Effect of coating architecture on impact stress distribution in particulate erosion conditions

M Bielawski and W Beres
NRC Institute for Aerospace Research, Ottawa, Ontario K1A 0R6 Canada
E-mail: mariusz.bielawski@nrc.gc.ca

Abstract. A computer simulation technique based on ABAQUS/Explicit was used to investigate stress and strain distribution at the surface and at the coating/substrate interface of multi-layer coatings under single particle impact. Eight different coating architectures and five material models were analyzed to determine possible stress reduction that could be obtained through a combination of layering patterns and material properties. Specifically, the elastic, elastic-plastic and brittle cracking coating models were used and coating response was analyzed using the surface tensile stress as a main evaluation criterion. It was found that stress reduction of up to 3.6 times was possible for the best configuration indicating that optimized coating architecture can significantly contribute to coating erosion performance.

1. Introduction
Erosion is one of the modes of material degradation that has a significant impact on safety and service life of gas turbine engines operated in dusty conditions. Wear caused by eroding particles, such as sand, dust or volcanic ash lowers engine power, decreases fuel efficiency and shortens service life. To protect gas path compressor components, complex filtration systems are used in some helicopter engines. Yet erosion-resistant (ER) coatings need to be applied to the most vulnerable components. The leading technology in this area is Physical Vapor Deposition (PVD). The PVD coatings, such as nitrides or carbides of transition metals, are much harder than most steels or specialized alloys and have substantially lower erosion rates. In addition to experimental developments, appreciable modelling and simulation have been carried out. These efforts have been directed at either modelling of erosion resistance of materials using the Monte Carlo method, or modelling of the coating response to eroding particle impact using the finite element (FE) method. The latter approach was adopted in this research. In particular, different coating architectures and material constitutive models were analyzed to determine their effect on the coating response to a single particle impact.

2. Modelling approach
The principal erosion mechanism for hard ceramic coatings such as TiN is brittle fracture. Under particle impact, multiple cracks are produced, which leads to material removal when the cracks propagate to the free surface or interlink. According to the Rankine criterion, cracks nucleate in the coating when the stress exceeds the tensile strength of the material. The amplitude of the tensile stress is obviously related to the kinetic energy of the impacting particle, while the cracking threshold is an intrinsic property of the coating material. Thus, the erosion resistance of brittle coatings can be linked to the magnitude of the surface stresses in the coating surface.
Detailed analysis of the stress field produced by a single particle impact demonstrated that six stress components (von Mises, radial S11, shear S12, axial S22, circumferential S33 and maximum principal SP3) at four critical locations need to be considered to fully characterize coating reaction [1]. The critical stress locations are shown in figure 1.

In this research, coating internal architecture (number of layers, individual layer thickness, layering pattern and total coating thickness) and Young’s modulus (E) of individual layers were optimized from the point of view of minimizing stresses in the critical locations.

2.1. FE model
A 2D axisymmetric model of a single particle impacting a multilayer coating on a steel substrate was developed using the finite element method based on ABAQUS/Explicit version 6.4. The interaction between the particle and the coating was modelled using the contact pair option with no friction. A constant initial velocity of 84 m/s was used for the particle in all calculations. Relevant material parameters were assigned to selected finite element cells to create the required coating/substrate internal architectures. Details of the model design were published elsewhere [2]. In all FE models, it was assumed that continuous solid mechanics principles still hold for the range of model dimensions.

2.2. Material models for coatings
The linear elastic models (EL) assumed Young’s modulus values from 200 to 800 GPa, while the elastic-plastic models (EP) were isotropic without strain hardening. The plastic part of the EP models included a perfectly plastic portion described by the yield stress $\sigma_y$ and the corresponding elastic strain $\varepsilon_y$. For the 300 GPa TiN coating, an $\varepsilon_y$ value of 1% was assumed [3]. Around these numbers, two series of EP material models were prepared. In the series EP-1, the yield stress $\sigma_y$ was assumed constant and in the series EP-2, the elastic strain $\varepsilon_y$ was assumed constant. In the brittle cracking models (BCM), post-failure stress-strain behaviour needed to be specified [1]. Since there is no such data for TiN, parametric studies were performed. Two types of BCM models were used: BCM-1 based on constant cracking stress and BCM-2 based on constant cracking strain. A BCM-1 model is presented in figure 2.
3. Results and discussion

3.1 Stress distribution
A basic coating configuration consisting of an elastic single-layer TiN on an elastic-plastic steel substrate was thoroughly analyzed to determine stress distribution in the coating/substrate system. The results are shown in figures 3 and 4.

