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MECHANICS AND TRIBOLOGY OF THIN COATINGS (FILMS)

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Abstract

The investigation on mechanics and tribology of thin-film coatings was presented in two different ways of analytical methods, i.e. mixed boundary value problems in elasticity and plasticity theories and simulations by finite element method. Boundary value solution for elastic double-layer problem investigated the mechanical and frictional properties of thin-film coating with elastic deformation and gave a few of useful insights for the indentation and sliding contact problems, such as contact pressure distribution, indentation approach. Finite element method has been used to model indentation and sliding processes in term of its advantages of solving non-linear contact problems. Elastic-plastic material model is usually used for thin-film coating made of metal or stiff material in finite element simulation, but it is not very effective for the coatings composed of polymers. The mechanics and tribology of thin-coatings made of metals has been well understood, but studies of mechanics and tribology for thin film coated by polymers, such as PTFE are still challenging because of their complicated microstructure and variable material response.

1. Introduction

Thin-film coatings have been extensively applied to industrial products such as magnetic storage devices, microelectro-mechanical devices with the emergence of micro- and nano-technology [1-3]. Therefore, the understanding of mechanical behaviors involved in the contact of layered media which include stresses and deformations produced by contacting bodies, elastic and plastic properties of materials, friction and wear etc. have been of great importance in practice and received considerable attentions. Indentation and sliding tests are two of experimental methods mostly applied to investigate the mechanical properties of thin coatings. Specifically, many efforts have been made on indentation to investigate the mechanical properties of material, such as elastic and plastic properties of the layer and substrate materials, effects of layer thickness on the contact pressure distribution, hardness measurement, adhesion effects, interfacial friction characteristics, etc. Additionally, mechanical behaviors of thin-film coatings during the indentation are also dependent on the material under test, the material of the indenter, the detailed shape and size of the indenter and the applied load. While the sliding contact problem of thin-film coatings is also of considerable interest, it is typically applied to examine the frictional characteristics of thin coatings, wear and durability of layered media, stresses and surface displacements at the contact region. In fact, early studies on mechanics and tribology of thin coatings focused on the mixed boundary value problem with the theories of elasticity and plasticity [4-6] and could only be applied to some limited cases with assumptions. Recently, finite element analysis has been a prevalent method to simulate the indentation or sliding process in terms of its advantage of solving non-linear contact problems since large strains and deformations as well as material nonlinearities are involved [7-10]. Based on the stiffness of thin coating compared to the substrate, the studies on mechanical and tribological behaviors of layered media can be classified as soft coating on hard substrate and hard coating on comparably softer substrate. Simulating the indentation or sliding on the thin-film coating made of different materials such as metals and polymers will require a variety of material models including non-linear material properties.

The following sections will examine the studies on the mechanics and tribology of thin coating from the perspective of different methods applied to analysis, i.e., analysis by the theories of elasticity and plasticity and analysis by finite element method.

2. Mechanics and Tribology of Thin Coatings Investigated by the Theories of Elasticity and Plasticity

As early as the 1970's, the issue of indentation on the layered elastic half-space was investigated by the theory of elasticity. Chen [4] studied the indentation of a medium consisting of one or two elastic layers bonded to a homogeneous half-space which was shown in Fig.1. Frictionless contact and indentation with a rigid axisymmetric punch were assumed to simplify such a mixed boundary value problem. The surface boundary conditions can be written as follows:

$$u_z(r,0) = a\varpi(r) = a[\delta - f(r)], 0 \le r \le a \tag{1}$$

$$\sigma_{zz}(r,0) = 0, r > a \tag{2}$$

$$\sigma_{rz}(r,0) = 0, r > 0 \tag{3}$$

where a is the radius of contact region, f(r) is the profile of the punch divided by a and δ is the ratio of the penetration of the punch to the contact radius. Over the interfaces $z=2h_1$ and $z=2(h_1+h_2)$ the surface traction and displacements must be continuous, i.e. on $z=2h_1$

$$\begin{aligned} u_z^{(1)} &= u_z^{(2)}, \\ u_r^{(1)} &= u_r^{(2)}, \\ \sigma_{rz}^{(1)} &= \sigma_{rz}^{(2)}, \\ \sigma_{zz}^{(1)} &= \sigma_{zz}^{(2)}, \end{aligned} \tag{4}$$

and on $z=2(h_1+h_2)$

$$\begin{aligned} u_z^{(2)} &= u_z^{(3)}, \\ u_r^{(2)} &= u_r^{(3)}, \\ \sigma_{rz}^{(2)} &= \sigma_{rz}^{(3)}, \\ \sigma_{zz}^{(2)} &= \sigma_{zz}^{(3)}, \end{aligned} \tag{5}$$

