Numerical simulation of deformation and fracture in a coated material using curvilinear regular meshes

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Abstract. This paper presents a computational analysis of the deformation and fracture mechanisms of a material with a porous polysilazane coating under tension and compression. A dynamic boundary-value problem in the plane strain statement is solved numerically by the finite-difference method. The coating-substrate interface and porous coating microstructure corresponded to configurations found experimentally are accounted for explicitly in the calculations. For this purpose an algorithm for curvilinear finite-difference meshing based on the solution of the elasticity theory has been developed. The algorithm implemented offers several benefits over the rectilinear meshing. Local regions experiencing bulk tension are shown to form along pore surfaces that control the fracture mechanisms at the mesoscale level.

1. Introduction
In recent years, advanced metal-ceramic composites have been widely used instead of pure metallic compounds and identified as important materials in high-precision manufacturing. Polysilazanes are extensively used to manufacture polymer-derived ceramics (PDCs), which can be employed to produce fibers, coatings and fiber-reinforced ceramic matrix composites. The resulting PDC-based coatings exhibit optimum adhesion ability, good corrosion and heat resistance [1]. However, due to the shrinkage occurring during the polymer-to-ceramic conversion, PDC coatings generally suffer from unwanted porosity, cracks and defects [2]. There is an increasing number of experimental and theoretical works devoted to investigation of pore characteristics and to analysis of methods to estimate the porosity and to produce porous coatings (see, e.g., [3]).

In this study we analyze numerically the mechanisms of deformation and fracture involved in material with a porous polysilazane-based ceramic coating under uniaxial tensile and compressive loading. A role of the geometry of the coating-substrate interface and of the porous coating microstructure is investigated. The simulated microstructure of the coated material corresponds to the experimental data on the composite (Figure 1a) and is accounted for explicitly in the calculations. In order to describe the mechanical behavior of the substrate and coating materials, we use an elasto-plastic model accounting for isotropic strain hardening and of a modified fracture criterion of the Huber type [4, 5].

There are two stages of the work. In stage 1, an algorithm for 2D regular curvilinear meshing based on the approach proposed in [6] is implemented, and a pertinent finite-difference solution is compared
to a solution obtained using a uniform rectilinear mesh (see, e.g., [4, 5]). The curvilinear mesh is shown to play an important role in the quality of the description of real pore shapes and geometry of the curvilinear coating-substrate interface. Stage 2 involves a numerical simulation study of the deformation and fracture of a mesovolume of the coated material subjected to compression and tension (Figure 1b), with the interfaces being taken into account explicitly.

![Figure 1. Scanning electron microscope image of a material with a porous ceramic coating [1] (a) and regular curvilinear mesh (b).](Image)

2. Algorithm of curvilinear mesh generation

In our previous work on numerical study of the deformation behavior of coated materials [4, 5], curvilinear interfaces are represented as step-wise lines of the rectilinear rectangular mesh (Figure 2a). The main idea of an approach proposed in [6] to generate 2D regular curvilinear meshes is to deform a regular curvilinear mesh (2) to a solution obtained using a uniform rectilinear mesh (see, e.g., [4, 5]). The curvilinear mesh is shown to play an important role in the quality of the description of real pore shapes and geometry of the curvilinear coating-substrate interface. Stage 2 involves a numerical simulation study of the deformation and fracture of a mesovolume of the coated material subjected to compression and tension (Figure 1b), with the interfaces being taken into account explicitly.

Here \( u_i \) and \( u_j \) are the displacement vector components, \( \vartheta \) is the computational parameter varying between 0 and 1. By specifying the boundary displacements \( u_{i,j}, u_{j,i} \) and \( u_{i,j}, u_{i,j} \), where \( i \) and \( j \) vary from 1 to \( n \), we define a curved geometry of boundary. The boundary displacements can be found analytically. The final configuration, i.e. the displacements of internal nodes (\( i = 2..n-1, j = 1..n-1 \)), is defined by solving Equation (1) numerically with the use of the finite-difference Seidel method. The following finite-difference approximation is considered:

\[
\frac{\partial^2 u_i}{\partial x^2} + \frac{(1 - \vartheta)}{2} \frac{\partial^2 u_i}{\partial y^2} + \frac{(1 + \vartheta)}{2} \frac{\partial^2 u_j}{\partial y^2} = 0
\]

\[
\frac{\partial^2 u_j}{\partial y^2} + \frac{(1 - \vartheta)}{2} \frac{\partial^2 u_j}{\partial x^2} + \frac{(1 + \vartheta)}{2} \frac{\partial^2 u_i}{\partial x^2} = 0
\]

