

Semi-Analytical Model for Rough Multilayered Contacts

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Abstract

This paper presents a new model for analysis of non-conformal rough surface contacts where one or both of the contacting bodies are coated with a multilayered coating. The model considers elastic contact of arbitrary geometry with real measured roughnesses and both normal and tangential surface loads. It predicts contact pressure distribution, surface deformations and full subsurface stress field. As such, the model offers an optimisation tool for analysis and development of multilayered coatings. Influence coefficients approach is utilised to obtain contact pressures and subsurface stresses while the contact solver is based on standard conjugate gradient method. To improve model efficiency, a semi-analytical approach is devised, where the influence coefficients for displacements and stresses are expressed explicitly by solving the fundamental equations in the frequency domain. Fast Fourier Transforms in conjunction with discrete convolution are then utilised to provide the solution in spatial domain. Selected results are presented to first validate the model and then illustrate the potential improvements that can be achieved in the design of multilayered coatings through application of the model.

Keywords: Coating, Contact Model, Roughness, Multilayered

Nomenclature

A_w - Influence coefficient matrix for surface displacements, $W_{\eta=0}$

A_s - Influence coefficient matrix for general stress, S

$A^{(k)}, B^{(k)}, C^{(k)}, D^{(k)}, F^{(k)}$ and $H^{(k)}$ - Solution constants. Superscript (k) indicates the layer

$E^{(k)}$ - Young's modulus for layer k (Pa)

$E^{*(1)}$ - Equivalent elastic modulus based on properties of counter face and layer (1),

$$E^{*(1)} = \left(\frac{1 - \nu_{counterface}^2}{E_{counterface}} + \frac{1 - \nu^{(1)2}}{E^{(1)}} \right)^{-1}$$

$$K^{(k)} = - \frac{\lambda^{(k)} + 3\mu^{(k)}}{E^{(k)}(\lambda^{(k)} + \mu^{(k)})}$$

L - Load (N)

P_{Hertz} - Maximum Hertz pressure (Pa)

S - Stress (Pa)

U, V, W - Normalised displacements, $u/l, v/l, w/l$ respectively in x-, y-, z- direction

a_{Hertz} - Hertz contact semi-width

f_r - Friction coefficient

$h^{(k)}$ - Thickness of layer k (m)

$$i = \sqrt{-1}$$

l - Semi-width in x and y directions of the surface discretization patch (m)

n - Number of layers, excluding the substrate

p - Contact pressure (Pa)

s, r - Fourier transform variables for ξ and γ direction respectively

x, y, z - Spatial coordinates (m)

$$\alpha_D = \frac{\Gamma(\kappa_S + 1) - (\kappa_L + 1)}{\Gamma(\kappa_S + 1) + \kappa_L + 1}, \beta_D = \frac{\Gamma(\kappa_S - 1) - (\kappa_L - 1)}{\Gamma(\kappa_S + 1) + \kappa_L + 1} \text{ - Dundur's parameters}$$

where $\Gamma = \frac{E_L(1+\nu_s)}{E_s(1+\nu_L)}$, $\kappa_s = 3 - 4\nu_s$, $\kappa_L = 3 - 4\nu_L$ (subscripts 's' and 'L' indicate substrate and coating in a single layered coating system).

$$\beta = \sqrt{s^2 + r^2}$$

ξ, γ, η = Normalised spatial coordinates; $x/l, y/l$ and z/l

$\lambda^{(k)}$ - Lamé's first constant $(= \frac{E^{(k)}\nu^{(k)}}{(1+\nu^{(k)})(1-2\nu^{(k)})})$ for layer k , (Pa)

$\mu^{(k)}$ - Lamé's second constant $(= \frac{E^{(k)}}{2(1+\nu^{(k)})})$ for layer k , (Pa)

$\nu^{(k)}$ - Poisson's ratio for layer k

σ_{ij} - Stress tensor (Pa)

Subscripts

i, j, k, l, m - Indices of the mesh positions in the discretized 3D domain

t - loop counter in the iterative process

Superscripts

(k) - Indicates the coating layer k

Other symbols

$\approx$ when placed over variable symbol, indicates double Fourier transformed variable in ξ and η direction

$$\Delta = \text{Biharmonic operator} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

1 Introduction

Surface coatings are widely employed in tribological components with the primary aim of protecting contacting surfaces from damage and/or reducing friction, particularly under poor lubrication conditions. Bearings, piston rings, fuel injectors and cams and followers are some of the mechanical components where tribological coatings are often employed. Relative to a homogenous contact, presence of a coating in general modifies the contact mechanics in two ways: contact pressures and areas are either increased or decreased depending on the coating properties relative to the substrate and the subsurface stress fields are modified not least due to the mismatch in elastic properties of the coating and the substrate. When carefully controlled, such changes can offer superior contact performance but when poorly understood they can lead to premature failure of coated contacts through mechanisms that may not have been expected in the equivalent homogenous contact, such as fracture, fatigue and delamination. Many modern coatings possess a multilayered structure, where the properties of each coating layer can be chosen to optimise the prevalent contact mechanics for improved tribological performance of the overall coating in terms of reduced friction and wear and extended durability. Such multilayered structures can therefore offer advantages over a single layer coating, but they also produce even more complex contact stress fields which need careful consideration. Accordingly, to maximise the benefits offered by multilayered coatings as well as minimising the risk of unexpected failures through undesirable stresses, a contact model which is able to predict contact pressures, deformations and subsurface stresses in rough multilayered contacts is needed.

The earliest contact model for coated surfaces was that of Burmister [1] who, as part of his studies into airport runway surfaces, produced a model for three-dimensional, single layered, smooth contacts subject to normal load. Over the following half a century several authors produced single-layered models capable of dealing with various levels of complexity. Dundurs [2] considered a smooth two-dimensional contact of coated surfaces and proposed two non-dimensional parameters to describe the material mismatch between the coating and the substrate. Gupta and Walowit [3] utilised Fourier transforms of Airy stress functions to provide a solution for deformations and stresses in a coated contact subject to unit pressure loading at the origin, which can then be utilised as an influence function for the said contact. O'Sullivan and King [4] included both normal and tangential loading in an influence coefficient based model, while Komvopoulos and co-workers [5] used finite element methods to study a similar contact configuration. Nogi and Kato [6], Kannel and Dow [7] and Cole and Sayles [8] provided full contact solutions for a layered contact of rough surfaces while others, such as Kadiric and co-workers [9], Ju and Chen [10] and Leroy et al [11] also considered in-contact thermal effects of the coating.

In recent years the layered contact analyses have been extended to include multilayered coating systems. Chen [12] used Fourier integrals to extend the single layered model of Burmister [1] to smooth bodies containing up to two layers. Elsharkawy and Hamrock [13] utilised the Gupta and Walowit [3] solution to develop a model for a dry, sliding contact

between two elastic bodies coated with a number of thin layers, both bodies possessing the same layer system. Their model is limited to two-dimensional contacts of two ideally smooth bodies while results are presented for contacts with up to two coating layers. A similar approach to that presented in this paper was used by Plumet and Dubourg [14], where the influence coefficients were first obtained for a multilayered contact in frequency domain by utilising Fourier transforms. Their method is limited to two smooth bodies, one of which is rigid and elliptical, while the presented results consider single-layered systems only. Cai and Bhushan [15, 16] considered one and two layered systems utilising Papkovitch-Neuber potentials to obtain influence coefficients and minimum complimentary energy principle to obtain the contact solution. They present results focusing on the effect of the material properties of the intermediate layer in a two layered coating.