The integral least square method was utilized to find out the contact pressure distribution under indenters in a variety of geometries such as circular flat-ended and parabolic which were shown in Fig.2 and 3. The results were also extended to apply to the impact problem of two solid bodies along the quasi-static assumption of the Hertz impact theory with experimental verification. However, a noticeable constraint on the choice of materials in experiment was that all materials involved must stay in the elastic range during impact. In the case of a thin stiff layer bonded to a soft stratum, the thin layer behaves like a plate and the surface pressure distribution may deviate substantially from the corresponding homogeneous half-space solution.

Considering the mechanical reliability of protective coating, it was of great importance to investigate the frictional contact stress field for normal and shearing surface traction. O'sullivan

[6] followed the theoretical procedure of analyzing elastic normal contact problems for layered media presented by Chen [4] and studied the quasi-static stress field generated by a sliding spherical indenter on an elastic substrate with a single layer. The configuration plot for this contact problem is shown in Fig.4. In the layer the stresses and displacements are taken as functions of x, y, and z_1, while in the half-space they are functions of x, y and z_2. The normal and tangential surface tractions are prescribed on $z_1=0$ as follows:

$$\sigma_{zz}{}^{(1)}(x,y,0) = -p(x,y), \quad \sigma_{zx}{}^{(1)}(x,y,0) = -q(x,y),$$
$$\sigma_{zy}{}^{(1)}(x,y,0) = 0 \tag{6}$$

The interface between the layer and half-space is required to have continuous tractions and displacements:

$$\sigma_{zx}^{(1)}(x,y,h) = \sigma_{zx}^{(2)}(x,y,0), \quad u_x^{(1)}(x,y,h) = u_x^{(2)}(x,y,0)$$
$$\sigma_{zy}^{(1)}(x,y,h) = \sigma_{zy}^{(2)}(x,y,0), \quad u_y^{(1)}(x,y,h) = u_y^{(2)}(x,y,0)$$
$$\sigma_{zz}^{(1)}(x,y,h) = \sigma_{zz}^{(2)}(x,y,0), \quad u_z^{(1)}(x,y,h) = u_z^{(2)}(x,y,0) \tag{7}$$

The superscripts (1) and (2) refer to the layer and half-space, respectively. The Papkovich-Neuber elastic potentials were employed to solve stress field for general surface loadings. In terms of the potentials φ and ψ_1, ψ_3, the stresses and displacements can be expressed as

$$2\mu u_i = \varphi_{,i} + x\psi_{1,i} + z\psi_{3,i} - (3-4\nu)\psi_i$$
$$\sigma_{ij} = \varphi_{,ij} - 2\nu(\psi_{1,1} + \psi_{3,3})\delta_{ij} - (1-2\nu)(\psi_{i,j} + \psi_{j,i}) + x\psi_{1,ij} + z\psi_{3,ij} \tag{8}$$

The traction boundary value problem solution is used in solving the case of an elastic spherical indenter contacting the layered half-space with contact radius a, the normal traction boundary condition on the surface of z1=0 is replaced by the mixed boundary condition:

$$u_z^{(1)}(r,0) + u_z^{(3)}(r,0) - u_z^{(1)}(a,0) - u_z^{(3)}(a,0) = W(r), |r| < a \tag{9}$$
$$\sigma_{zz}^{(1)}(r,0) = 0, |r| < a$$

where W(r) is the undeformed profile of the indenter, $u_z^{(3)}(r,0)$ is the surface deformation of the indenter, and $r = (x^2 + y^2)^{1/2}$ is the distance from the center of the contact zone.

The final results shown in Fig.5-7 demonstrated that the value of the thin-layer Young's modulus relative to the substrate had a strong effect on the potentials for yielding in both the layer and substrate as well as on the adhesion stresses at the layer/substrate interface. The maximum tensile stress on the film surface strongly depended on both the friction coefficient and the elastic modulus of layer relative to that of substrate.