The maximum compressive stress S22 was observed under the impact center, as expected. The magnitude of this stress was in the range of -36 GPa. Another critical area was the interface between the coating and substrate, where relatively high values of radial stresses S11 were present. Due to the model axial symmetry, some stress components were identical. In figure 4, the area of high tensile stresses S11 and S12 can be seen around the contact radius of the impacting particle. Outside the contact radius, there is an area of high radial stresses S11, in the range of 2 GPa. These tensile stresses in the coating surface are responsible for tensile cracking [4]. The high value of the shear stress S12 around the contact radius indicates presence of significant material deformation. In the case of an elastic coating, this deformation is only momentary and disappears when the impacting particle reflects from the surface. In the discussed example, this happened after approximately 15 ns.

3.2 Effect of coating architecture
The effect of coating architecture on impact stress magnitude in the TiN coating surface was investigated for eight different coating configurations. In this evaluation, tensile stress S11 at location No. 3 was used as an evaluation criterion. For Configuration No. 1 which was a single-layer TiN coating with E=200 GPa and total thickness of 10 µm, a stress value of 1.93 GPa was calculated. Adding a high-modulus second layer (Configuration No. 2) resulted in a decrease in surface stress magnitude to 1.08 GPa. Further optimization of the bi-layer coating through an increase in the second layer modulus (Configuration No. 3) reduced the stress value to 0.70 GPa, which was the lowest value for all examined configurations. Configuration No. 4 consisted of a series of 10 interchanging layers of low (200 GPa) and high modulus (400 GPa) TiN. In this case, a surface stress of 1.51 GPa was obtained. A similar value (1.49 GPa) was obtained for Configuration No. 5 where interchanging layers were replaced by a set of layers with gradually increasing (from top to bottom) modulus. However, when the order of layers was reversed (Configuration No. 6), a very high stress level was recorded (2.52 GPa), making this configuration the worst among those analyzed. In the next configuration (No. 7), a 1-µm thick high-modulus layer buried under the coating surface was modelled. This design produced a surface stress value of 2.1 GPa. The last configuration analyzed, No. 8, was a modification of Configuration No. 4 with four times thinner layers in the top section of the coating. This modification failed to deliver lower stress (1.83 GPa) than the original Configuration No. 4. Details of all coating designs can be found elsewhere [2].
Depending on the coating configuration and material properties used in calculations, the differences in tensile stress level between analyzed architectures were up to 3.6 times, indicating that optimized coating architecture can significantly contribute to coating erosion performance.

3.3 Effect of material model
FE calculations were performed for five different material models (EL, EP-1, EP-2, BCM-1 and BCM-2) for the multi-layered coatings described previously as Configuration No. 4. For each material model, stresses at four critical locations (see figure 1) were calculated. The results are summarized in table 1. Please note that compressive stresses were entered as negative numbers.

| Stress Component | Location | EL   | EP-1 | EP-2 | BCM-1 | BCM-2 |
|------------------|----------|------|------|------|-------|-------|
| S22              | 1        | -33.3| -7.51| -7.43| -31.2 | -31.3 |
| SP3              | 2        | 11.3 | 1.44 | 1.87 | 2.77  | 3.93  |
| S11              | 3        | 1.51 | 0.79 | 1.86 | 1.49  | 1.92  |
| S12              | 4        | 7.84 | 1.73 | 2.13 | 7.92  | 8.35  |

Overall, the highest stresses were recorded for the elastic model EL and the lowest stresses for the model EP-1. Noticeably, the differences between two EP models and between two BCM models were relatively small, with the exception of stress S11 that is responsible for tensile cracking in the coating surface. This stress appears to be the most sensitive to material model change. Thus, for brittle coatings where tensile cracking is the main failure mode, S11 can be used as a single evaluation criterion.

In summary, without experimental verification, it is difficult to judge which model is closer to reality. However, the elastic-plastic model EP-1 produced quite realistic stress values, comparable to those obtained from the quasi-static indentation experiments [5, 6].

4. Conclusions
Depending on the coating configuration and material properties used in calculations, the differences in tensile stress level between analyzed architectures were up to 3.6 times, indicating that optimized coating architecture can significantly contribute to coating erosion performance.

Material model selection strongly affects modelling results. As shown in FE calculations, the differences in stress values between models could be in the range of an order of magnitude. However, without experimental verification, it is difficult to judge which model is the most suitable. More efforts are needed to develop coating models allowing for quantitative calculations.

Acknowledgement
This research was performed with financial assistance from the Defence R&D Canada.

References
[1] Beres W and Bielawski M 2006 Proc. Int. Conf. on Aerospace Materials and Manufacturing: Emerging Materials, Processes, and Repair Techniques (Montreal, Canada 1–4 October 2006) ed M Jahazi et al (Montreal: Canadian Institute of Mining) pp 21–32
[2] Bielawski M and Beres W 2007 Wear 262 167–175
[3] Kolkman H J 1995 Surf. Coat. Tech. 72 30–36
[4] Zhang W and Subhash G 2001 Int. J. Solids Struct 38 5893–5913
[5] Rowcliffe D J 1992 Key Eng. Mat. 71 1–22
[6] Tang K C, Faulkner A, Schwarzer A N, Arnell R D and Richter F 1997 Thin Solid Films 300 177–188