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# Quantitative modeling of scratch-induced deformation in amorphous polymers

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ABSTRACT

In order to predict scratch performance of polymers, the present study focuses on quantitative assessment of various scratch-induced deformation mechanisms based on a set of model amorphous polymers *via* numerical modeling. A modification of Ree-Eyring theory is used to account for the rate dependent behavior of the model polymers at high strain rates using the experimental data obtained at low strain rates. By incorporating the rate and pressure dependent constitutive and frictional behaviors in the finite element methods (FEM) model, good agreement has been found between FEM simulation and experimental observations. The results suggest that, by including appropriate constitutive relationship and frictional model in the numerical analysis, the scratch behavior of polymers can be quantitatively predicted with reasonable success. Usefulness of the present numerical modeling for designing scratch resistant polymers is discussed.

## 1. Introduction

Scratch-induced surface deformation in polymeric materials is a complex mechanical process due to their strong rate, temperature and pressure dependent responses. The mechanical behavior of polymers generally exhibits strain softening-strain hardening phenomena, different constitutive behaviors under tension and compression, rate, temperature and pressure dependent yielding, and viscoelasticity. Surface friction also greatly influences the scratch-induced deformation features as changes in coefficient of surface friction alter the stress state polymer substrate experiences near the surface during the scratching process. Since the development of scratch-induced damage features in polymers involves large-scale deformation, close-form solutions are inadequate for modeling scratch behavior of polymers. Consequently, extensive research work has been carried out to study the evolution of scratch-induced deformation features and learn how they are affected by the bulk mechanical and surface properties [1–13].

Jiang et al. [1] showed that the development of different scratch-induced deformation features depends on the polymer type. The stress analysis using finite element methods (FEM) showed that the same material point could successively undergo tension and compression as the scratch tip passed through it. Based on their experimental observation, a polymer scratch damage evolution map was developed to qualitatively differentiate the scratch behaviors of polymers with variation in material constitutive relations. Similar scratch deformation maps, developed by Briscoe et al. [14,15] using conical indenter and constant/dead weight scratch normal load, showed evolution of different scratch-induced deformation to vary with the scratch speed due to changes in imposed strain rate. Using FEM parametric studies along with the ASTM scratch test [16] on a set of model polymers, Hossain et al. [4,5,8] showed that yield stress, strain at stress recovery and strain hardening slope beyond the strain at stress recovery in compression are the most important parameters that influence the residual scratch depth and shoulder height development along the scratch path. Tensile behavior has little influence on residual scratch depth and shoulder height formation but affects the surface roughness on the scratch groove along the scratch path, which was primarily caused by micro-cracking in the polymers investigated. Poisson's ratio and Young's modulus, in the range of 1.65 GPa–4 GPa, have shown not to significantly influence the residual scratch depth using FEM modeling [3]. Bucaille et al. [6] employed experimental work and FEM to conclude that a larger strain hardening led to greater elastic deformation, thus less

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cumulative plastic strain [6,17]. Bellemare et al. [18] reported a decrease in pile-up height (shoulder height) with the increase in strain hardening exponent using pure Copper and Copper/Brass alloy. Browning et al. [2] showed that, using experimental study on styrene-acrylonitrile (SAN) random copolymers, an increase in acrylonitrile (AN) content or molecular weight (MW) can have a positive effect on improving the scratch resistance as it increases the tensile strength and ductility.

Using their analytical expressions for stress field due to a circular contact region carrying a hemispherical Hertzian normal pressure and a proportionally distributed shearing traction, Hamilton and Goodman [19,20] showed that an increase in surface friction intensifies and moves the maximum stresses from sub-surface toward the surface, and, thus, inducing greater deformation. According to the study, a maximum tensile stress also develops at the rear end of the circular contact when increasing the surface friction, which can be thought of responsible for the ring crack observed in brittle materials. An extensive study [7] on the effect of surface friction on scratch depth and shoulder height development has shown that the coefficient of adhesive friction indeed affects the onset and extent of scratch depth and shoulder height, but the degree of influence can be altered by modifying the constitutive relation.

Most, if not all, of the experimental studies carried out by the researchers to correlate mechanical properties with the evolution of various scratch-induced deformation features can be considered qualitative since the bulk mechanical properties used to draw the conclusion were measured at a strain rate much lower than the rate polymer surface would experience at the imposed scratching speeds. Similar conclusion can be drawn in the case of FEM simulation efforts as most of the studies employed simplistic constitutive model in their analyses which did not take into account the rate, temperature and pressure dependent behaviors of polymers. Furthermore, simplistic description of the contact between the tip and the substrate was employed using the Coulomb's law of friction. As a result, most of the numerical analyses emphasize only on qualitative comparison between the FEM simulation and experimental findings.

