The influence of an interlayer on coating delamination under contact loading

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Abstract

The objective of this work is to study indentation induced delamination of a strong film from a two layer system. To this end our model is composed of an elastic diamond coating, and a chrome interlayer and a tungsten carbide substrate, both elastic-plastic. The interface between the coating and the interlayer is supposed weaker than between the interlayer and the substrate, thus the first one is modelled with a cohesive zone and a Xu-Needleman constitutive law while the second one is rigid. In addition only normal delamination is studied here, for in these conditions it always appears for a smaller indentation force than for shear delamination.

Delamination initiation is studied for several properties of the system through the evolution of the critical force with the interlayer thickness. Depending of the cohesive zone and the interlayer material properties, it is found that the critical force achieve a maximum with an interlayer thickness of a half to two times the coating thickness. The value of this maximum goes from two to five times the critical force for delamination of a two layer system. It is also demonstrated that this maximum tends to appear for smaller thickness if the cohesive zone is weaker, which could be very interesting for industrial applications.

Keywords: Adhesion; Coatings; Delamination
1. Introduction

Hard coatings are often used to improve the friction, wear, and contact fatigue resistance of surfaces that are subjected to contact loading. For example, ceramic coatings are used to protect a wide variety of automotive components, including pistons, valve heads, gears and bearings. In addition, diamond and diamond-like-carbon films are currently of great interest as protective coatings for machine tools, particularly for experimental dry machining processes. For example General Motors are developing tungsten carbide drills with diamond coating to bore aluminium without lubricating. Coatings subjected to contact loading suffer from a variety of failure mechanisms, including coating fracture, spalling, buckling, among many others [1-8]. Delamination of the coating from the substrate is a particular concern. Consequently, there is great interest in developing techniques to optimize coating adhesion. A variety of approaches may be exploited for this purpose, including selecting appropriately the elastic and plastic properties of the coating and substrate; optimizing the thickness of the coating, and modifying the chemistry of the coating/substrate interface itself. In this paper, we aim to contribute to this effort by predicting the influence of a transition zone between the coating and the substrate using a systematic set of computer simulations

To this end, we will present the results of a detailed parametric study that predicts the response of a hard elastic coating on an elastic-plastic two layer subsystem, composed of an interlayer and the substrate, to indentation loading. The problem to be solved is illustrated in Figure 1.1. A linear elastic coating is bonded to an elastic-perfectly plastic interlayer. The interface between them is modelled using a cohesive zone law [15], which allows the coating to separate from the interlayer, and is characterized by phenomenological constitutive equations relating the tractions acting on the two bonded solids to the separation between them. The substrate and the interlayer are rigidly bonded for the interface between them is supposed much stronger than the first one. The coating is indented by a rigid frictionless sphere.
Our goal is to compute critical force and depth $h_c$, which respectively specify the indentation force and depth needed to observe delamination at the coating/interlayer interface after complete unloading. Our main study will be the influence of the interlayer thickness, changing the interlayer mechanical properties, the indenter radius, and the strength and toughness of the interface. Our work builds on a study by Gao, Xia, Bower, Lev and Cheng [18], who used a similar model to study delamination mechanism maps for a two layer system. Convergence problems in finite element simulations used to restrict studies to a limited parameter space. Y.F. Gao and A.F. Bower have found a way to resolve these convergence problems [17] as it is described further below and it will be systematically used in our simulations.

The remainder of this paper is organized as follow. The next section summarizes the problem, its equations, its approximations and the cohesive surface model. Section three presents the model quantitatively, the concrete implementation of the cohesive zone and a dimensional analysis. Section four contains the results and their interpretations while section five is the conclusion.
2. Problem formulation

2.1. Governing equations

In this section the objective is to briefly define the general system, in order to find what data
the simulation is going to need and what are the basic phenomena at stake in the overall
behaviour. In addition it ensures a global understanding of the numerical process. Note that
section three presents the model used in our computations more precisely.

We consider a system comprising an elastic-perfectly plastic material (substrate) coated by an
elastic thin film, the two of them being separated by an elastic-perfectly plastic interlayer. The
part is indented by a spherical indenter. The indenter is assumed rigid and only characterized
by its radius $R$. Assuming the whole to be isotropic, the problem is axisymmetric, with radial
coordinate $r$ and axial coordinate $z$ in the indentation direction, as illustrated in Fig. 1. The
film is characterized by its thickness $t_c$ and is bonded to the interlayer by an interface, which
will be specified in the next subsection. The substrate is taken to have a height of $H - (t_c + t_i)$
and radius $L$, with $L$ large enough so that the solution is independent of $L$ and the substrate
can be regarded as a half space.

