The effect of double layer coatings of high modulus on contact stresses

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ABSTRACT
In an earlier paper (Van der Zwaag and Field 1982), we investigated, using finite element methods, the effect of a thin, hard coating on the stress field generated by a spherical indenter on a uniform halfspace. Of particular practical interest was the reduction in the maximum (radial) tensile stresses in the substrate solid as the modulus and thickness of the coating increased. Experimental support for the theoretical predictions was given by Van der Zwaag and Field (1983). In the present paper, the investigation is extended to examine the potential of double layer coatings of two different high modulus materials. It is shown that a suitable selection of the properties of the two layers can reduce the tensile stresses in the substrate solid compared to the values in an uncoated substrate. Two particular systems are examined in detail. Potential benefits of monolayer and multilayer coatings are discussed critically. The results have application to a range of practical problems.

§1. INTRODUCTION
In many high-technology applications a wide range of material properties is demanded for a single component. When such a range is unobtainable from a single material, surface coatings can assist in meeting the complex demands. Typical examples of well established types of coatings are low-friction, wear-resistant, corrosion-resistant and optical coatings.

Coatings have also been used to improve the rain-erosion resistance of exposed aircraft components. The present anti-rain erosion materials can be divided into two categories, namely compliant (elastomers) and rigid materials (metals and ceramics). It has been shown theoretically (Matthewson 1979, 1981, 1982) that a substrate is most effectively protected by a compliant coating when the Poisson’s ratio of the coating approaches 0.5. The observed excellent performance of neoprene-based coatings (Schmitt 1970) is in good agreement with these predictions.

In the case of hard coating materials, very good results have been obtained for nickel-plated fibre composites (Weaver 1967). However, the application of metallic coatings will be limited since metals are opaque over a wide range of frequencies, including the visible and radar spectrum.

In comparison with the other materials, ceramic coatings are still underdeveloped because of their brittle behaviour which causes serious problems in obtaining a perfect bond between coating and substrate. However, there are several applications such as infrared transparent windows where only ceramic coatings would meet the stringent optical requirements. So far, the development of ceramic coatings has been based

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primarily upon their optical properties and the resulting rain erosion protection has been shown to be small (Walton and Gorton 1970, Hackworth et al. 1979, Peterson 1979).

In order to determine the optimum mechanical properties for protective coatings, a finite element model, in which raindrop impact is simulated by a static spherical indentation, has been developed (Van der Zwaag and Field 1982). In this model, the effect of the elastic properties of the coating material and the coating thickness on the stresses in the coating and the substrate has been examined for coatings consisting of a single layer. Considerable reduction in the maximum tensile stress in the substrate, which is responsible for crack propagation in brittle materials, can be obtained with very rigid coatings of sufficient thickness.

Ball indentation experiments on carbon-coated germanium (Van der Zwaag and Field 1983) have shown that a thin coating (≤3 μm) can increase the critical load for crack nucleation up to 400%. The observed increase of the fracture load with the effective coating thickness was in good agreement with the theoretical predictions.

In the present work we have expanded the model to examine the potential of coatings consisting of two different rigid materials.

§2. The model

In the model, a circular area with a radius a is loaded normal to the coating surface. The pressure distribution over the contact area is given by

$$P(r) = P\left[(a^2 - r^2)/a^2\right]^{1/2},$$

where $r$ is the radial coordinate and $P$ the maximum pressure at the centre. This pressure distribution is identical to the pressure distribution in the case of Hertzian contact on a uniform halfspace (Hertz 1881, Huber 1904). Due to the circular symmetry of the problem the stress fields can be calculated using a two-dimensional finite element model. The elements are in the plane of a cross-section through the centre of contact.

The element distribution used is shown in fig. 1 (a). The elements are divided into three groups: one with the (fixed) substrate properties and two with the (variable) coating properties. Figure 1(b) shows a detail of the element distribution near the contact zone. The elements with the coating properties are shaded in this figure. The accuracy of the finite element programme has been tested by comparing the results for an uncoated halfspace (i.e. the properties of the two coating layers are equal to those of the substrate) with the analytical solution of the stress field. For the present element distribution, the difference between the two solutions is always less than 1%. Throughout the analysis the elastic properties of the substrate are kept constant with a Young's modulus of 61 GPa and a Poisson's ratio of 0.25 (i.e. typical values for a soda-lime glass). Young's moduli of the two coating materials were varied between two and ten times that of the substrate material. This range covers nearly all possible hard coating materials. Since the analysis for single layer coating systems has shown that the effect of the Poisson's ratio of the coating material on the stress field is small for Poisson's ratio varying from 0.20 to 0.30, the Poisson's ratio of all coating materials was kept constant at ν = 0.25.

