Predicting deformation-induced polymer-steel interface roughening and failure

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Predicting deformation-induced polymer-steel interface roughening and failure

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Abstract

A novel integrated framework is presented for the prediction of deformation-induced interface roughening and failure in polymer-coated steels. Crystal plasticity is employed to predict the change in steel surface roughness in-situ. The steel substrate is coated with a thin polymer layer and the polymer-steel interface is modeled using an exponential cohesive zone law. Uniaxial tensile simulations are performed and the results show that the predicted roughness increases with the applied deformation. The local changes in the steel surface profile result in initiation and growth of local interface failure. Furthermore, a compression simulation shows that the roughening rate of the steel is increased compared to tension, with an increase in the predicted interface damage as a result. The presented framework thus allows for a detailed numerical study of the initiation and growth of interface damage in polymer-coated steels during applied deformation. The incorporation of the crystal plasticity model to predict the changes in the steel surface profile complements the cumbersome measurements of detailed experimental displacement fields that accompany deformation-induced roughening and thus enables the analysis of deformation processes where measuring the steel surface profile is difficult if not impossible, e.g. industrial forming processes such as deep-drawing.

Keywords: polymer-coated steel; interface roughening; crystal plasticity; interface damage

1 Introduction

Deformation-induced surface roughening of steels and other crystalline materials is common in many engineering applications. This change in surface roughness can lead to several problems during manufacturing [2, 4, 16, 28], for example: (1) a detrimental effect on the surface finish of sheet metal; (2) a change in friction, wear and corrosion resistance; (3) localization phenomena which may lead to failure; or (4) local delamination of a coating.

In case of polymer-coated steels, the change in surface roughness may also result in local delamination of the coating. This is particularly the case for industrial manufacturing of food and beverage cans or canisters, see Fig. 1. To reduce the environmental impact of the production process, the Electrolytically Chromium Coated Steel (ECCS) sheet material is pre-coated with a Polyethylene Terephthalate (PET) layer prior to can production. Compared to the traditional manufacturing process of producing a blank steel can which is coated after production, using a pre-coated steel reduces the energy consumption and CO\textsubscript{2} emission with one third and the process water and resulting solid wastes to practically zero [1].

However, it is observed in practice that the polymer-steel interface is damaged due to the large deformations at high strain rates, temperatures and pressures during production. It has been shown experimentally that this is due to the evolving steel surface roughness. The food and beverage industry demands that the material does not exhibit any visible or invisible damage after production and during the prolonged shelf-life, as this compromises the quality of the canned content [6, 16].

The effect of deformation-induced roughening of the steel substrate was investigated in a numerical-experimental framework in [3, 4]. Experimental height profiles of a steel deformed in tension were used in a Finite Element based Digital Image Correlation (FE-DIC) calculation to extract the full-field displacement fields from height measurements [3]. These displacement fields were applied as boundary conditions in
Figure 1: Polymer-coated steel used in the manufacturing of food and beverage cans (after [10]).

a numerical analysis of a polymer coating and an interface model. It was thereby observed that the initiation and growth of interface damage is a result of the change in steel surface roughness [4].

However, applying the developed framework to other deformations than uniaxial tensile tests is infeasible. In-situ measurement of the evolving micro-scale surface height profiles in industrial forming operations like deep-(re-)drawing and wall ironing is not possible. To predict the change in surface roughness and the effect on the interface integrity of coated products during manufacturing, a predictive model for the evolution of the steel surface profile is desired.

Crystal plasticity can be used to predict the anisotropic crystallographic response of a metal [12]. Several authors have studied the applicability of these models for predicting deformation-induced surface roughening. Becker [2] and Wu & Lloyd [32] studied two-dimensional roughening and reported differences in the predicted roughness amplitude compared to experimental observations. Both authors concluded that the adopted two-dimensional assumption may well result in the observed difference. More recently, Zhao et al. [34] and Lim et al. [23] studied oligocrystals using three-dimensional crystal plasticity and compared the predictions with experiments. They found a relatively good comparison with the experiments for the displacement fields and resulting height profiles. However, small differences prevailed because discrete roughening phenomena, e.g. slip extrusions, can not be captured by the continuum model.

Strain gradient crystal plasticity modeling was also explored as a means of predicting the change in surface roughness. Borg & Fleck [7] and Nygård & Gudmundson [24] studied the effect of the internal length scale in the strain gradient model and found a strong dependency of the resulting profile on this length scale. However, so far no experimental comparison was made to determine the internal length scale.

These above mentioned studies focused on predicting deformation-induced surface roughening during uniaxial tension. Bending was recently studied by Rossiter et al. [28] for aluminium sheets using a crystal plasticity model. The simulations showed the formation of hills and valleys on the surface and the predicted roughness was found to depend on the subsurface grains. Finally, Šiška et al. [29] performed cyclic simulations on copper thin films. The roughness was found to increase with cycling and cycling between tension and compression resulted in a larger roughness than cycling in pure tension or pure compression. The predicted roughness was smaller than seen in experiments due to the limited number of simulated cycles.

