{I_i} \Delta t^2 \quad (2)$$

elastic-perfectly brittle force-displacement relations of each bond [9, 10]. In addition,  $m_i$  and  $I_i$  are the mass

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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 Tavaréz 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. Fig. 1 compares damage evolution, qualitatively and load-displacement curves, quantitatively.

In the remainder of the paper, two different coefficients of elastic mismatch ( $\alpha$ ) which is introduced in Ref. [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 Young's modulus of the constituents). In addition, the mechanical properties of the interface are the average properties of coating and substrate. Fig. 2 shows the damage evolution in all cases.

### 4. CONCLUSIONS

Damage evolution is simulated in the brittle coating/substrate structure to clarify the effects of the elastic mismatch and coating thickness. The results show that, when there is the high difference in mechanical properties of coating

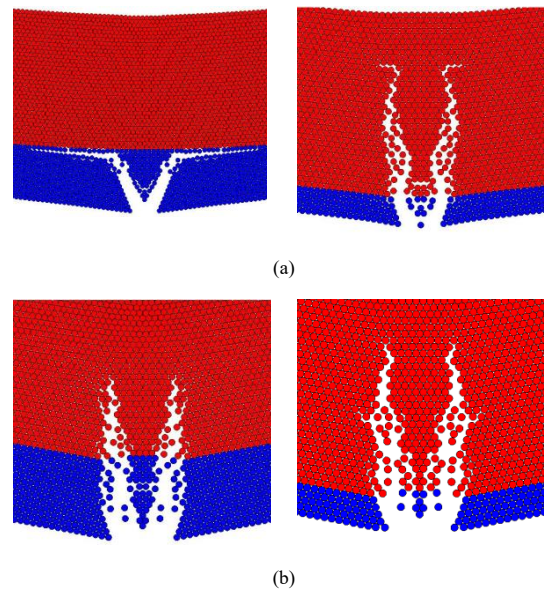


Fig. 2. Damage evolution in (a)  $\alpha=0.7$  and (b)  $\alpha=0$  with two different coating thicknesses

and substrate, for thick coatings, damage propagates at the interface but for thin coatings, damage propagation appears at the substrate. By reduction of their differences, no matter the coating thickness, damage propagates to the substrate.

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Table 1. Mechanical properties and dimensions [4]

100 GPa	Coating Young's modulus
200 GPa	Substrate Young's modulus
200 MPa	Coating tensile strength
350 MPa	Interface strength
15 mm	Length
3 mm	Width
1.5 mm	Thickness

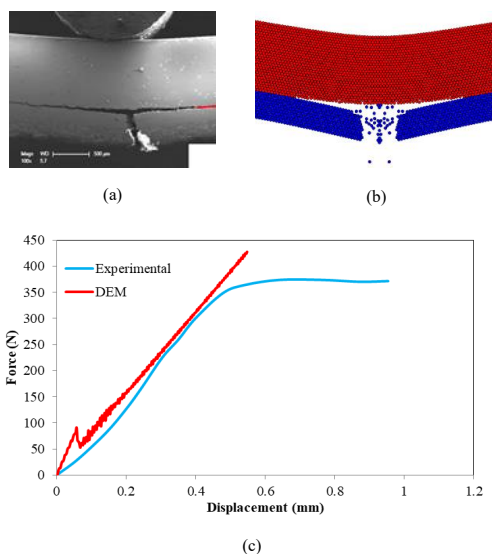


Fig. 1. (a) Experimental observation with 500  $\mu\text{m}$  coating thickness [4] (b) DEM simulation result and (c) load-displacement curves