From the discussion above it is evident that the existing multilayered contact models all suffer from one or more limitations in terms of either the number of layers they consider (generally one or two), the type of loading (commonly limited to normal load only) and/or the contact geometry (often only two dimensional line contacts or smooth bodies are considered). The current model attempts to address these deficiencies by providing an efficient semi-analytical contact model that considers two elastic bodies with any number of coating layers, normal and tangential loading, real rough surfaces and arbitrary (non-conformal) contact geometry. With the aim of illustrating the potential for optimisation of multilayered coatings in terms of produced contact stresses, the model is applied to an example coated contact containing 1, 2 and 4 coating layers of differing material properties and under normal as well as combined normal and tangential loading. Finally, the model is also used to study the effect of the relative interface positions and properties of intermediate layer in two-layered relatively stiff coating.

2 The Model

The method is based on linear elastic theory and utilises the influence coefficients approach to solve for contact pressures, deformations and subsurface stresses in a rough contact. The influence coefficients for displacements and stresses under normal and tangential loading are found semi-analytically by solving the Navier's generalized equation together with the bi-harmonic equation for displacements, through application of continuous Fourier transforms and a set of boundary conditions pertinent to a multilayered contact. The full contact pressure distribution in a rough contact under given loading is obtained through an iteration scheme based on conjugate gradient method and analytical expressions for the surface normal displacements. Finally, discrete convolution and FFTs are used to obtain the complete subsurface stress fields from the calculated stress influence coefficients and the contact pressure distribution. The rough multilayered contact problem for which the solution is sought is illustrated in Figure 1. One or both bodies may have a multilayered

structure. All layers and the substrate are assumed to exhibit linear elastic behaviour and the material properties within each layer are assumed homogenous. Each coating layer is given a finite thickness and is rigidly bonded to the adjacent layers. The substrate is regarded as a layer with infinite thickness. The coating layers are assumed to follow the original surface roughness profile so that the thickness of each layer is uniform. No assumptions about the roughness asperity shape or distribution are made and the model can deal with real, measured roughness profiles.

As shown in Figure 1b the potential contact area is discretized into square patches of finite width $2l \times 2l$, each carrying a uniform normal contact pressure, p_{ij} and uniform tangential stress, $f_r p_{ij}$ if in contact, and zero normal and tangential stress if not in contact. Displacement and stress influence coefficients are found by solving the governing equations for one such patch represented by a unit square pressure acting on a multilayered half-space at the origin as illustrated in Figure 1c.

As with any other numerical method, when choosing the appropriate size of a single discretized element there is a trade-off between computational efficiency and achieved accuracy. Owing to the use of efficient computational techniques and semi-analytical solution for influence coefficients in the current model, relatively fine discretization can be chosen where each micro-contact area in a rough contact is usually described by multiple square patches. Due to the use of standard FFT algorithms, it is necessary to use uniform element size in x and y directions, while non-uniform mesh can be implemented in z (depth) direction. This allows for stresses around the coating interfaces to be resolved accurately.

The chosen computational approach first seeks a fundamental solution for the displacements and stresses throughout the multilayered half-space due to a unit normal and tangential stress centred at the origin of the coordinate system (Figure 1c). This solution is used to form a matrix of influence coefficients, which relates displacement or stress at any point (k, l, m) in the domain to contact pressure at any surface point (i, j) . It can therefore be used together with complete contact pressure field, $p_{i,j}$ to determine the stresses and displacements throughout the domain through principle of superposition, so that for an example stress S : $S_{k,l,m} = \sum_i \sum_j A_{s,i,j,k,l,m} * p_{i,j}$, where A_s is the influence coefficient matrix corresponding to stress S .

Efficient and accurate determination of the influence coefficients is therefore central to this approach. The methodology adopted to calculate the influence coefficients is presented below.

2.1 Methodology for Obtaining the Influence Coefficients

The displacement and stress fields in a three-dimensional solid can be described by Navier's generalized equation, the biharmonic equation for displacements and Hooke's law relating stresses and displacements. Navier's equation can be written in tensor notation as:

$$(\lambda^{(k)} + 2\mu^{(k)}) \frac{\partial^2 u_i^{(k)}}{\partial x_i^2} + \mu^{(k)} \left(\sum_{j \neq i} \frac{\partial^2 u_i^{(k)}}{\partial x_j^2} \right) + (\lambda^{(k)} + \mu^{(k)}) \left(\sum_{j \neq i} \frac{\partial^2 u_j^{(k)}}{\partial x_j \partial x_i} \right) = 0 \quad 1$$

for $i=1-3; j=1-3$ and where superscript k indicates the coating layer.

The biharmonic equation for displacements is:

$$\Delta \Delta u_i^{(k)} = 0 \quad 2$$

for $i=1-3$

For simplicity, the coordinate positions $x_{i,j,k}$ as well as all displacements $u_{i,j,k}$ are normalised by half-width of the surface patch, l , as shown in Figure 1c. Using this normalisation scheme and expanding equation 1, three partial differential equations of the 2nd order for three normalised displacements U , V and W in three normalised independent variables, ξ , γ and η were obtained:

$$(\lambda^{(k)} + 2\mu^{(k)}) \frac{\partial^2 U^{(k)}}{\partial \xi^2} + \mu^{(k)} \left(\frac{\partial^2 U^{(k)}}{\partial \gamma^2} + \frac{\partial^2 U^{(k)}}{\partial \eta^2} \right) + (\lambda^{(k)} + \mu^{(k)}) \left(\frac{\partial^2 V^{(k)}}{\partial \xi \partial \gamma} + \frac{\partial^2 W^{(k)}}{\partial \xi \partial \eta} \right) = 0 \quad 3$$

$$(\lambda^{(k)} + 2\mu^{(k)}) \frac{\partial^2 V^{(k)}}{\partial \gamma^2} + \mu^{(k)} \left(\frac{\partial^2 V^{(k)}}{\partial \xi^2} + \frac{\partial^2 V^{(k)}}{\partial \eta^2} \right) + (\lambda^{(k)} + \mu^{(k)}) \left(\frac{\partial^2 U^{(k)}}{\partial \xi \partial \gamma} + \frac{\partial^2 W^{(k)}}{\partial \gamma \partial \eta} \right) = 0 \quad 4$$

$$(\lambda^{(k)} + 2\mu^{(k)}) \frac{\partial^2 W^{(k)}}{\partial \eta^2} + \mu^{(k)} \left(\frac{\partial^2 W^{(k)}}{\partial \xi^2} + \frac{\partial^2 W^{(k)}}{\partial \gamma^2} \right) + (\lambda^{(k)} + \mu^{(k)}) \left(\frac{\partial^2 U^{(k)}}{\partial \xi \partial \eta} + \frac{\partial^2 V^{(k)}}{\partial \gamma \partial \eta} \right) = 0 \quad 5$$

Similarly, expanding the biharmonic equation 2 for displacement U , gives a partial differential equation of the 4th order:

$$\frac{\partial^4 U^{(k)}}{\partial \xi^4} + \frac{\partial^4 U^{(k)}}{\partial \gamma^4} + \frac{\partial^4 U^{(k)}}{\partial \eta^4} + 2 \frac{\partial^4 U^{(k)}}{\partial \xi^2 \partial \gamma^2} + 2 \frac{\partial^4 U^{(k)}}{\partial \xi^2 \partial \eta^2} + 2 \frac{\partial^4 U^{(k)}}{\partial \gamma^2 \partial \eta^2} = 0 \quad 6$$

Identical equations are valid in all layers and the substrate provided that the corresponding material properties, $\lambda^{(k)}$ and $\mu^{(k)}$, for each layer are used.