Deformation-induced roughening and its influence on the interface integrity of a coating has not yet been investigated numerically using a predictive model for the steel roughening. In this work, a numerical framework is developed that enables study of deformation-induced interface roughening in polymer-coated steels. A crystal plasticity model [12] is employed to qualitatively predict the change in surface roughness of a polymer-coated packaging steel. The polymer coating is modeled using the Eindhoven Glassy Polymer model [11] to accurately predict the mechanical response of the coating. The interface between the polymer and steel is modeled using an exponential cohesive zone law [8], enabling analysis of the interface integrity during the deformation process. Uniaxial tension and compression simulations are performed and the results are qualitatively compared to a representative experiment of a packaging steel deformed in tension, where the surface roughness evolution was measured with high resolution [3]. The presented framework may be incorporated into a global-local approach to allow the analysis of a particular industrial forming processes such as deep-drawing, e.g. by embedding the modeled domain into a bulk simulation or a multi-scale approach. The objective of this paper is to investigate the feasibility of this approach. Some of the assumptions made impose limitations on the presented results, which require careful consideration for a quantitative analysis. In particular: 1) The continuum assumption in the crystal plasticity framework limits the predicted roughening to grain-scale features only, i.e. micro-scale discrete roughening phenomena are not incorporated into the current framework. 2) The adopted steel crystallography is numerically generated based on available experimental data using a representative method. However, this does not capture exactly the complete experimental texture.
Due to computational limitations, the finite element discretization is relatively coarse, limiting the amount of bending that can be described by the discretization. Nevertheless, it will be shown that the predicted roughness patterns do not change significantly upon mesh refinement.

The paper is organized as follows. The problem, constitutive models and computational procedures for the simulations are presented in section 2. The simulation results are discussed in section 3. The paper ends with a discussion and conclusion.

The following notations are adopted throughout the paper, where Cartesian tensors are used. A vector is denoted by \( \vec{a} = a_i \vec{e}_i \), a second-order and fourth-order tensor are denoted by \( A = A_{ij} \vec{e}_i \vec{e}_j \) and \( \mathbf{A} = A_{ijkl} \vec{e}_i \vec{e}_j \vec{e}_k \vec{e}_l \), respectively. The inner product is defined as \( \vec{a} \cdot \vec{b} = a_i b_i \), \( i = 1, 2, 3 \), the tensorial inner products as \( A : B = A_{ij} B_{jk} \vec{e}_i \vec{e}_k \) and \( \mathbf{A} : \mathbf{B} = A_{ij} B_{ji} \). The dyadic product is denoted as \( \vec{a} \otimes \vec{b} = a_i b_j \vec{e}_i \vec{e}_j \) and the outer product as \( \vec{a} \times \vec{b} = \vec{c} \). The transpose of a tensor is denoted by \( A^T \), the inverse of a tensor by \( A^{-1} \) and a material time derivative by \( \dot{\vec{a}} \) and \( \dot{\mathbf{A}} \). Finally, the absolute value is indicated by \( |a| \), the normalized value by \( \hat{a} \) and the spatial average value by \( \langle a \rangle \).

2 Constitutive and computational model

2.1 Problem statement

The studied material is a packaging steel used in the production of food and beverage cans known as TH340. The material consists of an Electrolytically Chromium Coated steel (ECCS) substrate, coated with a 15 \( \mu \text{m} \) thick PET coating, see also Fig. 1. A small block with in-plane dimensions 100 \( \times \) 100 \( \mu \text{m} \) of the packaging material is modeled, whereby the steel surface is initially flat (schematically shown in Fig. 2(a)). The steel thickness is 20 \( \mu \text{m} \). This block is assumed to be in-plane periodic (i.e. parallel to the interface). In addition to the in-plane periodic boundary conditions, rigid body rotations and global shear perpendicular to the interface are prevented, see Fig. 3(a). Furthermore, the presence of the bulk steel below the modeled block is incorporated by using appropriate boundary conditions that take into account the restrictions imposed by the bulk on the steel substrate. While different choices for these boundary conditions are possible, here parts of the bottom steel face (areas of 20 \( \times \) 20 \( \mu \text{m} \), i.e. an average of 2 \( \times \) 2 grains) are constrained with an average \( z \)-displacement of zero. The effect of this boundary condition was studied by varying the constrained domain size (from zero to the size of the modeled geometry) and it was found that the boundary condition does not significantly change the predicted results.

An average uniaxial tension and compression strain is applied at a linear strain rate of \( \dot{\varepsilon} = 3.75 \cdot 10^{-2} \text{ s}^{-1} \). The steel is modeled using the crystal plasticity model detailed in the next section. The polymer-steel interface is described using an exponential cohesive zone law, discussed further in section 2.3. The PET coating is modeled using the Eindhoven Glassy Polymer model described in section 2.4.