As the scale decreased to the nano level, the effects of adhesion should be studied because it affected the relationships among the applied force, the penetration of the indenter and the size of contact area. Sergici [1] applied a Maugis type of adhesion model to the contact of a spherical indenter with a layered elastic half-space and assumed that the elastic layer was perfectly bonded to the substrate and the contact at the interface between the indenter and layer was frictionless. As shown in Fig. 8, the boundary conditions at the interface (z=0) are listed as follows:

$$\begin{gathered} u_z^{(1)}(r,0) = u_z^{(2)}(r,0), r > 0 \\ u_r^{(1)}(r,0) = u_r^{(2)}(r,0), r > 0 \\ \sigma_{zz}^{(1)}(r,0) = \sigma_{zz}^{(2)}(r,0), r > 0 \\ \sigma_{zr}^{(1)}(r,0) = \sigma_{zr}^{(2)}(r,0), r > 0 \end{gathered} \tag{10}$$

and at the free surface (z=-h) are given by

$$\begin{gathered} \sigma_{zr}(r,-h) = 0, f > 0 \\ \left. \begin{gathered} u_z(r,-h) = \delta - f(r), r < a \\ \sigma_{zz}(r,-h) = \sigma_0, a < r < c \\ \sigma_{zz}(r,-h) = 0, r > c \end{gathered} \right\} \text{Mixed B.C.} \end{gathered} \tag{11}$$

Where f(r) is the shape of the indenter which, for a spherical indenter, is approximated by f(r) = $r^2/2R$.Using Hankel transform of order zero of the Papkovich-Neuber potentials, the non-dimensional normal force and penetration depth were calculated and plots of normal force versus contact radius and penetration depth were given. The effects of key parameters, such as elastic moduli ratio of the layer and the substrate, the dimensionless layer thickness, and the Maugis adhesion parameter on the curves of applied force versus contact radius and penetration depth were also investigated. It concluded that the thickness of the layer affected the combined stiffness of the layered elastic half-space. Increasing the layer thickness for compliant/stiff substrates increases/reduces the overall stiffness of the layered medium.

Although all contact problems presented in the aforementioned papers were assumed to have elastic deformations, a few of conclusions can also be applied to evaluate mechanical and tribological behaviors on thin-film coating with plastic deformations. Ogilvy presented a parametric elastic model for indentation testing of thin films [7]. It predicted that the formula of calculating contact radius and normal approach was effective for thinner film or larger spherical indenter at low loads with experimental verifications of lead films on steel substrate and rubber films on glass substrate. Expected effects of plasticity were provided to explain the increase of contact radius and normal approach relative to those expected from elasticity theory and the predicted contact radius was increased by the loss of adhesion due to the reduction in effective rigidity of the film while adhesion was lost.

Hereby, the analytical solutions obtained from the theories of elasticity and plasticity can be applied to the contact problems on soft thin-film or hard thin-film coatings with generality because stiffness and thickness of layer are not restrained. These results also provide valuable insights to the finite element method which has been widely employed to investigate mechanical and tribological behaviors of contact problems on thin-film coatings.

3. Mechanics and Tribology of Thin Coatings Investigated by Finite Element Method

3.1 Study of Mechanical and Tribological Behaviors of Thin Coating with Finite Element Analysis

Since the indentation or sliding contact is a highly non-linear problem in which large deformation, large strain, material nonlinearity and contact are all involved, it is difficult to study mechanical behaviors of thin coating in the analytical way. Thus, the finite element method is employed to simulate the contact problem of indentation or sliding.

Kral [8] presented the finite element method to analyze repeated elastic-plastic indentation of a homogeneous half-space by a rigid sphere. Both isotropic hardening and elastic-perfectly plastic material properties were used without other simplifying material assumptions. The contacting sphere was modeled with contact element, thus removing the need for assuming a particular contact pressure distribution. The particular mesh discretization was used to yield very fine elements near contact region between sphere ball and thin film to avoid possible convergence problems arising from sharp edges. As shown in Fig.9, the finite element discretization can also be referred as to model similar indentation cases for the contact of spherical ball on thin-film coating. The results demonstrated that the contact pressure was relatively insensitive to elastic properties while hardening produced significantly higher pressures and smaller contact radii at the interface. Additionally, the yielding behavior was caused by an increase in both the tensile hoop and compressive radial stresses upon the removal of the approximately uniform contact pressure.

Three-dimensional finite element simulation was performed to examine the surface deformation characteristics resulting from indentation and sliding contact on a layered half-space in Kral's paper [9]. A 30-nm-thick layer was modeled, with stiffness and yield stress both two and four times that of the substrate. Elastic and perfectly plastic material behavior was assumed throughout the analysis. Sliding was performed at two normal loads, both 100 and 200 times the yield load of the substrate material, and friction coefficients of 0.1 and 0.25 in order to determine the effect of the normal load and friction on the surface stresses and deformation of the layered half space. The three-dimensional finite element discretization of the layered half-space was given in Fig.10. All cases exhibited a substantial accumulation of plastic strain in the layer during the second load cycle, but only the higher load case exhibited significant accumulation of plastic strain in the substrate.