The analysis is carried out numerically using a finite strain, finite element method. It uses a
formulation in which equilibrium is expressed in terms of the principle of virtual work as:

$$
\int_{\Omega} \mathbf{T} : \mathbf{\varepsilon} \, dV + \int_{S} \mathbf{T} \cdot \Delta \, dS = \int_{\partial \Omega} \mathbf{\Gamma} \cdot \mathbf{\xi} \, dS
$$

Here, $\Omega$ is the total $H \times L$ region analyzed and $\partial \Omega$ is its boundary, both in the undeformed
configuration. $\mathbf{\xi}$ and $\mathbf{\Gamma}$ are respectively the displacement and traction vectors, $\mathbf{\sigma}$ is the stress
tensor while $\mathbf{\varepsilon}$ is the strain tensor. The second term in the left-hand side is the contribution of
the interface, which is here measured in the deformed configuration ($S_i = \{z = t_c\}$). The
traction transmitted across the interface is $\mathbf{T}$, while the displacement jump is $\Delta$. Here, and in
the remainder, the axisymmetry of the problem is exploited, so that $\mathbf{\xi}_\theta = 1^\theta = \mathbf{\sigma}_\theta = \mathbf{\varepsilon}_\theta = 0$. 

The precise boundary conditions are illustrated in Fig. 1.1. The indentation process is performed incrementally with a constant indentation rate $V_0$. Outside the contact area with radius $a$ in the reference configuration, the film surface is stress free:

$$\Gamma^*(r,0) = \Gamma^c(r,0) = 0 \text{ for } a \leq r \leq L.$$ 

Inside the contact area we assume frictionless conditions:

$$\Gamma^*(r,0) = 0 \text{ for } 0 \leq r \leq a.$$ 

The substrate is simply supported at the bottom, so that the remaining boundary conditions read:

$$\xi_s(0,z) = 0 \text{ for } 0 \leq r \leq L$$
$$\xi_s(r,-H) = \xi_s(r,-H) = 0 \text{ for } 0 \leq r \leq L$$
$$\xi_s(L,z) = \xi_c(L,z) = 0 \text{ for } -H \leq z \leq 0$$

However the sizes $L$ and $H$ will be chosen large enough that the solution is independent from the precise remote conditions.

These equations and boundary conditions need to be supplemented with the constitutive equations for the coating and the substrate, as well as the interface. As the latter is central to the results of this study, these will be explained in detail in the forthcoming subsection. The substrate and the interlayer are supposed to be elastic-perfectly plastic materials, with plastic flows being controlled by the rate-independent von Mises plasticity with yield stresses $\sigma_{ys}$ and $\sigma_{yi}$. The elastic part is given in terms of the Young moduli $E_s$ and $E_i$ and Poisson’s ratios $\nu_s$ and $\nu_i$ (subscript $s$ for substrate, $i$ for interlayer).

The coating is assumed to be a strong, perfectly elastic material with Young’s modulus $E_c$ and Poisson’s ration $\nu_c$ (subscript $c$ for coating). Finally noting $\mathbf{s} = \mathbf{\sigma} - tr(\mathbf{\sigma})I$ the deviatoric stress and $\sigma^* = \sqrt{\frac{3}{2}} \mathbf{s} : \mathbf{s}$ the Von Mises stress, we have:
\[ \sigma_s = E_s \varepsilon_s \quad \text{and} \quad \sigma_s^e \leq \sigma_{ys} \]
\[ \sigma_i = E_i \varepsilon_i \quad \text{and} \quad \sigma_i^e \leq \sigma_{yi} \]
\[ \sigma_c = E_c \varepsilon_c \]

The above equations, supplemented with the constitutive law for the interface to be discussed presently, form a non-linear problem. It is solved with the software *Abaqus v6.4* and an additional *Fortran* code which allows to implement the cohesive zone through user defined elements.
2.2. The cohesive surface model