An EBSD measurement was performed on the packaging steel to analyze the average grain size and distribution of Euler angles, see Fig. 2(b). The measurement revealed that the steel grains have a BCC ferrite crystal structure and are approximately equi-axed with an average grain diameter of about 10 \( \mu \text{m} \).

**Figure 2:** (a) Sketch of the modeled part of the polymer-coated steel; (b) results of an EBSD measurement on TH340 packaging steel; the colors indicate the crystal orientations.
2.2 Steel crystal plasticity framework

A conventional crystal plasticity model [12] is adopted for the BCC ferritic steel. Within this continuum approach, the effect of dislocation glide on slip systems is modeled in an average sense. Effects due to e.g. dislocation pile-ups are disregarded.

The deformation gradient \( F \) is multiplicatively split into an elastic \( F_e \) and plastic \( F_p \) contribution, i.e.

\[
F = F_e \cdot F_p. \tag{1}
\]

The multiplicative split introduces an intermediate configuration, which is distorted by the plastic deformation only. The elastic deformation, as well as rotations, are included in \( F_e \). The plastic part of the velocity gradient \( L \) is \( L_p = F_p \cdot F_p^{-1} \). In the crystal plasticity setting, the crystallographic decomposition of \( L_p \) is

\[
L_p = \sum_{\alpha=1}^{n_s} \tilde{\gamma}^\alpha P_0^\alpha, \tag{2}
\]

where \( P_0^\alpha = \tilde{s}_0^\alpha \otimes \tilde{n}_0^\alpha \) is the Schmid tensor of the slip system \( \alpha \), \( \tilde{s}_0^\alpha \) is the slip direction and \( \tilde{n}_0^\alpha \) the slip normal, both defined in the reference configuration, \( \tilde{\gamma}^\alpha \) is the plastic slip rate on slip system \( \alpha \) and \( n_s = 12 \) is the number of slip systems in the BCC crystal.

The elastic constitutive law is

\[
S = 4^4 C : \varepsilon_e, \tag{3}
\]

where \( 4^4 C \) is the fourth-order elasticity tensor, \( \varepsilon_e = \frac{1}{2} (F_e^T \cdot F_e - I) \) is the elastic Green-Lagrange strain and the stress \( S \) (similar to the Kirchoff stress) is

\[
S = F_e^{-1} \cdot \tau \cdot F_e^{-T}. \tag{4}
\]

The plastic slip rate \( \dot{\gamma}^\alpha \) is determined via a visco-plastic slip law [20],

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{\nu^\alpha} \right)^{\frac{1}{m}} \text{sign(} \tau^\alpha \text{)}, \tag{5}
\]

where \( \dot{\gamma}_0 \) is the reference slip rate, \( m \) is the strain rate sensitivity parameter, \( \tau^\alpha \) is the shear stress resolved on the slip system \( \alpha \), and \( \nu^\alpha \) is the current slip resistance. Schmid’s law is violated in BCC crystals and
thus non-Schmid effects are incorporated by redefining the resolved shear stress as
\[
\tau^\alpha = \left( F^T \cdot F_e \cdot S \right)^T : \left( P_0^\alpha + \eta^\alpha \right),
\]
(6)
where \( \eta^\alpha \) is defined by \[33\]
\[
\eta^\alpha = \eta_{ss} \vec{s}_0 \otimes \vec{s}_0 + \eta_{nn} \vec{n}_0 \otimes \vec{n}_0 + \eta_{zz} \vec{z}_0 \otimes \vec{z}_0.
\]
(7)
Here, \( \eta_{ss} \), \( \eta_{nn} \) and \( \eta_{zz} \) are three non-Schmid parameters and \( \vec{z}_0 = \vec{s}_0 \times \vec{n}_0 \). The evolution law of the current slip resistance \( \nu^\alpha \) is
\[
\dot{\nu}^\alpha = \sum_{\beta=1}^{n_s} h^\alpha_\beta |\dot{\gamma}|, \quad \text{(8)}
\]
where \( h^\alpha_\beta \) is a hardening matrix taken in the form
\[
h^\alpha_\beta = h^0 \left( 1 - \frac{\nu^\alpha}{\nu_\infty} \right)^a q^{\alpha\beta},
\]
(9)
with \( q^{\alpha\beta} \) a matrix with ones on the diagonal and everywhere else (\( q \) is the ratio of the latent hardening with respect to the self-hardening for non-coplanar slip systems), \( h^0 \), \( \nu_\infty \) and \( a \) are material parameters.

For BCC steel, only the \{110\}_x slip system family is assumed to be active at room temperature (e.g. [19, 13]).

The material parameters have been taken from literature [18, 30, 33] and are summarized in Table 1.