To determine the required displacement and stress influence coefficients the partial differential equations 3 to 6 must be solved subject to the boundary conditions listed in section 2.2 below. Although this solution could be obtained numerically, an analytical solution is obviously preferred for simplicity and efficiency of the overall model. To achieve this, these equations are first transformed to frequency domain by application of two-dimensional continuous Fourier transforms with respect to ξ and γ direction. This results in ordinary differential equations which can now be solved analytically. The two-dimensional Fourier transform of U , for example, with respect to ξ and γ is defined as:

$$F(U(\xi, \gamma, \eta)) = \tilde{\tilde{U}}(s, r, \eta) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(\xi, \gamma, \eta) e^{-is\xi - ir\gamma} d\xi d\gamma \quad 7$$

Where double tilde indicates transformed quantities, s and r are Fourier transform variables corresponding to ξ and γ direction respectively and $i = \sqrt{-1}$. V and W are transformed in the

same way. Fourier transform of the derivatives with respect to ξ or γ can be achieved through integration by parts to result in:

$$F\left(\frac{\partial^n(U,V,W)}{\partial(\xi)^n}\right) = \int_{-\infty}^{\infty} \left(\frac{\partial^n(U,V,W)}{\partial(\xi)^n}\right) e^{-is\xi} d\xi = (is)^n \left(\tilde{\tilde{U}}, \tilde{\tilde{V}}, \tilde{\tilde{W}}\right) \quad 8$$

$$F\left(\frac{\partial^n(U,V,W)}{\partial(\gamma)^n}\right) = \int_{-\infty}^{\infty} \left(\frac{\partial^n(U,V,W)}{\partial(\gamma)^n}\right) e^{-ir\gamma} d\gamma = (ir)^n \left(\tilde{\tilde{U}}, \tilde{\tilde{V}}, \tilde{\tilde{W}}\right) \quad 9$$

Where n is the order of the differential.

The application of the above transform to partial differential equations 3 to 6 results in the following ordinary differential equations for displacements $\tilde{\tilde{U}}, \tilde{\tilde{V}}, \tilde{\tilde{W}}$ with respect to one independent variable, η :

$$\begin{aligned} & -(\lambda^{(k)} s^2 + 2\mu^{(k)} s^2 + \mu^{(k)} r^2) \tilde{\tilde{U}}^{(k)} + \mu^{(k)} \frac{d^2 \tilde{\tilde{U}}^{(k)}}{d\eta^2} - (\lambda^{(k)} + \mu^{(k)}) sr \tilde{\tilde{V}}^{(k)} + \\ & is(\lambda^{(k)} + \mu^{(k)}) \frac{d \tilde{\tilde{W}}^{(k)}}{d\eta} = 0 \end{aligned} \quad 10$$

$$\begin{aligned} & -(\lambda^{(k)} r^2 + 2\mu^{(k)} r^2 + \mu^{(k)} s^2) \tilde{\tilde{V}}^{(k)} + \mu^{(k)} \frac{d^2 \tilde{\tilde{V}}^{(k)}}{d\eta^2} - (\lambda^{(k)} + \mu^{(k)}) sr \tilde{\tilde{U}}^{(k)} + \\ & ir(\lambda^{(k)} + \mu^{(k)}) \frac{d \tilde{\tilde{W}}^{(k)}}{d\eta} = 0 \end{aligned} \quad 11$$

$$i(\lambda^{(k)} + \mu^{(k)}) \left(s \frac{d \tilde{\tilde{U}}^{(k)}}{d\eta} + r \frac{d \tilde{\tilde{V}}^{(k)}}{d\eta} \right) - \mu^{(k)} \beta^2 \tilde{\tilde{W}}^{(k)} + (\lambda^{(k)} + 2\mu^{(k)}) \frac{d^2 \tilde{\tilde{W}}^{(k)}}{d\eta^2} = 0 \quad 12$$

$$\frac{d^4 \tilde{\tilde{U}}^{(k)}}{d\eta^4} - 2\beta^2 \frac{d^2 \tilde{\tilde{U}}^{(k)}}{d\eta^2} + \beta^4 \tilde{\tilde{U}}^{(k)} = 0 \quad 13$$

where $\beta = \sqrt{s^2 + r^2}$.

From equation 13 one obtains the general solution for $\tilde{\tilde{U}}^{(k)}$ to be:

$$\tilde{\tilde{U}}^{(k)}(s, r, \eta) = (A^{(k)} + B^{(k)} \eta) e^{\beta \eta} + (C^{(k)} + D^{(k)} \eta) e^{-\beta \eta} \quad 14$$

Substituting this into equations 10 and 11 the solutions for $\tilde{\tilde{V}}^{(k)}$ and $\tilde{\tilde{W}}^{(k)}$ are obtained as:

$$\tilde{\tilde{V}}^{(k)}(s, r, \eta) = \left(H^{(k)} + \frac{r}{s} B^{(k)} \eta \right) e^{\beta \eta} + \left(F^{(k)} + \frac{r}{s} D^{(k)} \eta \right) e^{-\beta \eta} \quad 15$$

$$\tilde{W}^{(k)}(s, r, \eta) = i \left[\left(\frac{A^{(k)}s}{\beta} + \frac{H^{(k)}r}{\beta} + \frac{K^{(k)}B^{(k)}}{s} + \frac{B^{(k)}\beta\eta}{s} \right) e^{\beta\eta} + \left(-\frac{C^{(k)}s}{\beta} - \frac{F^{(k)}r}{\beta} + \frac{K^{(k)}D^{(k)}}{s} - \frac{D^{(k)}\beta\eta}{s} \right) e^{-\beta\eta} \right] \quad 16$$

Where $A^{(k)}$, $B^{(k)}$, $C^{(k)}$, $D^{(k)}$, $H^{(k)}$, and $F^{(k)}$ are constants with respects to η but are functions of the Fourier variables s and r and , $K^{(k)} = -\frac{\lambda^{(k)} + 3\mu^{(k)}}{E^{(k)}(\lambda^{(k)} + \mu^{(k)})}$. The procedure for obtaining

the expressions for $\tilde{U}$, $\tilde{V}$ and $\tilde{W}$ is rather lengthy but the full details can be found in the PhD thesis of Nyqvist [17]. This solution applies to each layer since $A^{(k)}$, $B^{(k)}$, $C^{(k)}$, $D^{(k)}$, $H^{(k)}$, and $F^{(k)}$ have layer specific values.

2.2 Boundary Conditions

There are three boundary conditions at the surface and six at each layer interface. All boundary conditions are also transformed into frequency domain and stresses are expressed in terms of displacement differentials by using Hooke's law.

At the surface, $\eta=0$, the following three boundary conditions are imposed:

- The normal stress, $\sigma_{\eta\eta}$, at the surface ($\eta=0$) is equal to the unit contact pressure within the boundaries of square patch considered, $|\xi, \gamma| \leq 1$, and zero elsewhere. With application of Hooke's law and the above Fourier transforms this can be written as:

$$\begin{aligned} \tilde{\sigma}_{\eta\eta(\eta=0)}^{(1)} &= \left((-2is\mu^{(1)})A^{(1)} - \left(\frac{i}{s}(2\mu^{(1)} + \lambda^{(1)})(K^{(1)}\beta + \beta) + 2i\frac{\mu^{(1)}}{s}\beta^2\eta \right) B^{(1)} - 2ir\mu^{(1)}H^{(1)} \right) e^{\beta\eta} \\ &+ \left((-2is\mu^{(1)})C^{(1)} + \left(\frac{i}{s}(2\mu^{(1)} + \lambda^{(1)})(K^{(1)}\beta + \beta) - 2i\frac{\mu^{(1)}}{s}\beta^2\eta \right) D^{(1)} - 2ir\mu^{(1)}F^{(1)} \right) e^{-\beta\eta} \quad 17 \\ &= \tilde{p} = \frac{4}{sr} \sin(s)\sin(r) \end{aligned}$$

The details of the derivation of the double Fourier transform used in equation 17 can be found in the Appendix.