At each point of the interface $S$, define an orthonormal basis $\{n, t^{(1)}, t^{(2)}\}$, $n$ denotes the normal to $S$ and $t^{(\alpha)}$, where $\alpha = 1, 2$, denote two tangent vectors on $S$. Let $\xi(x)$ denote the (infinitesimal) displacement field in the solid, which is continuous everywhere except on $S$. Let $\xi^\pm(x) = \lim_{\varepsilon \to 0} \xi(x \pm \varepsilon n)$ denote the limiting values on each side of the interface. Therefore, the normal and tangential discontinuities across the interface are $\Delta_n = (\xi^+ - \xi^-) \cdot n$ and $\Delta_{ta} = (\xi^+ - \xi^-) \cdot t^{(\alpha)}$. Given the stress tensor $\sigma$ in the material, the normal and tangential tractions acting on $S$, denoted $\Delta_n$ and $\Delta_{ta}$, are: $T_n = n \cdot \sigma \cdot n$ and $T_{ta} = t^{(\alpha)} \cdot \sigma \cdot t^{(\alpha)}$. The cohesive interface law relates $(\Delta_n, \Delta_{ta})$ and $(T_n, T_{ta})$. For an ideal elastic interface, the relationship is defined by an elastic potential function $\Phi$ such that:

$$ T_n = \frac{\partial \Phi}{\partial \Delta_n} \quad T_{ta} = \frac{\partial \Phi}{\partial \Delta_{ta}} $$

Various forms of $\Phi$ have been used in numerical simulations. The one we will use is the one developed by Xu and Needleman:

$$ \Phi(\Delta_n, \Delta_{ta}) = \Phi_n + \Phi_n \exp\left(\frac{\Delta_n}{\delta_n}\right) \left[1 - r + \frac{\Delta_n}{\delta_n}\right] \left[1 - q + \frac{r - q}{r - 1} \frac{\Delta_n}{\delta_n}\right] \exp\left(-\frac{\Delta_{ta}^2}{\delta_{ta}^2}\right) $$

where $\Delta_r = \sqrt{\Delta_{11}^2 + \Delta_{22}^2}$. Further, $\Phi_n = \sigma_{\max} \delta_n \exp(1)$ is the energy required to separate the adjoining elements if the displacements are normal to the interface and $\sigma_{\max}$ is the maximum stress under normal displacement jump. If the displacements are tangential to the interface, the energy of separation is determined by $\Phi_t = q \Phi_n$. The other variables in the problem are $\delta_n$ and $\delta_{ta}$ which are respectively the characteristic normal and tangential length scales that enter into the problem. Finally, we have the parameter $r = \frac{\delta_t}{\delta_n}$ where $\Delta_{ta}^*$ is the value of $\Delta_n$ after complete shear separation with the normal force identically zero.
The relation between traction and displacement jumps therefore gives:

\[
T_n = \sigma_{\text{max}} \exp\left(1 - \frac{\Delta_n}{\delta_n}\right) \left[\frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_n^2}{\delta_n^2}\right) + \frac{1-q}{r-1} \left[1 - \exp\left(-\frac{\Delta_n^2}{\delta_n^2}\right)\right] \left[r - \frac{\Delta_n}{\delta_n}\right]\right]
\]

\[
T_t = 2\sigma_{\text{max}} \left(\frac{\delta_t}{\delta_n}\right) \left[\frac{\Delta_t}{\delta_t}\right] q + \left(\frac{r-q}{r-1}\right) \frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right) \exp\left(-\frac{\Delta_n^2}{\delta_n^2}\right)
\]

We eventually have the following graphs:

Figure 2.2.1: Traction-displacement separation law. In (a), \(\Delta_t = 0\), and in (b), \(\Delta_n = 0\).
3. Model

3.1. Presentation of the model

The system being axisymmetric, describing a plane is equivalent to describing the whole system. Figure 3.1.1 represents what is implemented in the finite element software. There are two instances, the indenter which is analytic rigid and the part which is deformable and divided in three regions. To be realistic the different regions must be bonded. Furthermore the bound between the coating and the interlayer is weaker than the one between the interlayer and the substrate so this is the delamination of the first one we are interested in. Thus the second one is modelled as rigid while a cohesive zone is implemented in the first one. This cohesive interface sticks the two regions together, allowing them meanwhile to separate as soon as stress becomes too important.

- Size problems

Taking in account the law of St Venant, the part will be taken with a very large size to prevent the boundary conditions from disturbing the results. Thus the length and the height will be respectively four times and two times the indenter radius.

The remaining size properties are as followed:

Coating thickness: $t_c = 1\mu m$

Indenter radius: $R = 10\mu m$

Part length: $L = 40\mu m$

Part height: $H = 20\mu m$

Interlayer thickness: $0 \leq t_i \leq 3\mu m$

In our Abaqus/CAE model one length unit correspond to $5\mu m$. 
• **Materials**

The diamond like carbon (DLC) coating is very hard and hardly plasticizes, thus it is modelled as an elastic material with a Young modulus $E_c = 1000 GPa$ and Poisson’s ratio $\nu_c = 0.2$.