The effect of the total coating thickness has been investigated for thicknesses up to 12% of the contact radius. In the following sections, the stresses are normalized to the maximum pressure at the centre of the contact area in such a way that positive values indicate tensile stresses and negative values compressive stresses. To distinguish between the various coating systems, the following notation is introduced: $E_i, E_s, t_i, t_s$
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Fig. 1

(a) Finite element distribution for double coating systems. (b) Detail of (a) near the contact area. The two coatings are indicated.

where $E_1$ and $E_2$ are the moduli of the outer and interlayer both normalized to the modulus of the substrate $E_s$ and $t_1$ and $t_2$ the corresponding thicknesses.

§ 3. Results

Elastic contact between an uncoated brittle material and an indenting or impacting particle can cause damage due to the development of radially oriented tensile stresses in a shallow surface layer around the contact area. The circumferential and axial stresses are compressive everywhere in and around the contact zone and do not contribute to the damage process. Also, in the case of the coated halfspaces investigated here, the finite element calculations have shown that the only stress which can be tensile and hence can cause crack propagation are the radial stresses. It is for this reason that this paper deals primarily with the effect of the various coating parameters on the radial stress field.

3.1. The radial stress fields in two example programmes

Before dealing with the results in a general way, the radial stress fields in two double layer coating systems are presented and discussed in detail. In the first demonstration
programme, the stresses are calculated for a 5/2/0.015a/0.015a coating system. The second demonstration programme deals with a 2/5/0.015a/0.015a system. Figures 2 and 3 show parts of the radial stress field at the surface, at the interlayer and at the substrate for the two coating systems.

The plotted radial stress for the interlayer is the stress field in the interlayer at the interface with the surface coating. Similarly, the plotted radial stress in the substrate is that which occurs in the substrate at the interface with the interlayer. In both figures the radial stress field which would occur in an uncoated halfspace of substrate material at the depth of the substrate interface is indicated by a dashed line. The figures show that both coating systems reduce the substrate stresses by an equal amount. For an uncoated specimen, the maximum radial stress at a depth of 0.03a below the surface is 0.078 P while for both coated specimens the maximum radial stress in the substrate is $\sigma_{r,\max}=0.043 P$. This value should be compared with $\sigma_{r,\max}=0.060P$ for a monolayer coating with $E_2 = 5E_0$ and a thickness of 0.015a and with $\sigma_{r,\max}=0.031P$ for a coating thickness of 0.03a. As expected intuitively the coating configurations in the example programmes are more effective than just a thin monolayer of the most rigid coating material and less effective than a monolayer of equal thickness to the sum of the outer and interlayer thicknesses.

![Figure 2](image)

The radial stress field outside the contact area at the surface, interface and substrate for a 5/2/0.015a/0.015a double layer coating system.
The radial stress field outside the contact area at the surface, interface and substrate for a 2/5/0.015a/0.015a double layer coating system.

When comparing the stresses at the surface and at the interlayer for the two coating systems of figs 2 and 3, large differences are observed. In the case of the rigid interlayer, the largest radial stresses occur below the surface while with the 5/2 system a more normal behaviour is observed. The largest radial stresses occur in the system with a rigid facing. The high stresses in the coatings are due to the relatively large deflections of the perfectly adhering substrate.

3.2. Effect of the coating parameters on the radial stress in the substrate

As was shown for the 5/2/0.015a/0.015a and 2/5/0.015a/0.015a coating systems (figs 2 and 3), the presence of a coating leads to a significant decrease of the radial stresses in the substrate. In fig. 4 the normalized maximum radial stress in the substrate is plotted versus the coating thickness for all coatings investigated. In all double layer coating systems the thickness of the surface layer equals that of the interlayer. The dashed line labelled 'Hertz' indicates the decay of the maximum radial stress with depth below the surface for a uniform halfspace with the properties of the substrate.