To quantitatively predict the scratch behavior of polymers using FEM, strain softening-strain hardening phenomena, asymmetric behavior in tension and compression, rate, temperature and pressure dependent behaviors, viscoelasticity, to name a few, will have to be incorporated in the constitutive relations. The contact between the tip and the polymer substrate has to be modeled properly to account for not only the coefficient of friction due to adhesion but also the friction developed due to large-scale material deformation. The scratch tip geometry and surface roughness of the polymer substrate also plays an important role during the contact between the rigid tip and polymer substrate. A quantitative model for predicting scratch behavior of polymers can then be developed if all these features can be included in the FEM simulation.

The objective of this study is to quantitatively predict the scratch-induced deformation of amorphous polymers *via* FEM by including the key characteristics of polymer constitutive behavior and an appropriate contact mechanics model. It is hoped that the present findings can facilitate development of scratch resistant polymers.

## 2. Theoretical consideration

During the scratching process, the effective strain rate on or near the surface can be approximated by Ref. [14]:

$$\dot{\varepsilon} = \frac{v}{w} \qquad (1)$$

Where, $\dot{\varepsilon}$ is the effective strain rate, $v$ is the scratch speed and $w$ is the scratch width. For a scratch speed of 100 mm/s and spherical scratch tip of 1 mm diameter, as recommended by the ASTM standard for automotive applications [16], the effective strain rate on or near the surface can reach at 100s to 1000s 1/s. Thus, to quantitatively predict the scratch-induced deformation of polymers using FEM, high strain rate constitutive behavior of polymers is needed. It should be noted that, since the strain rate varies from one position to another during the scratching process, the mechanical behavior only at a fixed strain rate is inadequate for modeling the scratch behavior. The constitutive behavior of the polymer substrate from low to high strain rate is needed along with an interpolation scheme to account for the wide strain rate range the material experiences.

For amorphous polymers, the yield stress generally increases with strain rate and a linear relationship can be established between the yield stress and logarithm of strain rate. However, the post-yield behavior can remain unchanged with the increase in strain rates [21–25]. To describe the rate dependent yield or flow stress for glassy, amorphous polymers, several theoretical models are available. Although based on specific molecular mechanisms involved in the yield behavior of polymers, Robertson [26] and Argon [27] models found only limited success in describing the rate dependent plasticity in amorphous polymers. Perhaps the most widely-accepted model to describe the rate dependent plasticity in amorphous polymers is the Ree-Eyring model [28], a modification of the original Eyring model [29]. The ability to change the slope at an intermediate strain rate distinguishes the Ree-Eyring model from Robertson and Argon models, and, thus, allows better prediction of the rate dependent plasticity in amorphous polymers from moderate to high strain rates. According to the formalism of the Ree-Eyring theory, yielding of amorphous polymers can be considered dependent on particular degrees of freedom in polymer chains, whose relaxation or activation depends on the applied strain rate and temperature. At low strain rates and/or high temperatures, pure viscous flow can be considered to take place at yielding due to jumps of segments of the macromolecule from one equilibrium position to another, called the $\alpha$ process. For high strain rates and/or low temperatures, the yield behavior of an amorphous polymer can be assumed of involving two rate processes, $\alpha$ and $\beta$, and the plastic flow due to these processes can be considered additive. At high strain rates and/or low temperatures, pure viscous flow also takes place at the yielding due to jumps of segments of backbone chain of the macromolecule from one equilibrium position to another similar to the single activated $\alpha$ process. But, the $\alpha$ process is hindered as the molecular movements are partially frozen even when the stress around the yield stress is applied. To activate these movements, it is necessary to supply additional energy by applying additional stress. Thus, at high strain rates and/or low temperatures, the observed yield stress can be considered as the sum of two stresses with respect to the $\alpha$ and $\beta$ processes.

Using the commercially available polycarbonate (PC) samples (Makrolon from Bayer), Bauwens-Crowet et al. [30] described the yield behavior of amorphous polymers by assuming the involvement of two different flow processes. They found success when compared their experimental data by curve-fitting using the Ree-Eyring model for multiple rate activated process. It was suggested [30] that the $\beta$ flow process observed at yielding is the same process observed in damping tests and can be correlated with the dynamic mechanical loss peak, i.e., loss tangent *vs.* temperature at a given frequency. They reported that the value of the activation energy $Q_\beta$ for PC was in agreement with the value reported from dielectric measurements [30]. They found similar results for PVC, as well [31]. According to Bauwens et al. [32], unlike $Q_\beta$, $Q_\alpha$ may not be compared with the activation energy related to the primary transition observed in dielectric or mechanical damping tests. Using PC, Bauwens [33] showed that the $\beta$ yield process and $\beta$ peak revealed