In this paper, the interlayer we are interested in is made of chromium which here is an elastic perfectly plastic material with $E_i = 250 GPa$, $\nu_i = 0.21$ and a yield stress $\sigma_{yi} = 1 GPa$.

The substrate is tungsten WC, here also elastic perfectly plastic with $E_s = 700 GPa$, $\nu_s = 0.26$, and $\sigma_{ys} = 2.7 GPa$.

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Figure 3.1.1 – Assembled model in Abaqus 6.4

Figure 3.1.2 – Material structures: DLC, chromium, tungsten carbide
• **Boundary conditions**

On the left boarder is applied an axisymmetric condition i.e. it can only move along $e_z$. The bottom and the right boarders are encastred, while the upper one is free and its interaction with the indenter is frictionless. Thus:

$$\Gamma^r (r, 0) = 0 \text{ for } 0 \leq r \leq a \text{ and } \Gamma^r (r, 0) = \Gamma^c (r, 0) = 0 \text{ for } a \leq r \leq L$$

$$\xi_e (0, z) = 0$$

$$\xi_e (r, -H) = \xi_e (r, -H) = 0$$

$$\xi_e (L, z) = \xi_e (L, z) = 0$$

![Frictionless contact](image)

**Figure 2 – Boundary conditions**

• **Load control versus displacement control**

Although we are mainly interested in the critical force for industrial applications, the load will be an imposed displacement of the indenter. It is indeed often observed that load control ends in convergence problems when the force curve is not a monotone function (the most famous example being buckling phenomena). Displacement control is therefore chosen here so we measure directly the critical indentation depth, and the applied force will be returned as an output by the finite element software, in order to finally obtain the critical force.
• **Finite elements**

The mesh is automatically produced by Abaqus/CAE. The choice we have made is four-node bilinear axisymmetric quadrilateral elements (CAX4R).

• **Mesh distribution**

The part is divided in two big regions for the mesh: the upper left corner, where the main deformations occur and the rest of the part. In the first one the mesh is fine and even finer when we get closer to the indenter in order to have a precise stress distribution near the indentation, while in the remainder it is rather coarse for deformation will be almost negligible. Quantitatively there are 960 elements in the first region and 160 in the second one. In addition the cohesive zone is only implemented between the coating and the interlayer of

![Mesh distribution](image)

**Figure 3.1.4 – Mesh distribution**
3.2. Implementation of the cohesive zone

- Parameters choice

In this case, as often, we will consider \( q = r = 0.5 \) which means \( \Phi_n = 2\Phi_t \) and \( \delta_n = 2\Delta_n^* \). The traction-displacement relation becomes:

\[
T_n = \sigma_{\text{max}} \exp\left(1 - \frac{\Delta_n}{\delta_n}\right) \left[ \frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_t}{\delta_t^2}\right) - 1 \right] \left[ 1 - \exp\left(-\frac{\Delta_t}{\delta_t^2}\right) \right] \left[ \frac{1}{2} \frac{\Delta_n}{\delta_n} \right]
\]

\[
T_t = \sigma_{\text{max}} \left(\frac{\delta_n}{\delta_t}\right) \frac{\Delta_t}{\delta_t} \exp\left(1 - \frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_t}{\delta_t^2}\right)
\]

The cohesive surface is represented by four-node elements with two integration points. The behaviour of these elements will condition the delamination.

- Introduction of a viscous term

  - Reasons

The problem with the cohesive zone is that, in many cases with a finite element code such as ABAQUS, it fails to converge due to an instability point when the crack initiates, which can be seen on Figure 3.2.1.