<table>
<thead>
<tr>
<th>( \nu_0 ) [MPa]</th>
<th>( \nu_\infty ) [MPa]</th>
<th>( h^0 ) [MPa]</th>
<th>( \dot{\gamma}_0 ) [s(^{-1})]</th>
<th>( m ) [-]</th>
<th>( a ) [-]</th>
<th>( q ) [-]</th>
</tr>
</thead>
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<tr>
<td>65</td>
<td>150</td>
<td>1000</td>
<td>0.01</td>
<td>0.20</td>
<td>1.50</td>
<td>1.40</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \eta_{ss} ) [-]</th>
<th>( \eta_{nn} ) [-]</th>
<th>( \eta_{zz} ) [-]</th>
<th>( C_{11} ) [GPa]</th>
<th>( C_{12} ) [GPa]</th>
<th>( C_{44} ) [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0544</td>
<td>-0.0293</td>
<td>-0.0267</td>
<td>233</td>
<td>135.5</td>
<td>118</td>
</tr>
</tbody>
</table>

### 2.3 Interface cohesive zone model

The PET-steel interface is modeled using a three-dimensional cohesive zone model. The mixed-mode exponential traction-separation law of Van den Bosch et al. [8] is used to model the PET-steel decohesion. In 3D, the cohesive zone opening vector \( \Delta \) is split into a contribution normal and tangential to the interface, i.e. \( \Delta = \Delta_n \vec{e}_n + \Delta_t \vec{e}_t \). Here, \( \vec{e}_n \) is normal to the interface and \( \vec{e}_t \) is an in-plane unit vector by projecting \( \Delta \) on the interface. The traction-separation law in the two directions is defined as
\[
T_n (\Delta_n, \Delta_t) = \phi_n \frac{\Delta_n}{\delta_n^2} \exp \left( -\frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right),
\]
(10)
\[
T_t (\Delta_n, \Delta_t) = 2 \phi_t \frac{\Delta_t}{\delta_t^2} \left( 1 + \frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_n}{\delta_n} \right) \exp \left( -\frac{\Delta_t^2}{\delta_t^2} \right),
\]
(11)
where \( \Delta \) is the cohesive zone opening, \( \phi \) is the work of separation and \( \delta \) is the characteristic opening length. The typical traction-separation response is shown in Fig. 4. This is a coupled law, as the maximum reached traction in one direction decreases with prior opening in the other direction. Note that in case of negative normal opening the coupling does not occur to simulate realistic interface closure.

The interface integrity is characterized by the parameter \( \xi \) which quantifies the fraction of the work of separation that is not yet dissipated in the cohesive zone element,
\[
\xi = 1 - \frac{\Omega}{\phi}, \quad \xi \in [0, 1],
\]
(12)
where $\Omega$ is the consumed work of separation in the cohesive zone [4].

The cohesive zone parameters (i.e. $\delta_i$ and $\phi_i$, $i = n, t$) have to be determined from dedicated experiments. However, the parameters may depend on the experiment used to determine them [31]. An example of two experiments of the same material which resulted in different values for the work of separation $\phi$ is the work of Fedorov et al. [17] and Van den Bosch et al. [10]. The differences arise from the dissipated energy in the process zone (i.e. the bulk material close to the interface). The simulations presented in this work require parameters that are characteristic for small-scale debonding [16], i.e. close to physical adhesion. Therefore, the material parameters used here are based on [17], see Table 2.

Table 2: Cohesive zone constants. Note that $\phi_n = \phi_t = \phi$ and $\delta_n = \delta_t = \delta$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_n$</td>
<td>2.5</td>
<td>J m$^{-2}$</td>
</tr>
<tr>
<td>$\phi_t$</td>
<td>2.5</td>
<td>J m$^{-2}$</td>
</tr>
<tr>
<td>$\delta_n$</td>
<td>0.25</td>
<td>$\mu$m</td>
</tr>
<tr>
<td>$\delta_t$</td>
<td>0.25</td>
<td>$\mu$m</td>
</tr>
</tbody>
</table>

### 2.4 Polymer constitutive model

The polymer coating investigated here is a 15 [$\mu$m] thick PET layer with several additives to improve adhesion [10]. PET is a glassy polymer and almost fully amorphous (crystallinity is approx. 8%). The typical intrinsic response of glassy polymers is shown in Fig. 5(a) for a uniaxial compression test. Initially, the response is nearly linear elastic (1), followed by non-linear visco-elasticity (2) up to yielding (3). Softening occurs directly after yielding depending on the age of the polymer (4). Finally, softening is overtaken by strain hardening at large strains (5). The yield point depends on the applied strain rate [11].

The model employed here to predict this complex mechanical behavior is the so-called “Eindhoven Glassy Polymer” (EGP) model. This model was shown to accurately capture the behavior of glassy polymers [11, 22]. While the EGP model is a multi-mode, multi-process constitutive model, here only one mode and one process are considered as only a limited set of PET parameters is known. The mechanical analogue of the single-mode, single-process EGP model is shown in Fig. 5(b) and detailed below.