The dashed lines labelled 2, 5 and 10E₁ indicate the stress reduction for the case of a monolayer coating with a Young's modulus of 2, 5 and 10 E₁ respectively. The conclusion from the two demonstration programmes in the previous section, that the radial stress field in the substrate is independent of the stacking of the two layers (i.e. a system with a rigid surface layer is as effective as a system with a rigid interlayer), is valid for all coating combinations investigated. Figure 4 shows that at a fixed total coating thickness the effect of a double layer system is always less than that for the case of a
monolayer of the more rigid coating material but more than that for a coating of the less rigid material.

This is shown in more detail in fig. 5 which shows the maximum radial stress at the substrate for five combinations of relative coating thicknesses at a fixed total coating thickness of 0.03a. Young's modulus of the surface layer is 5E_s and that of interlayer 2E_s. The calculations show a continuous decrease in maximum radial stress with increasing relative coating thickness of the more rigid coating material. Similar results are obtained for coatings of the 2/5 type.

It should be noted that the presence of a (single or double) coating increases the radial distance at which the maximum stress in the substrate occurs. Since the probability of propagating pre-existing defects in brittle materials depends on both the magnitude of the stress field and the size of the surface area stressed, the increase in distance reduces the effect of the coating. However, since the radial tensile stress is everywhere smaller than that for an uncoated substrate these hard coatings do indeed protect the substrate.

3.3. Effect of the coating parameters on the interlayer stresses

The maximum tensile stresses in the interlayer at the interface with the outer coating are plotted for the various coating systems in fig. 6 as a function of the total
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Fig. 5.

The maximum radial stress in the substrate as a function of relative coating thicknesses for 5/2 coatings. For \( t_1/(t_1+t_2)=0 \) or 1 the coating consists of a monolayer with \( E_1=2E_s \) and \( E_2=5E_s \), respectively. In all cases \( t_1 + t_2 = 0.03a \).

Fig. 6

The maximum radial stress in the interlayer versus the total coating thickness for various double layer coatings. In all cases \( t_1 = t_2 \).

coating thickness. The figure shows a rapid decrease of the maximum stress with coating thickness. In the case of a hard interlayer the stress level is high due to the limited protection offered by the outer coating while for the 10/2 and 5/2 systems the stresses in the interlayer are relatively low.

3.4. Effect of the coating parameters on the surface stresses

In contact problems involving brittle coating and substrate materials, failure of the total structure may be caused by propagation of flaws located either at the coating
surface or at the substrate. It is therefore important to examine stresses at the surface of the outer coating.

The maximum tensile stresses at the surface are plotted in fig. 7 as a function of the coating thickness. In all coating systems examined, the maximum tensile stress is higher than the value for a homogeneous halfspace $\sigma_{\text{max}} = 0.167 P$. The largest increase is found for coatings of the 10/2 type while the smallest increase occurs in the 2/10 systems.

For the double layer coatings examined here, the maximum radial stress for a given coating system is approximately constant for total coating thickness less than 0.12a. Calculations for monolayer coatings have shown that the maximum tensile stress in these cases increases with coating thickness. Unfortunately, with the present model no accurate calculations of the surface stresses are possible for coating thickness less than 0.015a.

3.5. Discussion

When an uncoated substrate is loaded the maximum tensile stress is $\sigma_{\text{r, max}} = 0.167 P$. In all coating systems examined here, higher values for the maximum stress are found, either in the interlayer (2/5 and 2/10 systems) or in the outer coating (5/2 and 10/2 systems). This indicates very clearly the point that only those materials which have a higher fracture stress than the substrate material can be used as a protective coating.

However, examination of the mechanical and elastic properties of various (infrared transparent) materials shows that in general the fracture stress $\sigma_f$ (for macroscopic specimens) increases with increasing Young's modulus as shown in fig. 8. Such a linear dependence between fracture stress and Young's modulus is also predicted by simple

The maximum radial stress in the outer coating surface versus the coating thickness for double layer and monolayer coatings. In the case of double layer coatings $t_1 = t_2$. 
models for the theoretical strength of solids which yields $\sigma_f = (E\gamma_0/r_0)^{1/2}$ where $\gamma_0$ is the fracture surface energy per unit area and $r_0$ the interatomic distance. The data compiled in fig. 8 can be described by $\sigma_f \approx E/1600$. Although such a simple relation is unlikely to hold true for very thin coatings of rigid materials, the general trend is probably correct. Also, our results for indentations on carbon-coated germanium support this prediction.