We will then use the solution proposed by Bower and Gao [17] which consists in adding small viscosity-like parameters \( \zeta_n \) and \( \zeta_t \) to the traction-displacement relations. The viscosity is not intended to model any physical energy dissipation process. The interfaces relations become:

\[
T_n = \sigma_{\text{max}} \exp\left(1 - \frac{\Delta_n}{\delta_n}\right) \left[ \frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_t}{\delta_t^2}\right) - 1 \right] \left[ 1 - \exp\left(-\frac{\Delta_t}{\delta_t^2}\right) \right] \left[ \frac{1}{2} \frac{\Delta_n}{\delta_n} \right] + \zeta_n \frac{d}{dt}\left(\frac{\Delta_n}{\delta_n}\right)
\]

\[
T_t = \sigma_{\text{max}} \frac{\delta_n \Delta_t}{\delta_t^2} \exp\left(1 - \frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_t}{\delta_t^2}\right) + \zeta_t \frac{d}{dt}\left(\frac{\Delta_t}{\delta_t}\right)
\]
The viscous term in the traction displacement relation becomes $\xi^r_B$ when computed, where $V$ is the displacement speed of the nodes. For our experiments $\xi^{r_B} = 10^{-4}, 10^{-4} \leq \xi^{r_B} \leq 5 \cdot 10^{-4}$ and the maximum relative displacement is around 0.2 per step, which lasts $1 \frac{h}{t_c}$ second, giving a maximum relative speed of 0.2. Therefore the maximum value of this term is around 0.2, which is very small compared to relative stresses going up to $\frac{\sigma_s}{\sigma_m} = 250$. Thus this term will not have any influence on our results. In fact, the viscous term $\xi$ can be made as small as desired, keeping its effect on convergence. Consequently, it will never affect our results.
3.3. Dimensional analysis

Further to this presentation all data and unknowns of the problems are identified, and due to the theorem Π it is now possible to express the critical indentation load and depth as functions of the following parameters:

\[
\frac{F_c}{\sigma_{ys} t_c^2} = \Pi_f \left( \frac{t_i}{t_c}, \frac{R}{t_c}, \frac{E_i}{\sigma_{ys}}, \nu_i, \frac{E_i}{\sigma_{ys}}, \nu_i, \frac{\sigma_yi}{\sigma_{ys}}, \nu_i, \frac{E}{\sigma_{ys}}, \nu_i, \frac{\sigma_{max}}{\sigma_{ys}}, \frac{\Phi_a}{\sigma_{ys} t_c}, \frac{\delta_i}{\delta_i}, q, r \right)
\]

\[
\frac{h}{t_c} = \Pi_h \left( \frac{t_i}{t_c}, \frac{R}{t_c}, \frac{E_i}{\sigma_{ys}}, \nu_i, \frac{E_i}{\sigma_{ys}}, \nu_i, \frac{\sigma_yi}{\sigma_{ys}}, \nu_i, \frac{E}{\sigma_{ys}}, \nu_i, \frac{\sigma_{max}}{\sigma_{ys}}, \frac{\Phi_a}{\sigma_{ys} t_c}, \frac{\delta_i}{\delta_i}, q, r \right)
\]

However the most interesting parameter is the relative interlayer thickness \(\frac{t_i}{t_c}\), and section four discusses its influence on the relative critical force, according to the values of the following dimensionless parameters i.e.:

- **geometry:** indenter radius \(\frac{R}{t_c}\)
- **materials:**
  - interlayer elasticity: \(\frac{E_i}{\sigma_{ys}}, \nu_i\)
  - interlayer plasticity: \(\frac{\sigma_yi}{\sigma_{ys}}\)
- **interface:**
  - cohesive zone strength: \(\frac{\sigma_{max}}{\sigma_{ys}}\)
  - cohesive zone toughness: \(\frac{\Phi_a}{\sigma_{ys} t_c}\)

The other ones being fixed: \(\frac{E}{\sigma_{ys}} = 370, \nu_c = 0.2, \frac{E_i}{\sigma_{ys}} = 260, \nu_i = 0.26, \frac{\delta_i}{\delta_i} = 1, q = r = 0.5\).
4. Results and discussion

4.1. Further information

Generally speaking, delamination is observed after one cycle of load-unloading which can be broken down in three steps. First the indenter is at a tangent to the part. Then we impose an axial indenter displacement \( h \) with a constant speed, and finally the indenter goes back to its initial position, with the same speed. Delamination is measured through the comparison between the displacement jump \( \Delta_n \) and the cohesive zone dimension \( \delta_n \): one can consider that delamination has occurred as soon as \( \Delta_n \geq \delta_n \).

This section tries to present enough results to fill in the parameter space, and to clearly show the influence of the interlayer thickness and its origins. In order to avoid mesh effects in our results, and to ensure the comparison between them is legitimate, all simulations have the same mesh distribution, the one presented in section three.