The 2-D and 3-D finite element method discussed above gave a few of useful insights to deal with the indentation and sliding contact problems on thin-film coating with the assumption of both isotropic hardening and elastic-perfectly plastic material properties. However, most of these studies for thin-film coatings were the cases of hard thin coatings on comparably softer substrate. In fact, softer thin coatings are also applied for reasons of performance, such as in electrical contact applications where gold is often used as a surface layer to improve electrical conductivity [11].

N. Panich [12] investigated the effect of penetration depth on indentation response of soft coatings on hard substrate using finite element method. It assumed that a soft coating was perfectly adhered to a harder substrate indented by a rigid indenter and the contact was frictionless. All thin-coating and substrate materials were assumed to be isotropic, elastic and perfectly plastic. The results shown in Fig.11 and 12 found out that the critical indentation depth below which the substrate has negligible effect on the loading curve increased with decreasing yield strength ratio of the coating to the substrate. The effect of the harder substrate on the indentation response of the coating-substrate system was two-fold, i.e. the initiation and propagation of plastic deformation in the substrate and the enhanced pile-up of the coating material around the indenter.

3.2 Material Models Applied in Simulations by Finite Element Method

Elastic and perfectly-plastic material model is commonly used in modeling the indentation or sliding problems of thin-film coating by finite element method. This material model has been proved effective in analyzing the contact problems of thin-film coating made of metals or very stiff materials. Recently, some fluoropolymers, such as PTFE (polytetrafluoroethylene), FEP (fluorinated ethylene propylene) and PFA (perfluoroalkoxy resin) are widely used as the coating materials due to the advantages of lower coefficient, chemical resistance and thermomechanical stability [14].

However, elastic and plastic material model is probably not good for studying the mechanical and frictional behavior of polymers because polymers, especially fluoropolymers exhibit a complicated nonlinear response when subjected to external loads. At small deformations, the material response is linear viscoelastic while at larger strains, the material undergoes distributed yielding, unrecoverable deformation, viscoplastic flow, and finally gradual material stiffening at large deformations until ultimate failure occurs [15]. Only recently the more advanced constitutive models for polymer material models have been developed by Khan and Kletschkowski [16-17]. Based on the observation that both viscoelastic and viscoplastic deformation of PTFE are time-dependent and nonlinear, Khan [16] presented a phenomenalogical viscoelasto-plastc constitutive model by a series connection of a viscoelastic deformation module (represented by three elements standard solid spring dashpot model) and viscoplastic deformation module by KHL model. The one-dimensional constitutive model is shown in Fig.13. Additionally, J.S. Bergström presented a new constitutive model called as Dual Network Fluoropolymer (DNF) model to predict the behavior of fluoropolymers subjected to multiaxial large-deformation thermomechanical loadings [15]. The DNF model shown in Fig. 14 incorporates experimental characteristics by using a decomposition of the material behavior into a viscoplastic response, corresponding to irreversible molecular chain sliding and a time-dependent viscoelastic response. The stress-strain plots were given to describe the tensile and compression behaviors of PTFE for various strain rates. The results of simulating small punch indentation were well matched with data obtained from the experiment, which was shown in Fig.15.

In terms of the feature complexity of the microstructure together with the broad range of usable temperature, the characteristic material response of fluoropolymers such as PTFE is still challenging to model.

4. Future Work and Conclusion

Therefore, two ways of studying the mechanical and tribological behaviors on thin-film coating have been investigated. Using the theories of elasticity and plasticity, it is of paramount importance to find out correct boundary conditions and governing equations for elastic double – layer problems. In fact, some numerical techniques, such as least square integral, Papkovich-Neuber potentials are also employed to obtain the solution of mixed boundary value problems. Finite element method has become prevalent to analyze the non-linear contact problem on thin-film coatings. Particular mesh discretization for the specific contact problem is required and proper material models should be taken into consideration to avoid convergence problem of solutions. In the past, elastic-plastic material model were widely used to investigate the mechanical behaviors for the coatings made of metal or stiff material. However, this model may not be good for simulating contact problems involved of polymers. Though a few of papers presented some new constitutive models for specific polymer, such as PTFE or other fluoropolymer, it is still challenging to precisely predict the characteristic material response of polymers by modeling due to the complicated features of microstructure at different temperatures and formation of components inside.