- The shear stress, $\sigma_{\eta\xi}$, at the surface in the sliding direction, ξ , is equal to the friction coefficient, f_r , multiplied by the applied pressure, p . As above, in the frequency domain this becomes:

$$\begin{aligned}
\tilde{\sigma}_{\eta\xi}^{(1)}(\eta=0) &= \left(\left(\frac{\mu^{(1)}}{\beta} s^2 + \mu^{(1)} \beta \right) A^{(1)} + (\mu^{(1)} K^{(1)} + \mu^{(1)} + 2\mu^{(1)} \beta \eta) B^{(1)} + sr \frac{\mu^{(1)}}{\beta} H^{(1)} \right) e^{\beta\eta} \\
&+ \left(- \left(\frac{\mu^{(1)}}{\beta} s^2 + \mu^{(1)} \beta \right) C^{(1)} + (\mu^{(1)} K^{(1)} + \mu^{(1)} + 2\mu^{(1)} \beta \eta) D^{(1)} - sr \frac{\mu^{(1)}}{\beta} F^{(1)} \right) e^{-\beta\eta} \quad 18 \\
&= f_r \frac{4}{sr} \sin(s) \sin(r)
\end{aligned}$$

- The shear stress, $\sigma_{\eta\gamma}$, in the direction transverse to sliding, γ , at the surface equals to zero, i.e. sliding in one direction only and no spin in the contact is assumed. Thus:

$$\begin{aligned}
\tilde{\sigma}_{\eta\gamma}^{(1)}(\eta=0) &= \left(\frac{\mu^{(1)}}{\beta} sr A^{(1)} + \left(\frac{r}{s} \mu^{(1)} + \frac{r}{s} \mu^{(1)} K^{(1)} \right) B^{(1)} + 2\mu^{(1)} \beta \frac{r}{s} \eta B^{(1)} + \left(\mu^{(1)} \beta + \frac{\mu^{(1)}}{\beta} r^2 \right) H^{(1)} \right) e^{\beta\eta} \\
&+ \left(- \frac{\mu^{(1)}}{\beta} sr C^{(1)} + \left(\frac{r}{s} \mu^{(1)} + \frac{r}{s} \mu^{(1)} K^{(1)} \right) D^{(1)} - 2\mu^{(1)} \beta \frac{r}{s} \eta D^{(1)} - \left(\mu^{(1)} \beta + \frac{\mu^{(1)}}{\beta} r^2 \right) F^{(1)} \right) e^{-\beta\eta} = 0 \quad 19
\end{aligned}$$

Layers are assumed to be rigidly bonded to each other so at each interface there is a continuity of displacements and stresses which can be expressed through the following six boundary conditions:

$$\begin{aligned}
\tilde{U}^{(k)} &= \tilde{U}^{(k+1)} & \tilde{V}^{(k)} &= \tilde{V}^{(k+1)} & \tilde{W}^{(k)} &= \tilde{W}^{(k+1)} \\
\tilde{\sigma}_{\eta\eta}^{(k)} &= \tilde{\sigma}_{\eta\eta}^{(k+1)} & \tilde{\sigma}_{\eta\xi}^{(k)} &= \tilde{\sigma}_{\eta\xi}^{(k+1)} & \tilde{\sigma}_{\eta\gamma}^{(k)} &= \tilde{\sigma}_{\eta\gamma}^{(k+1)}
\end{aligned} \quad 20$$

Finally the compatibility condition ensures that all displacements far away from the contact tend to zero:

$$\tilde{U} = \tilde{V} = \tilde{W} \rightarrow 0 \quad \text{as} \quad \xi, \gamma, \eta \rightarrow \infty \quad 21$$

The 6 constants, $A^{(k)}$ to $H^{(k)}$ are to be determined in each layer k including the substrate. To fulfil the condition of equation 21, constants A , B and H for the substrate must obviously be equal to zero. Hence, if the number of layers (excluding the substrate) is n , there are $(6n + 3)$ constants to be determined. Equations 17 to 20 result in a system of $(6n + 3)$ linear simultaneous equations which can then be solved to determine the $(6n + 3)$ constants for a given system as required. The system of equations that needs to be solved is illustrated in matrix form in equation 22. It is worth noting that since the constants, $A^{(k)}$ to $H^{(k)}$, are functions of s and r this system of equations needs to be solved for each point (s, r) in the frequency domain separately. In the present model the solution is computed using an LU factorisation implemented in NAG F07ADF routine in commercial NAG Fortran Libraries software and also available as an open source routine DGETRF.

$$\begin{bmatrix}
(a_{11}) & (a_{12}) & (a_{13}) & (a_{14}) & \dots\dots\dots(a_{1,6n+3}) \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
\vdots & & & & \\
(a_{6n+3,1}) & (a_{6n+3,2}) & (a_{6n+3,3}) & \dots\dots\dots a_{6n+3,6n+3}
\end{bmatrix}
\times
\begin{bmatrix}
A^{(1)} \\
B^{(1)} \\
C^{(1)} \\
D^{(1)} \\
H^{(1)} \\
F^{(1)} \\
A^{(2)} \\
\vdots \\
F^{(n)} \\
C^{(n+1)} \\
D^{(n+1)} \\
F^{(n+1)}
\end{bmatrix}
=
\begin{bmatrix}
(4/sr)\sin(s)\sin(r) \\
f_r(4/sr)\sin(s)\sin(r) \\
0 \\
0 \\
0 \\
0 \\
0 \\
\vdots \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\quad 22$$

The procedure outlined above is sufficient to define full influence coefficient matrices for any of the three displacements, U , V , W . The influence coefficients for stresses $\sigma_{\eta\eta}$, $\sigma_{\xi\xi}$, $\sigma_{\gamma\gamma}$, $\sigma_{\eta\xi}$, $\sigma_{\eta\gamma}$ and $\sigma_{\xi\gamma}$ can then easily be defined through direct application of Hooke's law. The resulting expressions are rather long-winded and the reader is referred to the PhD thesis of Nyqvist [15] for the full expressions.

It should be noted that at $s = 0$ and $r = 0$, the above solution is not defined as s and r appear in the denominator of the right hand side terms of equation 22. To work out the required values at these points a Gaussian interpolation scheme with 8x8 points is used in the model algorithm.

2.3 The Complete Contact Solver

Once the influence coefficient matrix for surface normal displacements $[A_w]$ is formed it can be used to relate the complete distribution of surface displacements $[W_{\eta=0}^{(1)}]$ to the contact pressure distribution $[p]$ through the convolution:

$$[W_{\eta=0}^{(1)}] = [A_w] \otimes [p] \quad 23$$

This convolution requires N^N operations. However, through use of discrete convolution theorem this operation can be performed in the frequency domain as:

$$[\tilde{W}_{\eta=0}^{(1)}] = [\tilde{A}_w] \bullet [\tilde{p}] \quad 24$$

which involves only $N \times N$ operations. This approach lends itself well to the current model since the influence coefficients matrix $[A_w]$ is already calculated in the frequency domain i.e. $[\tilde{A}_w]$ is known and hence the need for an extra Fourier transformation is avoided. The combination of semi-analytical calculation of the influence coefficients, as presented above, and the use of discrete convolution theorem, results in an efficient model which in turn enables increased accuracy and/or larger contact domain size to be used for a given calculation time.

Given that both surface displacements $[W_{\eta=0}^{(1)}]$ and pressures $[p]$ are unknown a-priori, a solution for contact pressures and displacements needs to be determined through an iterative process, in common with other contact solvers in the literature. The calculated contact pressure field must be such that $p_{ij} > 0$ at all contacting points, $p_{ij} = 0$ at all non-contacting points and the integral of pressure field over contact area must be equal to the applied load, L i.e.

$$\int p \, dx dy = 4l^2 \sum_{all \, i,j} p_{ij} = L \quad 25$$

In this work the contact solver utilises an iteration scheme based on a conjugate gradient method (CGM), similar to that presented, amongst others, by Stanley and Kato [18] and Ai and Sawamiphakdi [19].