In addition the reference set of data is given in Table 1:

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Materials</th>
<th>Interface</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{R}{t_c} = 10 )</td>
<td>( \frac{E_t}{\sigma_{ys}} = 92 ); ( \nu = 0.21 ); ( \frac{\sigma_{yi}}{\sigma_{ys}} = 0.39 )</td>
<td>( \frac{\sigma_{\text{max}}}{\sigma_{ys}} = 1 ); ( \frac{\Phi_n}{\sigma_{ys} t_c} = 3.73 \times 10^{-3} ) (( \Rightarrow \Phi_n = 10, J, m^{-2} ))</td>
</tr>
</tbody>
</table>

Table 1 – Reference data set for simulations

So that the final state of the system can be clearly seen, Figure 4.1.1 is an obvious delamination example, computed with the previous data set and a corresponding indentation depth \( \frac{h}{t_c} = 1.5 \). Figure 4.1.2 is the corresponding evolution of the normalised axial force imposed to the indenter according to its normalised displacement.
Figure 4.1.1 – Stress fields observed after delamination:
(a) Von Mises and (b) $\sigma_{zz}$ component

Figure 4.1.2 – Force-displacement graph
4.2. Results

Our results not only display the critical force, which is the most interesting parameter for industrial applications, but also the critical indentation depth, which is more intuitive. In addition we systematically have computed the asymptote for infinite thickness, which corresponds to the case of a chrome substrate. Indeed the position of the asymptote of the critical force curve compared to the value for no interlayer, i.e. $t_{c} = 0$, indicates the more efficient material for coating adhesion.

- Reference result

Our reference result is Figure 4.2.3 which has been computed with the data set given in Table 1 and $0 \leq \frac{t}{t_{c}} \leq 3$. 

![Graph](image-url)
The first part of the curve and the asymptote position confirm the intuition: the insertion of a chrome interlayer increases the critical force and depth. However $h_c$ and $F_c$ then exceed the asymptote values, to form peaks at about $\frac{t_i}{t_c} = 1.9$, which is a surprise. In addition it is interesting to note that a very small interlayer does not seem to affect the system strength. It is in fact contrary to common experimental results, which leads to assume that its influence is actually due to chemistry effects, and not mechanical. For bigger interlayers the presence of a peak suggests that several phenomena are at stake. The further results aim to isolate the influences of the different parameters and thus to discover the general behaviour of the system.

- **Influence of the Young modulus**

To understand the influence of elasticity the following graphs have been made with the same data except for the interlayer which is now a fictitious material with $E_i = E_s$.
The general curve shapes are the same but the amplitudes are far smaller when the Young modulus is higher i.e. when the material of the interlayer is less elastic. Furthermore the peak is translated towards smaller thicknesses. Thus elasticity amplifies the phenomenon although it does not create it.

Figure 4.2.2 – Critical force (a) and depth (b) vs. interlayer thickness with $E_i = E_s$
- Influence of yield stress

Here the only change compared with the data set of Table 1 is that we have a fictitious interlayer material with $\sigma_{yi} = \sigma_{ys}$.

![Graph](image)

Figure 4.2.3 - Critical force (a) and depth (b) vs. interlayer thickness with $\sigma_{yi} = \sigma_{ys}$

Obviously yield stress is behind the observed phenomenon: a high yield stress smoothes the curve, and implies a monotonous transition between a system with tungsten only and one with chromium only. This lets suppose that plasticity is at stake in the general behaviour, and creates the phenomenon.
• Influence of the indentation sphere radius

Here is the result of a simulation with \( \frac{R}{t_c} = 2.5 \)

![Graph (a)](image)

![Graph (b)](image)

Figure 4.2.4 - Critical force (a) and depth (b) vs. interlayer thickness with \( \frac{R}{t_c} = 2.5 \)

The sphere being smaller, so is the area of contact between the part and the indenter. Thus the critical depth increases, while the associated critical force increases, by comparison with the reference simulation. This simulation confirms that the indenter dimensions do not affect our results.
Influence of the cohesive zone properties

Here are respectively the results for
\[
\frac{\sigma_{\text{max}}}{\sigma_{y_s}} = 0.5, \frac{\Phi_n}{\sigma_{y_s}t_c} = 1.86 \cdot 10^{-3} \] \Leftrightarrow \Phi_n = 5Jm^{-2} \text{ and}
\[
\begin{align*}
\frac{\sigma_{\text{max}}}{\sigma_{y_s}} &= 0.5, \\
\frac{\Phi_n}{\sigma_{y_s}t_c} &= 3.73 \cdot 10^{-2} 
\end{align*}
\Leftrightarrow \Phi_n = 100Jm^{-2}.
\]

(a)

(b)

Figure 4.2.5 - Critical force and depth vs. interlayer thickness with
\[
\frac{\sigma_{\text{max}}}{\sigma_{y_s}} = 0.5, \frac{\Phi_n}{\sigma_{y_s}t_c} = 1.86 \cdot 10^{-3} \]
Here one can see that the tougher the cohesive zone is, the higher the critical force and depth are, which could have been predicted. However the peak also translates to the thicker interlayers. Finally it seems that the cohesive zone toughness effects are the same as elasticity ones.