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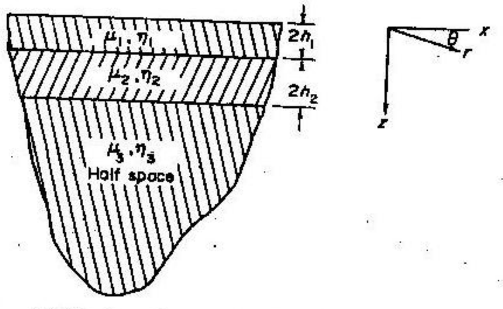
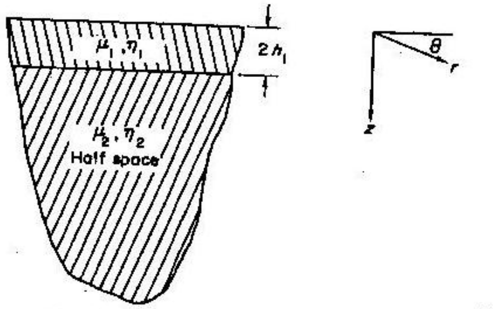


(a) Two layers bonded to half space



(b) One layer bonded to half space

Figure 1 Configuration of multi-layer media. Originally from Chen et al. 1972[4]

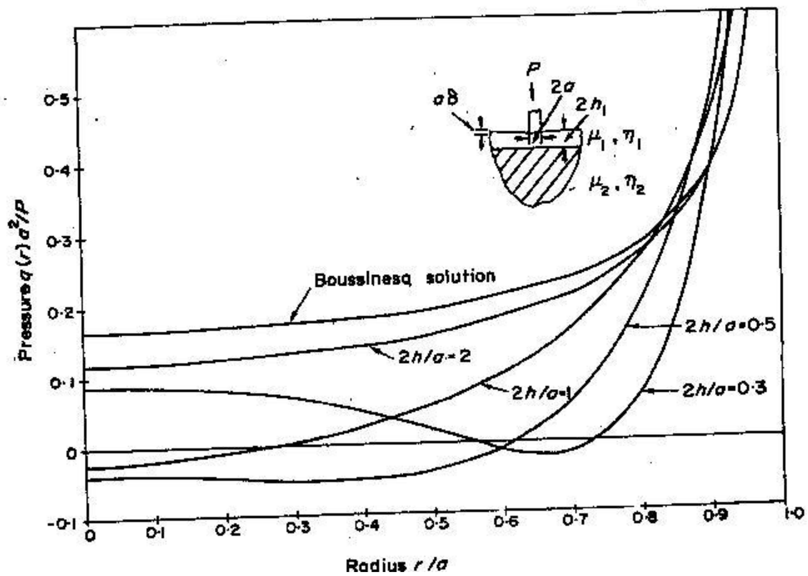


Figure 2 Dimensionless pressure distribution under the flat ended punch. Originally from Chen et al. 1972[4]

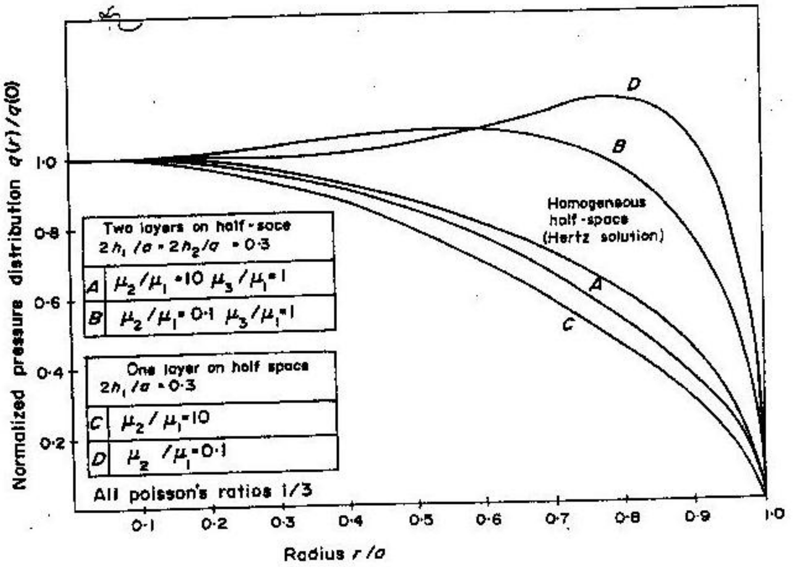


Figure 3 Normalized surface pressure distribution under parabolic punch. Originally from Chen et al. 1972[4]