The CGM algorithm is implemented through the following steps:

- Initiate the pressure field, $[p_t]$, that meets the equality and inequality constraints above. Usually a Hertzian pressure distribution is a good start.
- Calculate a candidate pressure array $[p_{t+1}]$ as (in general, $[p_{t+1}]$ will violate the constraints):

$$[p_{t+1}] = \left(\frac{[p_t]}{E^{*(1)}} \right) - [Grad] \quad 26$$

Where:

$$[Grad] = \frac{[W_{\eta=0}^{(1)}] + [gap]}{l} \quad 27$$

and 'gap' is the geometrical overlap of the surfaces. $[W_{\eta=0}^{(1)}]$ is calculated as outlined above using the matrix $[\tilde{A}_w]$, discrete convolution theorem and double inverse Fast Fourier Transform (FFT⁻²) algorithm for implementation of inverse discrete Fourier transform in two dimensions i.e.:

$$[W_{\eta=0}^{(1)}] = FFT^{-2} \left[\tilde{W}_{\eta=0}^{(1)} \right] = FFT^{-2} \left(\left[\tilde{A}_w \right] \bullet \left[\tilde{p} \right] \right) \quad 28$$

- To satisfy the pressure constraints, $[p_{t+1}]$ is moved uniformly up or down so that the sum of the positive pressures equals to the applied load while the shape of $[p_{t+1}]$ is not changed. Set all negative elements of $[p_{t+1}]$ to zero.
- Increment the index t and repeat the loop until convergence criteria are satisfied, which in the present algorithm occurs when the integral of pressures over contact area is equal to the applied load within 0.5% and all pressures at contacting points are positive and zero elsewhere.

Once the contact pressure distribution is determined it is straight forward to calculate the complete stress fields throughout the three-dimensional domain by convolving the appropriate influence coefficient matrix with the predicted pressure distribution. Once again, the process is made more efficient by completing the convolution in the frequency domain first, before transforming the required stress field back to the spatial domain through the use of inverse FFTs. For a particular stress field, S , and associated influence coefficient matrix, A_s , this can be written as:

$$[S] = FFT^{-2} \left[\tilde{S} \right] = FFT^{-2} \left(\left[\tilde{A}_s \right] \bullet \left[\tilde{p} \right] \right) \quad 29$$

The complete algorithm that implements the above methodology to predict surface pressures and displacements as well as complete stress field in a rough multilayered contact is illustrated in the flowchart of Figure 2.

FFT algorithms have been used by many authors to improve efficiency for general contact solvers [11, 12, 13, 18]. As noted in those works, FFTs can lead to an error, referred to as periodicity error, in predictions when applied to non-periodic functions such as stresses and displacements in a concentrated contact. One way to minimise the periodicity error is to increase the size of the calculation domain to many times the contact size, effectively zero-padding the domain outside the immediate contact area. Polonsky and Keer [20] provide a good analysis of the potential errors when using FFTs in contact analysis and recommend that the calculation domain be 8 times the contact size for an acceptable periodicity error with accuracy on par with that provided by multi-level-multi-integration techniques. Given the efficiency of the present semi-analytical model a large calculation domain can be accommodated without significant increase in computing times, especially given that the FFT algorithm itself is very efficient. Various domain sizes have been implemented from which it was found that for most applications the domain size (in x and y directions) equal to 5 times the nominal contact width provides a good balance between computational efficiency and accuracy.

3 Validation of the Model Predictions

The predictions of the current model were validated against a range of existing analytical and numerical solutions and selection of these comparisons is presented here. The

predictions for influence coefficients were validated against the analytical solution for a square unit pressure acting on a homogenous half space produced by Love [21]. In order to make this comparison possible, the current model was run with the multilayered half space possessing 4 layers but with all layers having identical properties ($E = 207$ GPa and $\nu = 0.3$). Figure 3 plots the three direct stresses, $\sigma_{\eta\eta}$, $\sigma_{\xi\xi}$ and $\sigma_{\gamma\gamma}$ at the origin ($\xi = 0$, $\gamma = 0$) against the depth coordinate η obtained through the current model and Love's solution. Similarly, Figure 4 plots the predictions for the surface normal displacements from the two approaches. A very good agreement between the two predictions is evident in the figures. These comparisons were repeated with multiple configurations of the multilayered half space to ensure the accuracy is not affected by the number of layers or individual layer thicknesses. In all cases, the difference between the present model and Love's analytical solution was below 0.5%.

In addition to the above validation against a homogenous half-space solution, it is obviously desirable to validate the predictions of the model for an actual multilayered half-space where the layers have differing properties. In order to achieve this comparison, an FE model of a large square body with two layers and a substrate was set-up in a commercially available FE package, ABAQUS v6.11. A small square pressure patch was applied in the middle of the surface of this body, with the dimensions of the patch being much smaller than the overall dimensions of the body in order not to violate the half-space assumption. The body was designed to consist of two layers of 5 μm each with the top layer having elastic modulus $E^{(1)} = 621$ GPa and the second layer having elastic modulus $E^{(2)} = 414$ GPa, on top of a substrate with elastic modulus $E^{(s)} = 207$ GPa. All Poisson's ratios were equal to 0.3. The finite element model consisted of a quarter-space with symmetry planes. The model had dimensions of 0.1 mm x 0.1 mm x 0.2 mm using symmetry planes which represented a cubical volume of 0.2 mm x 0.2mm x 0.2mm. A uniform square pressure source of side length 2 μm was applied at the origin. The domain was meshed with Linear Tetrahedral elements. The mesh was designed to be very dense within the layers and near all interfaces, while being less dense in the substrate.

Figure 5 and Figure 6 compare the predictions from this FE solution and the current model for direct stresses $\sigma_{\xi\xi}$ and $\sigma_{\eta\eta}$ respectively. Once again, a very good agreement between the two approaches is evident. Figures also clearly show the discontinuity in the $\sigma_{\xi\xi}$ stress at both interfaces, while the $\sigma_{\eta\eta}$ stress is continuous across the interface as may be expected given the boundary conditions.

Finally, the predictions of the complete model, including the contact solver, for a ball on a multilayered half-space were compared to Hertzian solution for smooth contact, Figure 7, and West and Sayles [22] solution for a rough contact, Figure 8. As above, although the half-space consisted of a number of layers of varying thickness, the material properties of each layer were set to be the same in order to enable the comparisons with the existing models which are only applicable to homogenous bodies. As evident in Figure 7 and Figure 8, the

predictions of the current model for both smooth and rough three-dimensional contacts agree well with the existing solutions.

4 Results and Discussion

The presented model is intended as a tool to help optimise the design of a multilayered coating in terms of contact pressures and areas and subsurface stress fields for given loading, roughness and counter face properties. This should in turn help to ensure that the resulting coating is less likely to suffer failure through mechanisms such as delamination, cracking or fatigue while still offering the intended benefits of reduced wear and/or friction through control of surface pressures and real contact areas. The model allows for studies of the influence of various factors including the number of layers, individual layer elastic properties and layer thicknesses, surface roughness, counter-face properties etc. However, the number of cases that can be studied within the scope of the current paper is obviously limited and the analyses below focus on selected cases which serve to illustrate the capabilities of the model while offering further insight into the effects of selected parameters on the behaviour of multilayered coating systems.

4.1 Case Study on Optimising the Subsurface Stresses Through Coating Design

As discussed in the introduction chapter, the presence of a surface coating can significantly modify the stress fields in the contact, which in turn may lead to failure modes that would not have been expected in an equivalent homogeneous contact. Various studies [3, 23] have for example found that the yield load for a surface with a relatively stiff single-layered coating is lower than that in a homogenous contact made of substrate material alone. Oliveira and Bower [24] present an extensive study of fracture and delamination in single-layered coatings and find that the fracture load can increase or decrease by a factor of 5 due to the mismatch in elastic properties of layer and substrate.