Figure 4.2.6 - Critical force and depth vs. interlayer thickness with $\left( \frac{\sigma_{\text{max}}}{\sigma_{\text{yy}}} = 0.5, \frac{\Phi}{\sigma_{\text{yy}}t_c} = 3.73 \cdot 10^{-2} \right)$
• Global results

Finally in order to clearly see the different influences Figure 4.2.14 represents all previous results together.

Figure 4.2.7 – Global results: critical indentation force (a) and depth (b) vs. interlayer thickness
4.3. Discussion

- General behaviour

The previous results have demonstrated that the general behaviour of the system is far from being trivial, for it depends on all the parameters at stake. However a close look to the stress field evolution during the indentation allowed us to propose the following analysis, when there are only two layers: the substrate and the coating.

When the indentation begins, the substrate goes through elastic deformation and then rapidly plasticizes as the stress field increases to \( \sigma_{ys} \). The coating, purely elastic and very strong, bends but does not deform much. At the end of the load the strain is at its maximum in the substrate. During the unloading there are two phases: first the stress field decreases everywhere until it reaches zero in the substrate, and its deformation is then equal to the plastic strain. Because of the bound between them the coating is still bended so that its stress field is still high. Then the second phase begins: the coating tends to go back to its initial position, and pulls the substrate. The stress field increases along the interface and the substrate plasticizes once again, this time reducing its strain compared to its initial shape. Finally when the interface stress field is too high delamination occurs: it allows to reduce stress in the coating and in the substrate at the same time. Finally the crack dimension is directly linked to the final remaining strain \( \varepsilon_f \). This cycle is illustrated in a stress-strain graph in Figure 4.3.1.

![Figure 4.3.1 – Load cycle of the substrate](image-url)
Within this framework, we can now assume intuitively that the insertion of an interlayer which is more elastic and has a smaller yield stress than the substrate - which is the case of chromium - would reduce the plastic strain due to the load. It would then decrease the stress field along the interface after the unloading, when the coating pulls back. Consequently the critical indentation depth would be higher, proportionally to the thickness of this interlayer. However this type of material is more easily compressed, so the evolution of the critical force is far harder to predict, for it then depends of two antithetical phenomena. The previous results are consistent with this whole analysis and in addition, they confirm the above remark. Indeed although the plastic strain reduction usually dominates, implying in our graphs that the asymptote is above the value for no interlayer (i.e. \( \frac{1}{\gamma} = 0 \)), one can see the contrary in Figure 4.2.5(b) where compressibility is slightly stronger.

- **The appearance of a peak**

The insertion of the interlayer makes the system unquestionably more complex, for an unpredictable peak appears in our previous simulations. An explanation can be found thanks to three points: the comparison of the strain-stress graphs for chromium and tungsten (Figure 4.3.2), a very useful energetic point of view and the observation of the stress fields. First it is important to note that the elastic strain is almost the same but that the elastic energy that tungsten can absorb is far higher.

![Figure 4.3.2 – Stress-strain curves for tungsten and chromium](image)
Now take an energetic point of view: delamination occurs when the work $W_0$ needed to lead the material to no strain is higher than the coating/substrate bound energy $\varphi_0$. Note $W_0^C$ the corresponding work with chromium only and $W_0^T$ the one with tungsten only. In Figure 4.3.3 we find that $W_0^C \leq W_0^T$, which conforms to intuition and results.