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\[
(u_{i,j})_{i,j} = \frac{1}{A_i} \left( \frac{2}{\Delta x_i} \left( \frac{(u_{i,j})_{i,j} - (u_{i,j})_{i,j+1}}{\Delta x_i} + \frac{u_{i,j}}{\Delta y_j} \left( \frac{(u_{i,j})_{i,j+1} - (u_{i,j})_{i,j}}{\Delta y_j} + \frac{u_{i,j}}{\Delta y_j} \left( \frac{(u_{i,j})_{i,j+1} - (u_{i,j})_{i,j}}{\Delta y_j} \right) \right) \right) \right)
\]

\[
\left( \frac{1}{\Delta x_i} \left( \frac{(u_{i,j})_{i,j} - (u_{i,j})_{i,j+1}}{\Delta x_i} + \frac{u_{i,j}}{\Delta y_j} \left( \frac{(u_{i,j})_{i,j+1} - (u_{i,j})_{i,j}}{\Delta y_j} + \frac{u_{i,j}}{\Delta y_j} \left( \frac{(u_{i,j})_{i,j+1} - (u_{i,j})_{i,j}}{\Delta y_j} \right) \right) \right) \right)
\]

Here \( \Delta x_{i+1} = x_{i+1} - x_i, \Delta y_{j+1} = y_{j+1} - y_j, \Delta x = x_{i+1} - x_i, \Delta y = y_{j+1} - y_j \), and

\[
A_i = \frac{2}{\Delta x_i} \left( \frac{1}{\Delta x_i} + \frac{1}{\Delta x_i} \right) + \frac{1}{\Delta x_i} \left( \frac{1}{\Delta x_i} + \frac{1}{\Delta x_i} \right), B_{i,j} = \frac{2}{\Delta y_j} \left( \frac{1}{\Delta y_j} + \frac{1}{\Delta y_j} \right) + \frac{1}{\Delta y_j} \left( \frac{1}{\Delta y_j} + \frac{1}{\Delta y_j} \right)
\]
Figure 2b shows the algorithm output for a rectangular region of the coating material with a single perfectly round pore at the centre. A curvilinear mesh corresponding to the experimental microstructure of the coated material containing multiple pores in the coating and a curvilinear coating-substrate interface is presented in Figure 1b.

3. Statement of the mechanical problem

The coated material deformation was simulated in the plane strain formulation. A total system of equations of mechanics includes equations of motion and continuity, expressions for components of the strain rate tensor and constitutive relations [4, 5]. Numerical solutions were performed in terms of Lagrangian variables using the finite-difference method of the second-order of accuracy [7].

**Figure 2.** Rectilinear (a) and curvilinear (b) meshes for a region with a single pore in the center.

For plane strain the following non-zero components of the strain rate tensor are given by

\[
\dot{\varepsilon}_{xx} = \frac{\partial u}{\partial x}, \quad \dot{\varepsilon}_{yy} = \frac{\partial u}{\partial y}, \quad \dot{\varepsilon}_{xy} = \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right).
\]

The upper dot stands for the time derivative. The mass conservation law and equations of motion in the absence of body forces take the forms:

\[
\dot{V} / V = \dot{\varepsilon}_{xx},
\]

\[
\dot{\sigma}_{xx} + \dot{\sigma}_{yy} = \rho \ddot{u}, \quad \dot{\sigma}_{xy} + \dot{\sigma}_{yx} = \rho \ddot{v},
\]

where \( V \) is the specific volume, \( \sigma_{ij} \) are the stress tensor components, \( \rho \) is the mass density. Taking into account the stress tensor decomposition in the spherical and deviatoric part \( \sigma_{ij} = -P \delta_{ij} + S_{ij} \), the strain tensor decomposition in the elastic and plastic part \( \varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p \), and the hypothesis of plastic incompressibility \( \dot{\varepsilon}_{kk}^e = 0 \), we get the pressure rate and deviatoric stress rate components

\[
\dot{S}_{ij} = 2\mu \left( \dot{\varepsilon}_{ij} - \frac{1}{3} \dot{\varepsilon}_{kk} \right), \quad \dot{P} = -K \dot{\varepsilon}_{kk},
\]

where \( K \) and \( \mu \) are the bulk and shear moduli, \( \dot{\varepsilon}_{ij}^p \) is the plastic strain rate tensor, \( \omega_{ij} \) is the material spin tensor. Summation is implied over the repeated index.