Many practical situations adopt a design where a hard, stiff coating layer is deposited on a more compliant substrate, usually steel. Due to their high hardness such layers generally serve to reduce surface damage such as wear. However, their comparatively high elastic modulus also creates tensile stresses at the coating-substrate interface and within the coating itself [3, 12, 22, 23]. Such tensile stresses are undesirable as they can promote coating failure through fatigue, fracture or delamination. From a practical point of view, it is therefore useful to study how such tensile stresses can be controlled by application of a multilayered coating. The coating system of interest would therefore retain the high stiffness (and hardness) top surface layer to provide low wear, but would now include a varying number of intermediate layers with changeable properties with the aim of reducing or eliminating internal tensile stresses. This section presents a case study of such a system.

For the purpose of the study, the overall thickness of the coating was fixed at 12 μm and the applied load and counter face properties were kept constant, while four different

multilayered systems were studied: homogenous case, a single layered, a two layered and a four layered case where the intermediate layers possess gradually changing elastic modulus. The four cases studied are illustrated in Figure 9 including material properties of all layers and the loading conditions. Ideally smooth surfaces are modelled in all cases so that roughness effects do not obscure the effects of layer properties. A mesh of 1024 x 1024 elements in x-y plane was used while 30 points were used in the depth direction, z, resulting in the z resolution of 0.5 μm

In all cases the substrate is given the properties of steel ($E^{(s)} = 207 \text{ GPa}$) and the elastic modulus of the very top layer is kept constant at $E^{(1)} = 621 \text{ GPa}$, highest of all layers present. The chosen multilayered structures then represent the situation where the material properties of the top stiff layer do not change but the intermediate layers are introduced with elastic moduli in between the compliant substrate and the stiff top layer so that the elastic mismatch at each interface is moderated even though the total coating thickness is unchanged and the benefits of the top hard layer are maintained.

Figure 10 shows the contact pressure distribution for all four cases. As may intuitively be expected, given that all layers are stiffer than substrate, all coating systems produce higher maximum contact pressure and the correspondingly lower contact area than the homogeneous case. From the practical point of view, the reduced contact area would help to reduce overall contact friction while the very hard coating would help reduce surface wear. In a coated system, the extent of deviation in maximum pressure and contact area from those predicted for a homogenous case depends on the ratio of the thickness of the coating to the contact radius as this determines whether the coating, substrate or combined properties play the dominant role in contact mechanics. For these contact conditions all three multilayered systems produce very similar maximum pressure and correspondingly reduced contact area. The ratio of the top layer thickness to the contact radius in the 3 coated cases studied varies between 0.07 and 0.25 and it seems that throughout this range it is the properties of the top layer (where elastic modulus is always $E^{(1)} = 621 \text{ GPa}$) that largely determine the contact pressures in the current set-up.

Figure 11 shows contour plots of the σ_{xx} direct stress in the plane $y=0$ for all four cases studied. For homogenous case (Figure 11a), σ_{xx} is compressive throughout the domain without any discontinuities as may be expected. For a single layered case (Figure 11b) the modifications to the stress field due to the presence of the coating are very apparent. The region of compressive σ_{xx} stress has now been reduced but more significantly, tensile stresses are introduced in the coating near the coating-substrate interface and at the interface itself ($z = 12 \mu\text{m}$). The reason for occurrence of tensile stresses is that upon loading the relatively more compliant substrate ($E^{(s)} = 207 \text{ GPa}$) induces tensile forces on the stiffer coating ($E^{(1)} = 621 \text{ GPa}$) above it through the rigidly bonded interface. In this example the tensile stress is caused by a mismatch in the elastic moduli but similar situation may be expected to arise for the mismatch in the Poisson's ratio [24].

The present model allows us to study how these tensile stresses may be affected by the presence of intermediate layers in multilayered coating. To this effect, Figure 11c shows the contours of the σ_{xx} for Case 3 where there are two coating layers present, each with 6 μm thickness. The very stiff top layer has been retained but an intermediate layer with intermediate stiffness ($E^{(2)} = 414 \text{ GPa}$) has now been introduced. The results show that the magnitude of the tensile stress at the lowest interface ($z = 12 \mu\text{m}$) has now been reduced and no new tensile stresses at the other interfaces are introduced. Finally, Figure 11d illustrates the case with four coating layers where the layers have gradually reducing stiffness from the same top layer with $E^{(1)} = 621 \text{ GPa}$, then $E^{(2)} = 517 \text{ GPa}$, $E^{(3)} = 414 \text{ GPa}$, $E^{(4)} = 310 \text{ GPa}$ down to the substrate where $E^{(s)} = 207 \text{ GPa}$ as before. The results show that despite the fact that the overall coating thickness and the properties of the top stiff layer and the compliant substrate have remained unchanged, the tensile stresses that were present in a single coating case have now been completely eliminated. This result suggests that this particular four-layered design of the coating may offer all the advantages of the single-layered hard surface coating as intended, while eliminating the risk of failure through unwanted tensile stresses in the subsurface.

Coatings are often used in applications where liquid lubrication is unsatisfactory. Consequently, coated contacts are commonly subjected to significant frictional forces. In order to establish whether the general trends provided by the above study, where only the normal load was considered, is also valid in the presence of friction, the same four cases were analysed with an additional tangential load due to friction coefficient of 0.2. Figure 12 presents the contour plots of σ_{xx} stress that are equivalent to those shown in Figure 11 but now include the additional tangential load. As may be expected, the results indicate that friction produces a region of tensile stress at the trailing edge of the contact for all four cases analysed including the homogenous contact. In addition, tensile stresses in the coating due to elastic mismatch are still present. The results in Figure 12 confirm that the effect of chosen intermediate layers on the magnitude of the tensile stress near the coating-substrate interface is similar in this case as that observed for the normal load only i.e. the tensile stresses that are introduced by a stiff layer on a compliant substrate in a single-layered system are again eliminated in the four-layered system.

These results indicate that for stiff coatings under normal and tangential load there are two competing areas of tensile stresses, one at the trailing edge near the surface due to friction and the other nearer the coating-substrate interface due to elastic mismatch. Which of these stresses would be more likely to cause the first failure depends on their relative magnitudes, and this would change for different coating designs and friction coefficients. Oliveira and Bower [22] provide results to indicate the influence of coating properties on the magnitude of the contact pressure that would be expected to cause coating fracture from an existing short crack as well as whether such fracture would occur at the surface or in the subsurface region. Although their results are for single-layered coatings only, it is interesting to attempt to relate them to the results shown here. To describe the elastic

mismatch between the coating and the substrate Oliveira and Bower use Dundurs' parameters, α_D and β_D . Dundurs' parameters are defined for a single layered coating as a function of elastic modulus and Poisson's ratio of the two materials (see nomenclature for definition). Definitions are such that for all material combinations $|\alpha_D| \leq 1$ and $|\beta_D| \leq 0.5$ and for a layer stiffer than the substrate $\alpha_D > 0$.

Unfortunately, Dundurs' parameters cannot be calculated for a multilayered coating. In order to make rough comparisons with Oliveira and Bower's data, the value of the 'local' Dundurs' parameters at the last interface ($z = 12 \mu\text{m}$) will be used here, that is the quoted values of α_D and β_D are worked out by using the elastic properties of the substrate and the layer immediately adjacent to it. This seems a sensible approach given that any tensile stresses of interest are present near this particular interface in the presented examples (Figure 11 and Figure 12). Using this convention, α_D is 0.5, 0.33 and 0.2 for Cases 2, 3 and 4 respectively. Given the Poisson's ratio of 0.3 used here, $\beta_D = \alpha_D/3.5$ in all cases. This is not too dissimilar from $\beta_D = 3$ used by Oliveira and Bower. However, it must be stressed that due to the differences in the two studies, any comparison between the results can only be considered as a rough guide to the apparent trends.