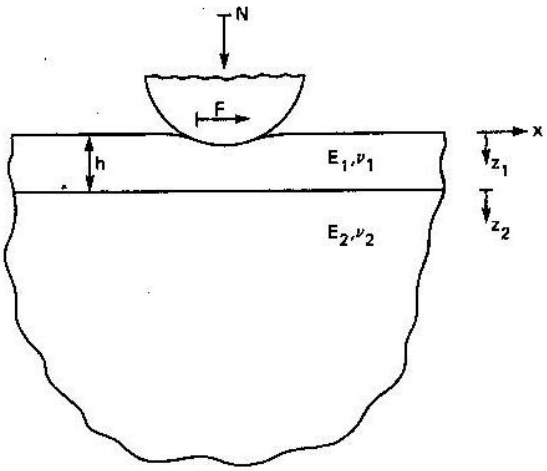


Figure 4 Contact problem cross-sectional geometry in the x-z plane and notation. Originally from O'Sullivan et al. 1988[6]

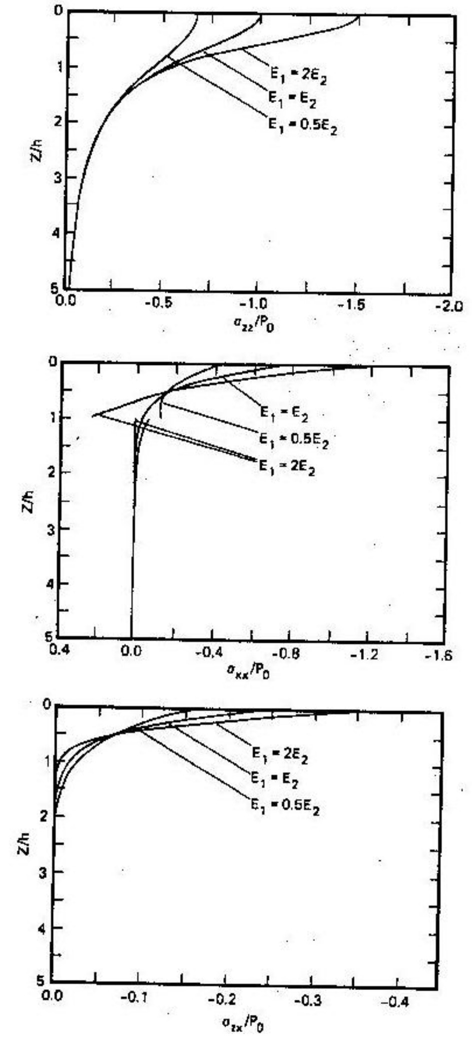


Figure 5 Stresses along the z-axis under combined normal and sliding contact. Originally from O’Sullivan et al. 1988[6]

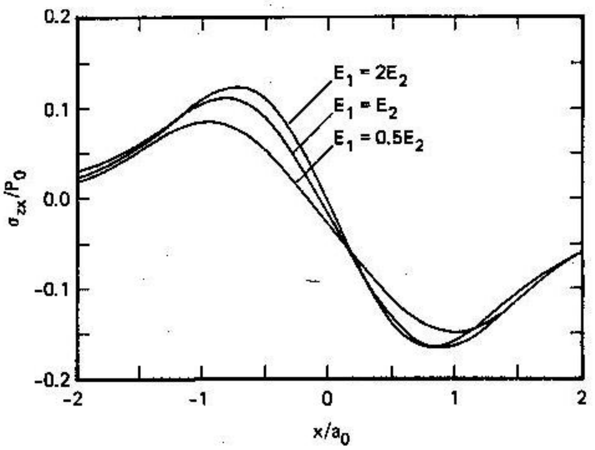


Figure 6 Interfacial shear stress along the x-axis at z_1=h for E_1/E_2. Originally from O’Sullivan et al. 1988[6]

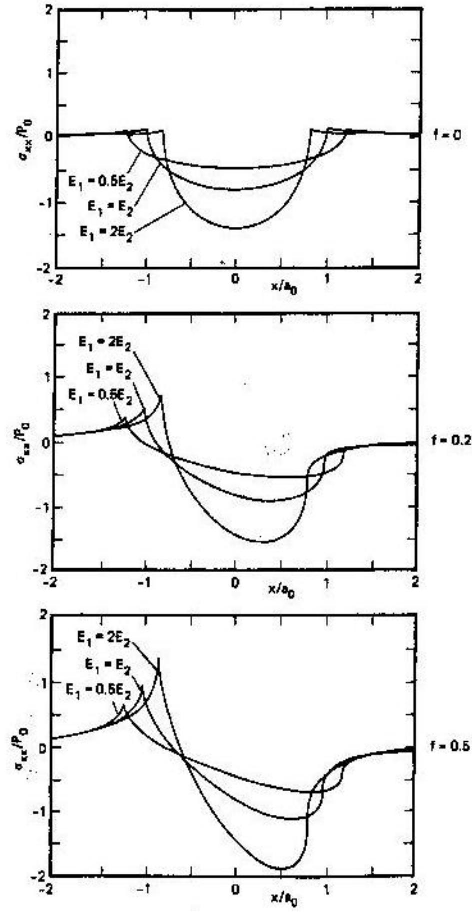


Figure 7 Variation of σ_{xx} on the surface along the a-axis for different values of the friction coefficient f and E_1/E_2. Originally from O'Sullivan et al. 1988[6]