The coating is elastic-brittle ceramics. The substrate material is assumed to be isotropic and follow the von Mises yield criterion with isotropic hardening. In order to describe the plasticity of the steel substrate, we use the plastic flow law \( \dot{\varepsilon}_{ij}^p = \dot{\lambda} \dot{\sigma}_{ij} / \partial \sigma_{ij} \) associated with the von Mises yield condition \( f(S) = \sigma_{eq} - Y_0(e_{eq}) = 0 \), where \( \lambda \) is a scalar parameter, \( \sigma_{eq} \) and \( e_{eq} \) are the equivalent stress and equivalent plastic strain, respectively. The strain-hardening function for the high-strength austenitic steel used as the substrate material is given in [8] as
$$\sigma_r(e_{eq}^p) = \sigma_r - (\sigma_s - \sigma_y) \exp\left(-\frac{e_{eq}^p}{e^p_r}\right),$$  \hspace{1cm} (9)

where $\sigma_r$ and $\sigma_y$ are the ultimate tensile and yield strengths, respectively, $e^p_r$ is the reference value of the plastic strain.

To describe the fracture of the PDC-based coating, use was made of a maximum distortion energy criterion of Huber type accounting for crack initiation and growth in local regions experiencing bulk tension. According to this criterion, fracture occurs in any local coating region if the equivalent stress $\sigma_{eq}$ reaches its critical value: $\sigma_{ten}$ or $\sigma_{com}$ in local tension or compression cases, respectively. Local tension means that the cubic strain $e_{kk}$ takes on a positive value. Here, $\sigma_{ten}$ and $\sigma_{com}$ are the constants that characterize the tensile and compression strength of porous ceramic coating, respectively.

The boundary conditions on surfaces $\Gamma_1$ and $\Gamma_3$ of the computational domain simulate uniaxial tension/compression along the $X$-axis. The bottom surface $\Gamma_4$ is the symmetry line and the top surface $\Gamma_2$ is free from loads (Figure 1b).

4. Simulation results

4.1. Convergence analysis
For convergence test we have performed two sets of numerical simulations for rectilinear and curvilinear meshes (see Figure 2) that approximate a rectangular region with a single perfectly round pore under tensile loading. Material inside the pore region possessed very low elastic properties.

The calculated equivalent stress patterns for the models with rectilinear and curvilinear meshes are shown in Figure 3a-b. Comparison of the stress measured along $A-A'$ and $B-B'$ lines is illustrated in Figure 3c-d to confirm the robustness of the implemented approach. Convergence of the numerical solution was found for both cases (Figure 4). The total number of nodes per pore diameter along the $X$-axis was varied from 10 to 300. Due to the fact that the geometry of the pore material is accounted for more accurately in the calculations, the use of the curvilinear mesh allows accelerating the approach of a maximum stress concentration to a saturation physical value.

Figure 3. Equivalent stress patterns obtained from the rectilinear (a) and curvilinear models (b) and
equivalent stress values taken along $A-A'$ midlines ($c$) and $B-B'$ diagonals ($d$).

Figure 4. Maximum equivalent stress versus the number of nodes per pore diameter.

4.2. The deformation and fracture of the steel substrate with porous PDC-based coating

Let us analyse the mechanisms for stress concentration in the porous coating using the coated material (Figure 1a) approximated by the curvilinear mesh (Figure 1b). At earlier stages of the deformation, both the tensile and compressive stresses are found to occur along pore surfaces in both cases of external tension or compression. In both cases, cracks originate in regions of local tension. Under tension and compression tensile regions occur at different points. On further loading tensile cracks originate and propagate in different ways, i.e., along the loading axis in the case of external compression (Figure 5b, d) and in the perpendicular direction in the case of external tension (Figure 5a, c).

Figure 5. Calculated equivalent stress, plastic strain and fracture patterns of the coating of a composite material for the case of tension ($a, c$) and compression ($b, d$).
5. Conclusions
An algorithm for 2D curvilinear finite-difference meshing based on the solution of the elasticity theory has been implemented that allows describing the pore shape and geometry of the curvilinear coating-substrate interface more precisely. The convergence of the numerical solution has been verified for both rectilinear and curvilinear model, while the use of the curvilinear mesh is shown to accelerate an approach of the maximum stress concentration to a saturation physical value dictated by the geometry of the pore material. Using the curvilinear model, we have performed numerical simulations of tension and compression of coated steel specimens by solving a dynamic boundary-value problem. The pores in coating are shown to be the sources of a geometrical stress concentration on mesoscale level, where thereafter cracks originate. Both under external tension and compression, cracks in the coating tend to originate in the regions experiencing tensile loading. The fracture patterns depend heavily on the type of the applied load, that coming from different locations of local tensile regions under different types of the external loading.

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