The total stress is separated into two contributions, i.e. a driving stress $\sigma_s$ and a hardening stress $\sigma_r$ (see also Fig. 5(b)),

$$\sigma = \sigma_s + \sigma_r.$$  \hspace{1cm} (13)

Hardening originates from the oriented entangled network and is modeled by a neo-Hookean relation,

$$\sigma_r = G_r \bar{B}^d,$$  \hspace{1cm} (14)

where $G_r$ is the strain hardening modulus and $\bar{B}^d$ the deviatoric part of the isochoric left Cauchy-Green

Figure 4: The coupled exponential traction-separation law of Van den Bosch et al. [8], using the parameters of Table 2.
deformation (Finger) tensor. The intermolecular interactions are modeled via the driving stress,

\[ \sigma_s = \sigma_s^h + \sigma_s^d = \kappa(J - 1)I + G\tilde{B}_e^d. \]  \(15\)

Here, \(\sigma_s^h\) and \(\sigma_s^d\) are the hydrostatic and deviatoric stresses, respectively, \(\kappa\) is the bulk modulus, \(J\) is the volume change ratio, \(I\) is the second-order unity tensor, \(G\) is the shear modulus and \(\tilde{B}_e^d\) is the deviatoric part of the elastic isochoric Finger tensor. The kinematic evolution of \(J\) and \(\tilde{B}_e\) is given by

\[ \dot{J} = J\text{tr}(D), \]  \(16\)

\[ \dot{\tilde{B}}_e = (\tilde{L} - D_p) \cdot \tilde{B}_e + \tilde{B}_e \cdot (\tilde{L}^T - D_p). \]  \(17\)

Here \(\tilde{L}\) is the isochoric velocity gradient tensor and \(D\) the deformation rate tensor and \(D_p\) is the plastic deformation rate tensor, which is coupled to \(\sigma_s^d\) via a non-Newtonian flow rule,

\[ D_p = \frac{\sigma_s^d}{2\eta}, \]  \(18\)

with viscosity \(\eta\)

\[ \eta = \eta_{0,ref} \frac{\tau_{eq}/\tau_0}{\sinh(\tau_{eq}/\tau_0)} \exp\left(\frac{\mu p}{\tau_0}\right) \exp(S), \]  \(19\)

where \(\eta_{0,ref}\) is the reference zero-viscosity, \(\tau_0\) is the characteristic equivalent stress and \(\mu\) captures the pressure dependency. The total equivalent stress, \(\tau_{eq}\) and the pressure, \(p\), are defined as

\[ \tau_{eq} = \sqrt{\frac{1}{2} \sigma_s^d : \sigma_s^d}, \]  \(20\)

\[ p = -\frac{1}{3} \text{tr}(\sigma). \]  \(21\)

The thermodynamic state parameter \(S\) typically depends on the equivalent plastic strain \(\varepsilon_{p,eq}\) \([11]\). However, previous research revealed a dependency of the interface damage on the initial thermodynamic state of the polymer coating \([4]\), i.e. the dependence on the initial value of \(S\). Deformation-induced interface roughening was investigated in a two-dimensional numerical-experimental framework. The simulations predicted that a rejuvenated coating shows noticeably less interface damage compared to an aged coating. The change in steel surface profile triggers localization in an aged coating, which results in interface damage. The localization is significantly less for a rejuvenated coating resulting in less damage. Here it is assumed that the polymer has been rejuvenated (i.e. \(S = 0\)) prior to can manufacturing, e.g. via a pre-conditioning treatment \([5]\). The material parameters for the PET coating are listed in Table 3 and the corresponding mechanical response is shown in Fig. 5(a).
Table 3: Material properties of PET for the EGP model.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_r$ [MPa]</td>
<td>4.7</td>
</tr>
<tr>
<td>$\kappa$ [MPa]</td>
<td>1800</td>
</tr>
<tr>
<td>$G$ [MPa]</td>
<td>812</td>
</tr>
<tr>
<td>$\eta_{0,ref}$ [MPa·s]</td>
<td>$3 \cdot 10^8$</td>
</tr>
<tr>
<td>$\tau_0$ [MPa]</td>
<td>1.262</td>
</tr>
<tr>
<td>$\mu$ [-]</td>
<td>4.8</td>
</tr>
</tbody>
</table>

2.5 Computational model

The modeled domain (see Fig. 2(a)) is discretized using three-dimensional linear cube elements to create a regular finite element grid, similar to [28], which results in non-conforming grain boundaries. Another possible discretization relies on using tetrahedral elements (similar to e.g. [23, 34]), which accommodate conforming grain boundaries. However, this requires a large number of elements, which drastically increases the computational cost. The adopted finite element discretization is shown in Fig. 6.

The dominant Euler angles and their respective fractions are extracted from the EBSD measurement shown in Fig. 2(b) using the methodology proposed by Jöchen & Böhlke [21]. The representative Euler space (the rotation angles $\phi_1$, $\Phi$, $\phi_2$) is divided into 432 ($24 \phi_1$, $3 \Phi$ and $6 \phi_2$ divisions) boxes within which the average Euler angle and fraction is calculated. This results in a set of 333 unique Euler angles with their associated volume fractions. Using this reduced set of Euler angles and fractions, the experimental Orientation Distribution Function (ODF) is approximated within a 5% error of the L2 norm.