![Figure 4.3.3 – Load cycle if there is no delamination](image)

In addition analyse what happens when there’s a chrome interlayer on a tungsten substrate. The work provided by the indenter is absorbed by the part. A rough approximation would be that stress is dispatched in a spherical way. One can then deduce that there are spherical plastic limits for each material: before it is elastic and beyond it plasticizes (Figure 4.3.4 (a)). Now for the same indentation depth, the more chromium there is in the part, the smaller $W_0$ is. Thus as $t_i$ increases, the chromium/tungsten boarder heads for the bottom of the part while the plasticizing limits heads for the top (Figure 4.3.4 (a) and (b)). When the chrome interlayer is thick enough to reach the tungsten plasticizing limit, the latter does not plasticize and only absorb energy elastically, which does not participate in delamination during unloading. On Figure 4.3.4 we see that the peak must be between (b) and (c) which is consistent with the reference curves shown above. Finally when the chromium/tungsten boarder is under the
tungsten plasticizing limit, the chromium plasticizes in places where tungsten did not with a smaller $t_i$. Consequently $W_0$ increases again (Figure 4.3.4 (c)) until it reaches its maximum when there is chromium only (Figure 4.3.4 (d)). This therefore explains the peak seen in our results, the shape of the critical force and depth being the same as $W_0$.

Figure 4.3.4 – Von Mises stress fields just after load for $\frac{h}{t_c} = 0.24$ and

(a) $\frac{t_i}{t_c} = 1.5$; (b) $\frac{t_i}{t_c} = 1.875$; (c) $\frac{t_i}{t_c} = 2.625$; (d) $\frac{t_i}{t_c} = \infty$
• **Influence of the Young modulus**

As we could expect now the shape of the curve is the same when the interlayer elasticity decreases but so does the efficiency. Indeed for the same indentation depth the fictitious material has a bigger plastic strain and \( W_0 \) is much higher while \( \phi_0 \) is the same, as seen in Figure 4.3.5. In addition the peak appears for smaller interlayer thicknesses since the fictitious material plasticizes earlier.

![Figure 4.3.5 – Influence of the Young modulus](image)

• **Influence of yield stress**

It appears that the interlayer has almost no effect when the yield stress is too large. This is easily explained with the same energetic point of view. This time the plasticizing limits for the interlayer material and tungsten are the same, but the fictitious material, although it is still more efficient than tungsten, is far less efficient than chromium, as seen on Figure 4.2.10. Therefore in comparison with the first simulation, corresponding to Table 1, the asymptote is lower, and the curve is monotone.
In the simulation corresponding to Table 1 $\Phi_n = 10 \, J \, m^{-2}$ while in Figure 4.2.5 $\Phi_n = 5 \, J \, m^{-2}$ and in Figure 4.2.6 $\Phi_n = 100 \, J \, m^{-2}$. So basically in the second graph the bound is weaker and in the third it is much higher. So the results are as expected: the critical force and depth are proportional to $\Phi_n$, i.e. the stronger the bound is, the greater the work must be in order to break it.

An interesting fact appears though: the critical force peak translates towards the smaller thicknesses when the cohesive zone is weaker, which is consistent with the explanation given above. A weaker bound implies a smaller $W_0$ critical and thus the plasticizing zones in the interlayer and the substrate are reduced. Consequently the optimal interlayer thickness is smaller.

This could lead to industrial applications for even a very thin interlayer could have a positive effect on the strength of the coating. Therefore the interlayer would mainly reinforce the cohesive zone where defects are located.
5. Conclusion

Numerical simulations have been carried out of the indentation process of a coated material with an interlayer by a spherical indenter. The interface between the film and the interlayer was modelled by a cohesive zone, with a Xu-Needleman constitutive law. A parametric study has been carried out to investigate the influence of interfacial strength, interlayer yield strength and elasticity on delamination. Delamination mechanism is found to be mainly by the plastic deformation in both interlayer and substrate.

Observation of stress fields allowed us to propose a general behaviour of the system during indentation, and the study of the evolution of critical force and depth with the interlayer thickness showed the existence of optimal properties in order to enhance coating adhesion. We also found chromium between diamond like carbon and tungsten carbide seems particularly efficient if its thickness is about twice the coating one. Moreover small Young modulus and yield stress tend to increase this efficiency. Finally the optimal efficiency tends to appear for smaller interlayer thicknesses if the cohesive zone is weaker.

It bears emphasis at this point to recall that the coating is assumed to be elastic and strong. Deviations from this, such as plasticity of the coating or cracking, may affect our findings. In addition, it is obvious that all results must be taken in account qualitatively. Indeed for simplicity, the present simulations have assumed perfect plasticity for the substrate and the interlayer. Strain hardening of the substrate will, obviously, change the quantitative results.

Actually our main goal was to find if an interlayer had an effect on coating delamination. A more in depth study, backed by experiments, would probably lead to the properties of optimal interlayer material, which could be used for industrial applications.

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References