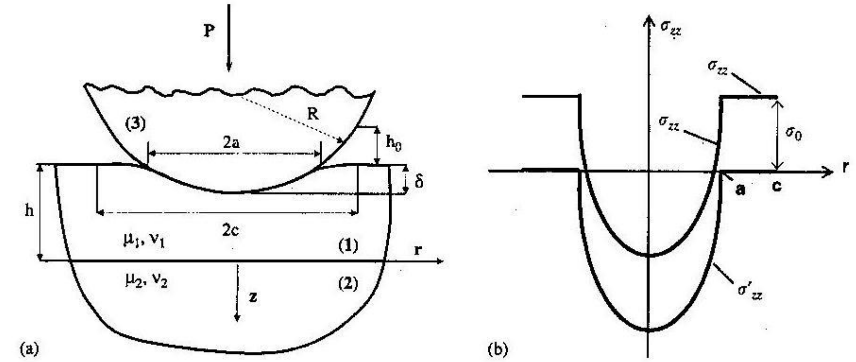


Figure 8 Indentation of an elastic layered media by a rigid spherical indenter. Originally from Onur et al. 2006[1]

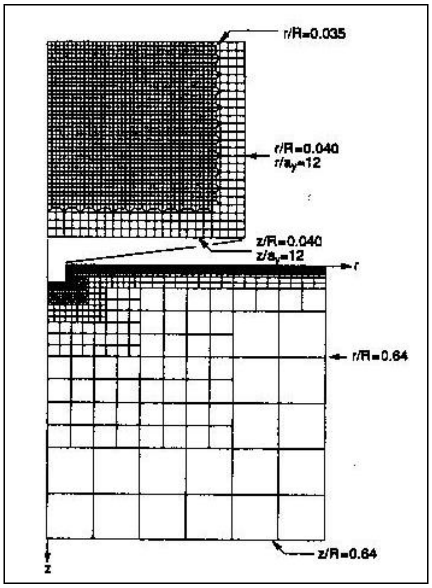


Figure 9 2-D finite element discretization of layered half-space. Originally from Kral et al. 1993[8]

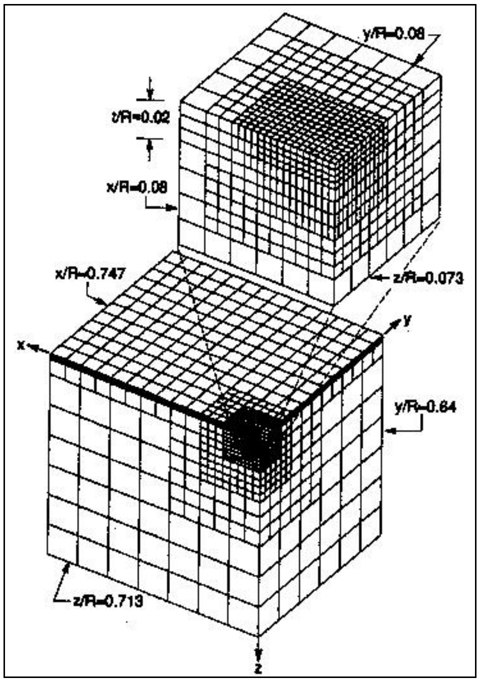


Figure 10 3-D finite element discretization of layered half-space. Originally from Kral et al. 1996[9]

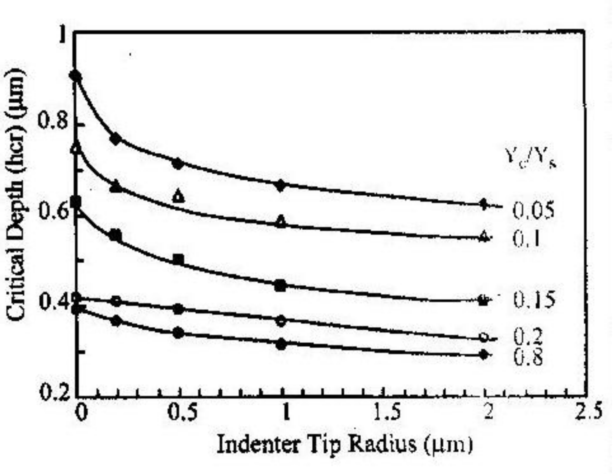


Figure 11 Critical indentation depth below which the substrate effect on loading is less than 5%, as a function of indenter tip radius. Originally from Panich et al. 2003[12]