As the subsurface crystallographic steel microstructure is not readily available, a Voronoi tessellation is used to generate realistic grain geometries. The Voronoi tessellation is performed using the Neper software package [26]. The average grain size is taken from the EBSD measurement and equals 10 [$\mu$m]. Within the modeled domain, 200 grains are generated for the steel substrate using an equi-axed, in-plane periodic tessellation. An example of one of the tessellations is shown in Figure 6.

Figure 6: Example of a Voronoi tessellation and the finite element discretization used in the tension and compression simulations; colors only serve to distinguish the respective grains.

3 Results

3.1 Deformation-induced roughening

Four tensile simulations were performed along the $x$-direction of the material using different tessellations and Euler angles. The resulting height profiles for the tessellation shown in Fig. 6 at an average strain of $\varepsilon = 7.5\%$ and $\varepsilon = 15\%$ are shown in Fig. 7(a) and (b), respectively. The results show the formation of hills and valleys on the steel surface. The roughness pattern grows in amplitude with increasing deformation, but reveals the same qualitative behavior. The size of the roughness features varies and depends on the size of the grains.

The root-mean-square (RMS) roughness value of the resulting height profile of the four simulations...
is compared to experimentally obtained values in earlier work [4]. The RMS value is defined as

$$\text{RMS} = \sqrt{\langle u_z(x)^2 \rangle},$$

(22)

where $\langle ... \rangle$ indicates the spatial average of the top steel surface. The evolution of the RMS value (with thick lines to indicate the minimum and maximum) for the different simulations, together with the experimental result, as a function of the applied average strain is shown in Fig. 8.

The results show that varying the grain geometry and orientations affects the predicted roughness amplitude and roughening rate ($\partial \text{RMS}/\partial \varepsilon$), leading to a spread in the predicted RMS values. The microstructure clearly influences the predicted roughness. Comparing the two curves shows that the RMS values predicted by the simulations display the same qualitative trend as the experiment. In both cases, the RMS increases approximately linearly with the applied strain. A quantitative comparison is not pursued because of the limited amount of (experimental) data.

Figure 7: Surface roughness at different strains in a tensile simulation of a polymer-coated steel; the microstructure is shown in Fig. 6.

Figure 8: Evolution of the RMS values predicted in four tensile simulations for different underlying steel microstructures; the thick lines correspond to the lower and upper bound of the simulations.

3.2 Interface integrity

The interface integrity ($\xi$, see Eq. 12) at $\varepsilon = 7.5\%$ and $\varepsilon = 15\%$ for the tensile simulation is shown in Fig. 9. At a strain of $\varepsilon = 7.5\%$ the interface is still almost fully intact. However, at $\varepsilon = 15\%$, damage has clearly initiated locally, see Fig. 9(b). This is visible in the localized regions where the interface integrity tends towards zero. The evolution of the average interface integrity ($\langle \xi \rangle$) in the four simulations is shown in Fig. 10(a) and the minimum integrity $\xi_{\text{min}}$ is shown in Fig. 10(b). The average interface integrity
Figure 9: Interface integrity $\xi$ at different strains in a tensile simulation of a polymer-coated steel; the microstructure is shown in Fig. 6.

Figure 10: The average and minimum interface integrity for four tensile simulations of a polymer-coated steel; the thick lines correspond to the lower and upper bound of the simulations.

remains relatively high for all simulations, even at a strain of $\varepsilon = 15\%$. Clearly, the interface fails locally as is visible in the rapid decay towards zero of the minimum value.

The correlation between the roughness profile in Fig. 7(b) and the interface integrity in Fig. 9(b) is investigated next. To this end, the local deformations at the interface are decomposed in three characteristic scalar (but position dependent) quantities: (a) the positive out-of-plane displacement field which forms hills (Eq. 23); (b) the absolute out-of-plane displacement field that forms valleys (Eq. 24); and (c) the local in-plane displacement field (Eq. 25).

$$u_{\text{hill}} = \frac{1}{2} (u_z + |u_z|)$$

$$u_{\text{valley}} = \frac{1}{2} (|u_z| - u_z)$$

$$u_{\text{in-plane}} = \sqrt{(u_x - u_{x,\varepsilon})^2 + (u_y - u_{y,\varepsilon})^2}$$

Note that in Eq. 25, the average surface strain due to the applied tension ($u_i, \varepsilon$, $i = x, y$) is removed via linear regression. These displacement fields are normalized and multiplied by the loss in the interface integrity (i.e. $1 - \xi$) yielding the correlation factor $\chi$

$$\chi = \hat{u} (1 - \xi).$$

Here, $\hat{u}$ is the normalized displacement field for each of the individual measures of Eqs. 23-25. Thus only a large displacement combined with a low interface integrity results in $\chi \gg 0$. The result of the correlation analysis is shown in Fig. 11. The correlation factor of the positive out-of-plane displacement field and the interface integrity (Fig. 11(a)) shows that no clear correlation exists between the formation
of a hill on the steel surface and the interface integrity. This is explained by the fact that the formation of a hill is accompanied by interface closure in the interface normal direction. The correlation factor for the formation of a valley (Fig. 11(b)) and the factor for the in-plane displacement field (Fig. 11(c)) show high values in several locations. Furthermore, the formation of valleys or the in-plane displacement field alone cannot describe the interface damage, see the arrows in Figs. 11(b) and 11(c). Clearly, the formation of valleys together with the in-plane displacement field determines the resulting interface integrity profile.

