PREDICTION OF THE THERMO-MECHANICAL CONTACT BEHAVIOUR OF A GRADED COATING/SUBSTRATE SYSTEM USING ADVANCED NUMERICAL TECHNIQUES

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ABSTRACT
Coatings or coating combinations are widely used to increase operating life and running performance of engineering materials. Nevertheless, the development and choice of coatings is a very complex and costly task. This selection and optimization is thus based on a recursive procedure combining experimental tests and modeling. Numerical simulation is used to analyze coating behavior, tune the geometrical configuration and define optimal thermo-mechanical properties in relation with the applied stress. The objective of the current work is to develop a 3D thermo-elastic model for coatings with graded properties. Former models dealt with isotropic layers with constant properties adhering perfectly. These last assumptions result in discontinuities in stress and temperature fields at the interface between successive layers. The increasing use of interface layers between coatings and substrates requires theoretical models to predict the thermomechanical behavior of such graded coatings. The gradation in properties of the material reduces induced thermo-mechanical stress discontinuities. Multigrid techniques are used to improve solver efficiency, reduce CPU time and thus permit the use of fine grids to accurately describe the variations in elastic properties.

INTRODUCTION
Numerical simulation of thermo-elastic loading on elastic bodies becomes very difficult when considering thin coatings with varying properties. Models usually consider isotropic layers with constant properties. Those models [1, 2] are based on integral transform methods combined with Fast Fourier Transform algorithms. These techniques cannot handle 3D thermomechanical problems, as the corresponding equations do not verify the assumption of displacement biharmonicity. Functionally graded materials (FGM) are commonly used nowadays to protect surfaces from mechanical and tribological damage. They may be either coating materials or interface regions between successive coatings with varying properties. The optimum protection depends on the wear resistance of the surfaces, the thermal barrier of the components, the bond strength increase and the reduction of internal stresses... Deposition processes, characterization techniques and numerical models are the three basic abilities to create the optimum FGM adapted to substrate and operating conditions. The numerical model presented here can handle any kind of depth dependence of the material properties. The heat conduction and Navier’s equations are discretized through a finite difference (FD) or a finite element (FE) formulation. The mesh size is governed by the interface layer thickness but also by the characteristic loading dimensions. Multigrid techniques [3] are used to improve the solver efficiency, which is important as the number of variables is very large.

1 Thermoelastic model
The objective of this work is to solve the thermal and the elastic problems in a solid with varying properties under a given thermal and mechanical loading. The main assumptions are small strains and linear elasticity. The temperature field is unaffected by the mechanical loading.

1.1 Thermal equation
Let us consider a solid with varying properties in the x-direction (figure 1). Both continuous or discontinuous variations can be modeled. The heat conduction equation is written as [4]:
\[
\Delta T + \frac{1}{k} \left( \frac{\partial k(x)}{\partial x} \frac{\partial T}{\partial x} \right) = 0
\] (1)

with \( \Delta \) the Laplace operator and \( k(x) \) the thermal conductivity. The boundary condition can be an imposed heat flux or an imposed boundary temperature.

### 1.2 Generalized elasticity equations

The displacement based equilibrium equations are solved with the corresponding boundary conditions. The solution of this set of equations automatically satisfies the compatibility equations.

The equilibrium equations, accounting for the anisotropic properties of the solid, are the generalized Navier equations:

\[
\frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu}{2} \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial u_j}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left( (3\lambda + 2\mu) \alpha T \right) \quad i = 1, 2
\] (2)

with \( \lambda(x) \) and \( \mu(x) \) the Lamé’s coefficients:

\[
\lambda = \frac{E \nu}{(1 + \nu)(1 - 2\nu)} \quad \mu = \frac{E}{2(1 + 2\nu)}
\] (3)

The Young’s Modulus \( E(x) \) and the Poisson’s ratio \( \nu(x) \) are a function of \( x \) depending on the deposition technique and the material composition. Stress-based boundary conditions are expressed in terms of displacements and strains using the stress/displacement relations.

### 2 Numerical results

Equations (1) and (2) are discretised on a uniform grid by second-order central finite differences. The classical solution of the problem using Gauss-Seidel relaxation is very time consuming. Multigrid methods are used to accelerate the convergence. First, the temperature field is calculated using equation (1) with the appropriate thermal boundary conditions. Then, the set of equations (2) is solved with the mixed boundary conditions. Finally, the stresses in the solid are calculated using the displacement/stress relations.

#### 2.1 Applications

As an example, a 10mm*10mm solid is submitted to a hertzian contact \( (P_0 = 200 \text{MPa}, \ a = 0.28 \text{mm}) \). The layer thickness is 100\( \mu \)m. Two cases are considered. In the former the coating has constant properties \( (E_c = 600 \text{ GPa}, \ \nu_c = 0.2) \) with a stepwise transition. In the latter the interfacial layer has graded properties \( (E_c = 602 \text{ GPa}, \ \nu_c = 0.3) \) varying linearly between the coating and the steel \( (E_s = 202 \text{ GPa}, \ \nu_s = 0.3) \) properties. Figure 2 shows the different Von Mises stress fields for a hertzian contact.

![Figure 1. Young’s Modulus and Poisson’s ratio with graded interphase](image1)

![Figure 2. Von Mises stress (MPa) in a coated solid with stepwise (above) and linear transition of the mechanical properties](image2)

#### 2.2 Conclusion

The method proposed in the current study allows a detailed analysis of the stress field inside and near a coating layer. It was shown that the interfacial layer reduces the stress discontinuity near the coating-substrate boundary. This stress reduction confirms the usefulness of such a layer.

### REFERENCES