As mentioned earlier, not only the magnitude of the stress field is important but also the spatial distribution of the tensile stresses. Whilst the maximum tensile stress is almost independent of the total coating thickness, the distribution of the radial stress changes markedly with coating thickness. This is illustrated in fig. 9 where the radial stress outside the contact area is plotted for three different coating thicknesses. In all cases $E_1 = 5E_s$, $E_2 = 2E_s$ and $t_1 = t_2$. In these figures the decay of the radial stress with radial distance for an uncoated halfspace ($\sigma_r = \sigma_{r,\text{max}} a^2/r^2$ for $r > a$) is indicated with a dashed line. For the thin coatings the relatively large deflections of the interlayer cause a significant increase in the area stressed by relatively large tensile stresses. For brittle materials, such an increase is clearly detrimental. Similarly, in the case of a rigid interlayer the tensile stresses in the outer coating decay more rapidly than in the case of an uncoated halfspace.

It should be mentioned here that in the model it is assumed implicitly that there is a perfect bond at the various interfaces. In practice, however, delamination can occur which will reduce the effect of the coating considerably and will lead to coating removal and a complete loss of protection. Examination of the interfacial shear stresses for several single and double-layered systems has shown that the magnitude and spatial
The radial stress field on the coating surface outside the contact area for three 5/2 type coatings with $t_1 = t_2$, (a) $t_1 + t_2 = 0.03a$; (b) $t_1 + t_2 = 0.06a$; (c) $t_1 + t_2 = 0.12a$. The dashed lines indicate the hertzian decay for an uncoated halfspace.

The distribution of the interfacial shear stresses do not vary much between the different systems. This means that the interfacial bond strength rather than the coating properties will determine the likelihood of delamination. Since the bond strength depends on technological parameters and the reactivity of the compounds and not on the elastic properties, no suggestions can be made for coating systems with a high resistance against coating delamination.

Finally, the problem of the correct layer sequence of a double coating is addressed. While the sequence of coating layers will often depend on technological feasibility and/or restrictions due to optical requirements, the stress analysis presented here, in conjunction with the assumed linear dependence of fracture stress on Young’s modulus, suggests that coatings with a rigid outer layer and an interlayer of intermediate stiffness are likely to perform better than coatings with a rigid interlayer.
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This preference for rigid outer layer coatings is based on the ratios of the maximum surface stresses. For example, for coatings of the 10/2 type \( \sigma_{s,\text{max}} = 0.62P \) and for coatings of the 2/10 type \( \sigma_{s,\text{max}} = 0.23P \) (fig. 7). The ratio of the two stresses is less than the predicted ratio between the fracture stresses of the two materials (which is 5). The relatively large area with high tensile stresses for coatings with a rigid outer layer (fig. 9) reduces the difference between the two types of coating.

§4. Conclusions

It has been shown that thin, hard coatings, either consisting of a monolayer or a double layer, reduce the maximum tensile stress in the substrate compared to the values for an uncoated halfspace under the same loading conditions. Thin, hard coatings can therefore in principle be used to protect brittle materials against elastic contact damage. Comparison of double layer coatings with monolayer coatings shows that for a given total coating thickness the substrate stresses are more effectively reduced by a monolayer of the hardest of the two materials used in the double layer. However, for the double layer coatings the surface stresses in the outer coating are lower than in the case of monolayer coatings, in particular for larger coating thickness. A further important practical advantage is that thick monolayers are difficult to fabricate without developing residual stresses which encourage delamination. A multilayer system with layers of different modulus could, in principle, be built up to relatively large thicknesses without delamination.

Although the performance of a coating depends on a number of factors other than just the stresses, such as fracture strength and toughness of coating and substrate material, interfacial strength, pre-existing stresses and flaw statistics, the calculations suggest that double layer coatings might perform better than monolayer coatings. The best results are predicted for the coatings with a rigid outerlayer and an interlayer of intermediate stiffness.

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References


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