Figure 11: Correlation (\(\chi\)) between the normalized displacement field (\(\hat{u}\)) and the loss of interface integrity (1 − \(\xi\)) for three different displacement measures in the tension simulation shown in Figs. 7(b) and 9(b); arrows indicate differences between \(\chi_{\text{valley}}\) and \(\chi_{\text{in-plane}}\); note that the colorbar was adjusted for clarity (the maximum for each measure is indicated in the respective captions).

### 3.3 Tension-compression comparison

Tension and compression simulations are next compared to study the interface integrity for different loading conditions. The roughness profile predicted for a uniaxial compression simulation at \(\varepsilon = -15\%\) is shown in Fig. 12(a) for the steel crystallography in Fig. 6. The tension results were presented earlier in Figs. 7 and 9. Comparing the roughness patterns predicted in tension (Fig. 7(b), repeated in Fig. 13(a)) and compression shows clear differences. Apparently, different hills and valleys form on the steel surface due to the applied deformation. However, a clear relation exists between the valleys that form in compression and the hills that form in tension, and vice versa. This is obvious from Fig. 13 where the roughness profile in compression was inverted for clarity (Fig. 13(b)). The two roughness profiles qualitatively match in terms of the predicted surface heights. However, the in-plane deformations are different due to the prescribed compression and tension. Clearly, the slip activity on the active slip systems in the crystal plasticity model are reversed in compression, resulting in a nearly inverse roughness profile. Fig. 14 shows the evolution of the extreme values of the RMS roughness value for four tension and four compression simulations. The results show that, in compression, the average slope of the RMS value increases compared to tension. In compression, the steel surface material extrudes out of the surface to accommodate compression, while in tension, the surface is stretched, reducing the roughness pattern.
The interface integrity at a strain of $\varepsilon = -15\%$ is shown in Fig. 12(b). Similar to the predicted roughness profiles, a difference is visible in the predicted integrity patterns. Different locations of the PET-steel interface initiate damage. Similar to the result in tension, the correlation analysis showed that a correlation emerges between the in-plane and negative out-of-plane displacement fields and the predicted interface damage. The evolution of the extremes of the average and minimum interface integrity as a function of the applied strain is depicted in Figs. 15(a) and 15(b), respectively. The average integrity again remains relatively high, indicating that interface failure occurs locally. The interface damages faster in compression as a result of the increased roughening rate. Furthermore, the minimum interface integrity decays more rapidly towards zero in compression than in tension. Obviously, uniaxial compression results in an increase in the predicted interface damage compared to uniaxial tension.

![Figure 12](image_url) (a) Surface roughness and (b) interface integrity for a compression simulation at $\varepsilon = -15\%$; the used tessellation and grain orientations are identical to the tension simulation in Fig. 7.

![Figure 13](image_url) (a) Surface roughness profile for a tension simulation at $\varepsilon = 15\%$ (identical to Fig. 7(b)), and (b) the inverted roughness profile for a compression simulation at $\varepsilon = -15\%$; the used tessellation and grain orientations are consistent with the tension simulation.

4 Discussion

The presented numerical framework enables prediction of deformation-induced roughening of a steel substrate and the effect thereof on the polymer-steel interface integrity. The simulations predict the initiation and growth of interface damage, whereby the tensile results of the evolving steel surface qualitatively match experimental results. Furthermore, a comparison between uniaxial tension and compression shows that in compression, the roughening rate is increased with an increase in predicted interface failure as a result.

The continuum assumption within the crystal plasticity model limits the simulated height profile evolution to continuum phenomena occurring at the grain-scale or above. The effect of micro-scale events,
e.g. the formation of crystallographic slip steps is not predicted in the current framework. Recent results of Faber et al. [16] showed that during production, the polymer-steel interface may locally delaminate due to micro-scale roughening. Clearly, incorporating the micro-scale roughening phenomena into the presented framework poses a great challenge.

While discrete slip events occurring at the free surface are not incorporated in a crystal plasticity approach, the slip activity on the different BCC slip planes is still predicted in an average sense. The average slip activity may serve as an indicator for discrete surface events. Micro-scale slip steps can be assessed via a different numerical simulation (e.g. Discrete Dislocation Dynamics) on the basis of the predicted slip activities found here.