Considering Oliveira and Bower's results for the normalised coating thickness (h/a_{Hertz}) of 0.27, which is the total coating thickness studied here (total thickness = $12 \mu\text{m}$, $a_{\text{Hertz}} = 44 \mu\text{m}$): for frictionless contact at $\alpha_D = 0.5$ Oliveira and Bower predict that coating fracture will occur in the subsurface and that the contact pressure needed to cause fracture is reduced by a factor of about 2 to 3 compared to a homogenous case, whereas for $\alpha_D = 0.2$ no significant change in pressure for fracture is predicted. These general trends seem to be in line with the trends in current predictions for σ_{xx} for frictionless contact, where for $\alpha_D = 0.5$ (Case 2, Figure 11b) significant tensile stresses exist in the subsurface, while for $\alpha_D = 0.2$ (Case 4, Figure 11d) no tensile stresses are observed and therefore no increased likelihood of coating fracture is expected.

For a friction coefficient of 0.1, and $\alpha_D = 0.5$ Oliveira and Bower predict no significant change in fracture pressure, while this point lies very near their boundary between surface and subsurface coating fracture. For $\alpha_D = 0.2$, they predict that the presence of a stiff coating actually slightly increases the fracture pressure and surface fracture is predicted. The results presented in Figure 12 here, although they are for friction coefficient of 0.2 (Olivier and Bower do not present results for friction coefficient of 0.2), reveal similar trends: For $\alpha_D = 0.5$ (Case 2, Figure 12b) tensile stresses of similar magnitude exist both at surface and subsurface while the magnitudes of tensile stresses in coated and homogenous contacts are very similar – this is in line with Oliveira and Bower prediction that failure could be initiated at either location and that there is no significant change in fracture pressure. For $\alpha_D = 0.2$ (Case 4, Figure 12d) on the other hand, tensile stresses exist only at the surface (Figure 12a) – in line with Oliveira and Bower's prediction of surface initiated fracture.

The analysis presented above intentionally used ideally smooth surfaces so that the effects of the coating layers are not hidden by the effects of any surface roughness characteristics. However, in many practical applications it is necessary to consider the interaction of coating parameters (particularly layer thickness) in relation to surface roughness. In the cases illustrated in Figure 11 and Figure 12, the stress concentrations at the coating-substrate interface ($z = 12 \mu\text{m}$) are the result of the overall (macro-) contact stress field. In the presence of roughness, each asperity micro-contact creates a micro-stress field that is situated much nearer to the surface, and therefore there could be significant interactions of these shallower stress fields and any coating interfaces that happen to lie in the vicinity. This effect was studied by Kadiric and Sayles [25] for a single layered coating. To illustrate this in the current example, the four layered problem of the study above (Case 4 in Figure 9) is analysed again but now in presence of a roughness profile. Figure 13 shows the predicted pressure distribution for this contact, while Figure 14 shows the contours of the predicted σ_{zz} stress in this case. It is evident that the maximum asperity contact pressure in the rough contact is about four times the maximum Hertz pressure in the equivalent smooth contact. But more importantly, Figure 14 shows that asperity micro-contacts cause local stress concentrations to the depth reaching the second layer interface at $6 \mu\text{m}$. Such stress concentrations at the interface are obviously undesirable and may lead to premature coating failure. This simple example illustrates that in a real rough layered contact, consideration should be given to both the macro stress fields caused by elastic mismatch between the coating layers as well as the interaction of layer interfaces with micro stress concentrations caused by asperity contacts. In reality, due to the random features in the roughness structure it is difficult to provide general guidelines for the effect of roughness on the performance of coatings and each case of interest should ideally be analysed in a similar manner as that presented in Figures 13 and 14 before suggesting an optimum multilayered coating system for given roughness and loading conditions.

4.2 Parametric Study of the Influence of Layer Properties on Subsurface Stresses

The case study presented in the previous section indicated the significant influence that the layer properties may have on the subsurface σ_{xx} stress distribution and consequently on the overall performance of the multilayered coating. This section will attempt to obtain some general trends in this respect that may be useful to engineers choosing an appropriate coating for their application. Given the number of variables in a multi-layered contact that can be studied, the present analysis must inevitably impose some constraints on the coating system to be studied. The intention here is to offer some insight in how a multilayered structure may help to optimise the stress distribution within a fixed total thickness of a relatively stiff coating. These limitations are often present in practice where the dimensional tolerances of the component may restrict the total thickness of the coating that can be applied, while stiff, hard coatings are often used for wear and friction control. The chosen system is illustrated in Figure 15. It consists of a multilayered half-space with two relatively stiff layers on a steel substrate; The elastic moduli of the top layer and the substrate are

kept constant while that of the intermediate (2nd) layer is varied; Poisson's ratio is 0.3 for all materials; The position of the second interface is fixed at $\eta = (h^{(1)} + h^{(2)}) / l = 1$ (i.e. the total coating thickness is fixed), while the position of the first interface is varied; The half-space is subjected to a uniform pressure over a square patch of width $2l$ located at the origin, i.e. surface pressure distribution is kept constant in all cases rather than the applied load. This approach was chosen in order to make the relative comparisons between the resulting subsurface stresses more realistic – if the load was fixed the actual contact pressure would change with the coating design (stiffer coating would increase the pressure and reduce the contact area while the more compliant coatings would have the opposite effect).

This set-up allows for analysis of the influence of the position of the intermediate interface and properties of the intermediate layer on the subsurface stress distribution, with all other parameters being constant. Since the direct stress in x direction, σ_{xx} was shown to be important for the performance of layered system the study will once again focus on the magnitude of this stress.

Figure 16 shows the trend in σ_{xx} stress at the first layer interface ($z = h^{(1)}$) and $x = y = 0$ for all studied combinations of elastic modulus of the intermediate layer, $E^{(2)}$, and position of the first interface, $h^{(1)}$. The results are plotted in terms of ratio $E^{(1)} / E^{(2)}$ and $E^{(2)} / E^{(s)}$ and normalised thickness of first layer, $h^{(1)} / l$. It is evident that when the thickness of the first layer is $h^{(1)} / l = 0.4$, the σ_{xx} stresses at the first interface are compressive for all combinations of $E^{(1)} / E^{(2)}$ studied. For the case of $h^{(1)} / l = 0.6$, tensile stresses occur only for relatively large elastic mismatch between the two layers, $E^{(1)} / E^{(2)} > 1.5$, and their magnitude grows as the elastic mismatch increases. Finally, for the thickest first layer ($h^{(1)} / l = 0.8$) first interface experiences tensile stresses for all considered combinations of $E^{(1)} / E^{(2)}$.

Figure 17 shows the values of σ_{xx} stress at the second interface ($\eta = 1$) for all studied cases. It is apparent that σ_{xx} stress at this position is almost always tensile and that the thickness of the first layer has no influence on the magnitude of this stress. The elastic mismatch at this interface, $E^{(2)} / E^{(s)}$, on the other hand has a large influence with the magnitude of tensile stresses increasing with increasing mismatch.

The values of 'local' Dundurs' parameters at this interface are $\alpha_D = 0, 0.2, 0.33, 0.43$ and 0.5 for cases studied while $\beta_D = \alpha_D / 3.5$. From Figure 17 it is evident that tensile stress exist for $E^{(2)} / E^{(s)} > 1.5$ corresponding to α_D greater than about 0.2 . Using these local values of Dundur's parameters the results can once again be compared to the analysis of Oliveira and Bower [22] in a manner described in the previous section. Oliveira and Bower results for the coating thickness of $h / l = 1$ suggest that the contact pressure which would be expected to cause subsurface fracture is only significantly reduced in a coated contact relative to a homogenous contact, when α_D is greater than about 0.3 . This is supported by the current results where significant tensile stresses exist at the interface only for $\alpha_D > 0.2$. As noted

above, Oliveira and Bower's analysis was for a frictionless, single-layered, Hertzian line contact and therefore the comparison provided here should be treated with caution.