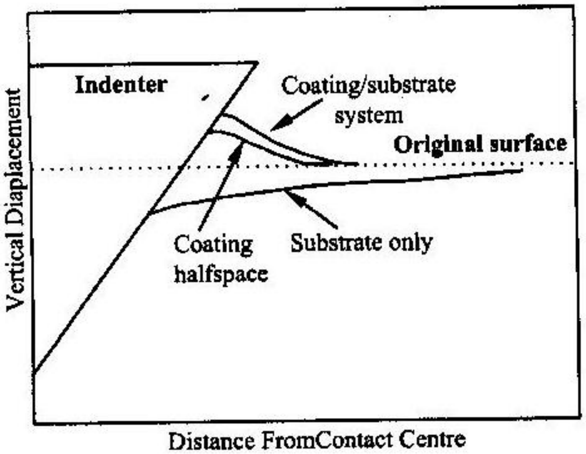


Figure 12 Surface profiles of the indented coating/substrate system and corresponding substrate and coating halfspaces, showing enhanced pile-up in the coating/substrate system. Originally from Panich et al. 2003[12]

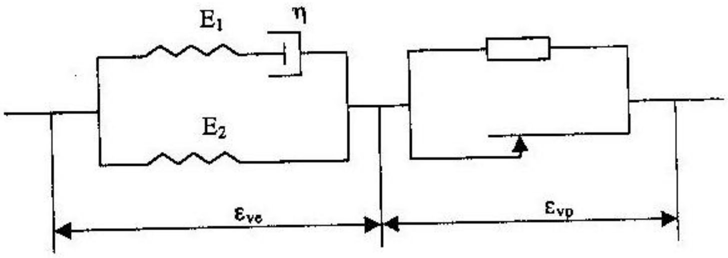


Figure 13 One dimensional rheological representation of the constitutive model. Originally from Khan et al. 2001[16]

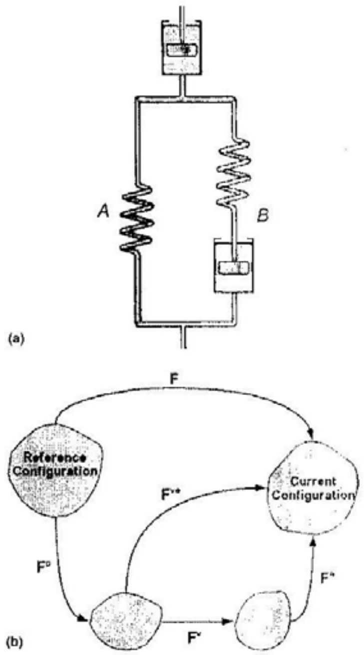


Figure 14 (a) Rheological representation of the constitutive model; (b) Kinematics of deformation. Originally from Bergström et al. 2005[15]

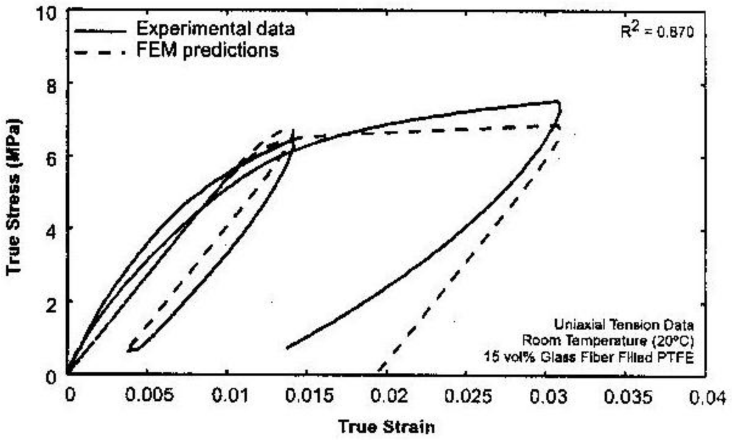


Figure 15 Comparison between experimental data and predicted behavior in uniaxial tension at different strain rate. Originally from Bergström et al. 2005[15]