To incorporate the roughening events near grain boundaries, e.g. due to dislocation pile-ups, a strain gradient crystal plasticity approach can be considered. Borg & Fleck [7] studied roughening near a grain boundary of a bi-crystal of FCC aluminium and found that the predicted roughness profile depends on the internal length scale. Nygårs & Gudmundson [24] also studied roughening using a strain gradient crystal plasticity model. Their simulations revealed a strong dependence of the predicted roughness on the internal length scale. However, these results were not yet compared to experiments, and are therefore still limited to interpretations.

It is also possible to incorporate the misorientations inside the steel grains into the grain orientations. Currently, all material points inside the modeled steel grains have an identical grain orientation. The effect of internal grain misorientations was investigated by Cheong & Busso [14]. Their simulations showed that including the local misorientations into the crystal plasticity simulations may change the local strain distribution and thus also the predicted roughness.

The comparison with experiments presented in this work is limited to a qualitative comparison in
terms of the average roughness evolution. The simulations were compared to a single tensile experiment performed on a packaging steel, revealing that the evolution of the average roughness compares well to experiments. However, to quantitatively predict deformation-induced roughening, experiments and simulations need to be based on the same orientation distribution and grain morphology. An example of such a comparison is the work of Zhao et al. [34] and Lim et al. [23], who compared the experiments and simulations on aluminium oligocrystals. Their results suggest that the predictions compare adequately to the experiments. Quantitative predictions of the roughness evolution are feasible by incorporating the complete measured steel crystallography in the presented framework.

In the presented results, the steel thickness was taken equal to 20 [µm]. The influence of the modeled steel thickness was analyzed by studying the evolution of the extremes of the RMS values as a function of the average applied strain for four simulations of a polymer-coated steel with a steel thickness of 20 [µm] and 30 [µm], the results of which are shown in Fig. 16. On average, the predicted roughness in the simulations with a steel thickness of 30 [µm] is smaller compared to the simulations with a steel thickness of 20 [µm] and the variation between the simulations decreases as more grains are incorporated. Clearly, to accurately predict the steel roughness evolution, a sufficient amount of grains must be considered.

![Figure 16: Evolution of the minimum and maximum RMS values for four simulations using a steel thickness of 20 [µm] and 30 [µm] and different steel microstructures; the thick lines correspond to the lower and upper bound of the simulations.](image)

Finally, from a computational perspective, the discretization is limited by the computational costs. Here, the discretization is taken relatively coarse, which may artificially stiffen the response. To assess the limitations of this approximation, a mesh convergence study was performed using tensile simulations on three geometries: 1) a small block of steel with dimensions 40 × 40 × 20 [µm], 2) a thin strip of steel with dimensions 40 × 1 × 40 [µm], and 3) a thin strip of steel with dimensions 20 × 20 × 2 [µm]. The second, quasi-3D, configuration has infinitely long grains along the y-direction (as a result of the in-plane periodic boundary conditions) and multiple grains through the thickness. The third geometry accounts for the three-dimensional nature, but with only a single grain through the thickness. Together, these three configurations cover all possible features influencing mesh convergence with a reasonable computational effort. The roughness profiles for the simulated small block of steel for a coarse and refined discretization are shown in Fig. 17. The results show that the predicted roughness patterns remain qualitatively the same upon mesh refinement, indicating that the predicted interface integrity patterns are not affected by further mesh refinement. Fig. 18 shows that, for completely different realizations, the adopted boundary conditions representing the underlying bulk give an adequate value for the RMS for a rather coarse discretization.

5 Conclusion

A three-dimensional numerical framework for the prediction of deformation-induced interface roughening and interface failure was presented. The framework was applied to a polymer-coated packaging steel. Simulations of uniaxial tension and compression were performed for different steel grain geometries and orientations. Some conclusions are drawn from the analysis.
Figure 17: Roughness profiles at $\varepsilon = 15\%$ for two different finite element discretizations (a) roughness, 4,000 elements. (b) roughness, 32,000 elements.

Figure 18: The evolution of the RMS roughness for the thin strips – cases 2 (solid) and 3 (dashed) – for different refinement steps. The geometrical configurations are indicated next to the plot.

- The predicted roughness evolution in tension qualitatively agrees with tensile experiments performed on a packaging steel. Furthermore, the simulations predicted the initiation and growth of local interface failure.
- Compared to tension, compression simulations showed an increased roughening rate with an increase in the predicted interface damage as a result.
- The developed framework enables study of the local initiation and growth of interface damage during deformation-induced roughening of a polymer-coated steel.

The incorporation of a predictive steel model, i.e. crystal plasticity, complements the cumbersome measurements of detailed experimental displacement fields that accompany deformation-induced roughening and thus enables the analysis of deformation processes where measuring the steel surface profile is difficult if not impossible, e.g. industrial forming processes such as deep-drawing. The framework may be extended to simulate industrial forming conditions, e.g. repeated deep-(re-) drawing and wall ironing, to investigate the interface integrity during forming. Due to the computational cost of the simulations, this may be accomplished by incorporating the framework into a global-local approach, e.g. by embedding the modeled domain into a bulk simulation or via a multi-scale approach.
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