The presented results suggest that the elastic mismatch at the lower interface can have a significant influence on the σ_{xx} stress at the interface above. This influence increases as the distance between the two interfaces reduces. For example, interfacial σ_{xx} stress for $h^{(1)} / l = 0.8$ is tensile for all values of $E^{(2)}$ studied i.e. even when there is no elastic mismatch between first and second layer (case of $E^{(1)} / E^{(2)} = 1$) as shown in Figure 16. This suggests that the tensile stress here was purely caused by the presence of tensile stress zone at the lower interface. On the other hand for $h^{(1)} / l = 0.4$ the stresses are always compressive for all values of $E^{(1)} / E^{(2)}$ used here, suggesting that at this shallower depth, the first interface is sufficiently removed from the tensile stress zone of the second interface for its effect to be insignificant. Conversely, the stress at the second interface (Figure 17) is not affected by the depth of first interface at all, rather the magnitude of σ_{xx} here is largely determined by the 'local' elastic mismatch at this interface, being most tensile for $E^{(2)} / E^{(s)} = 3$ and compressive for $E^{(2)} / E^{(s)} = 1$.

Therefore, from practical point of view, within the range of values of E and h considered here, the behaviour of the last interface in a multilayered coating can to large extent be determined by considering the local elastic mismatch at this interface alone, while the behaviour of the intermediate interface can only be determined by considering not only the local elastic mismatch but the also the relative position of the two interfaces.

5 Conclusion

This paper presents a new three dimensional model for non-conformal contacts of multilayered rough surfaces subject to normal and tangential surface loads. Contacting bodies are assumed to be elastic half-spaces consisting of any number of individual layers that are rigidly bonded at all interfaces. Material properties within each layer are assumed to be homogenous and the thickness of each layer is assumed uniform. The model is capable of dealing with real measured roughnesses and arbitrary contact geometry provided the half-space assumption remains valid. Model inputs consist of the geometry of the contacting bodies, normal load, friction coefficient and elastic properties of all layers. The model predicts contact pressures, real areas of contact and the complete subsurface stress field. The model algorithm is based on the influence coefficients approach. For improved efficiency, a semi-analytical approach is adopted where the influence coefficients for all displacements and stresses are obtained by first solving the fundamental differential equations analytically in frequency domain through use of continuous Fourier transforms. These solutions are then transformed back to spatial domain by application of Fast Fourier Transform algorithm. The solution for contact pressures is obtained through an iterative scheme based on conjugate gradient method.

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4 The model predictions are validated firstly against a range of existing analytical solutions for
5 homogenous contacts by assigning identical properties for each layer in a considered
6 multilayered half space, and secondly, against a finite element predictions for a multilayered
7 body.
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10 Through its ability to predict contact stress fields, the model offers a tool for analysis and
11 optimisation of multilayered coating systems that can help coating designers maximise the
12 potential benefits offered by multilayered coatings while minimising the risk of coating
13 failure.
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16 Results are presented to illustrate important aspects of sub-surface stress distribution in a
17 multilayered contact. In particular, it is shown how subsurface tensile stresses that can be
18 created, even under pure normal load, by a stiff single-layered coating on a more compliant
19 substrate, can be minimised by the application of a suitable multilayered coating while still
20 retaining the benefits provided by the same stiff top layer on the chosen substrate. Finally,
21 selected results are presented to indicate trends in subsurface tensile stresses in an example
22 two-layer coating system, where the overall coating thickness and the properties of top
23 layer and substrate are fixed, while the elastic properties and the thickness of the
24 intermediate layer are varied. The results indicate that the elastic mismatch at layer
25 interfaces, as well as the relative position of interfaces in a multilayered coating plays an
26 important role in determining the subsurface stresses. It is shown that the behaviour of
27 stresses at the deepest interface is largely determined by the local mismatch in the elastic
28 properties at this interface while the stress behaviour at the intermediate interface is
29 influenced not only by the local mismatch in elastic properties at this interface but also its
30 proximity to, and conditions at, the interface below it.
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Appendix

Obtaining the Fourier transform of unit square pressure ($p = 1$) acting over a square patch

$|\xi| \leq 1$ and $|\gamma| \leq 1$ at the origin as used in Equations 17 and 18

$$\tilde{\tilde{p}} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (p e^{-is\xi} e^{-ir\gamma}) d\xi d\gamma = \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} p e^{-is\xi} d\xi \right) e^{-ir\gamma} d\gamma \quad A1$$

By definition $p = 1$ for $|\xi| \leq 1$ and $|\gamma| \leq 1$ otherwise $p = 0$, so:

$$\begin{aligned} \tilde{\tilde{p}} &= \int_{-1}^1 \left(\int_{-1}^1 1 e^{-is\xi} d\xi \right) e^{-ir\gamma} d\gamma = \int_{-1}^1 \left[\frac{e^{-is\xi}}{-is} \right]_{-1}^1 e^{-ir\gamma} d\gamma = \int_{-1}^1 \frac{1}{is} (e^{is} - e^{-is}) e^{-ir\gamma} d\gamma \\ &= \frac{1}{is} (e^{is} - e^{-is}) \left[\frac{e^{-ir\gamma}}{-ir} \right]_{-1}^1 = \frac{1}{is} \frac{1}{ir} (e^{is} - e^{-is}) (e^{ir} - e^{-ir}) \\ &= -\frac{1}{sr} (e^{is} - e^{-is}) (e^{ir} - e^{-ir}) \end{aligned} \quad A2$$

Given that $\sinh(x) = \frac{1}{2}(e^x - e^{-x})$ and substituting in Equation A2:

$$\tilde{\tilde{p}} = -\frac{1}{sr} (2\sinh(is) 2\sinh(ir)) = -\frac{4}{sr} \sinh(is) \sinh(ir) \quad A3$$

Finally, substituting $\sinh(ix) = i \sin(x)$ into Equation A3:

$$\tilde{\tilde{p}} = -\frac{4}{sr} i \sin(s) i \sin(r) = \frac{4}{sr} \sin(s) \sin(r) \quad A4$$

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Figure 2. Flow chart illustrating the basic steps of the complete algorithm implemented in the current model to predict contact pressures and sub-surface stress fields in a rough, multilayered contact.

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Figure 5. Comparison of direct stress $\sigma_{\xi\xi}$, along the line $\xi = \gamma = 0$ from the FE solution and the current model for a uniform square pressure patch ($p = 1\text{GPa}$) of size $2l \times 2l$ acting at the origin of half space made up of two $5 \mu\text{m}$ thick layers ($E^{(1)} = 621$, $E^{(2)} = 414$ and $\nu = 0.3$) on an infinitely thick substrate ($E^{(s)} = 207 \text{ GPa}$ and $\nu^{(s)} = 0.3$)

Figure 6. Comparison of direct stress $\sigma_{\eta\eta}$, along the line $\xi = \gamma = 0$ from the FE solution and the current model for a uniform square pressure patch ($p = 1\text{GPa}$) of size $2l \times 2l$ acting at the origin of half space made up of two $5 \mu\text{m}$ thick layers ($E^{(1)} = 414$, $E^{(2)} = 207$ and $\nu = 0.3$) on an infinitely thick substrate ($E^{(s)} = 207 \text{ GPa}$ and $\nu^{(s)} = 0.3$)

Figure 7. Comparisons of predictions for surface displacements ($W_{\eta=0}$) and pressures (p) obtained with the current model with those from a Hertzian solution for a rigid ball on an elastic flat contact. The multilayered model was run with all layers having identical properties. (Ball radius = 5 mm, Load = 5 N, $E = 207$ GPa, $\nu = 0.3$)

Figure 8. Comparisons of predictions for surface geometry and pressures obtained with the current model with those obtained using West and Sayles ('W&S' in the legend) [22] model for a smooth rigid ball on an elastic rough half-space. The multilayered model was run with all layers having identical properties. (Ball radius = 5 mm, Load = 5 N, $E = 207$ GPa, $\nu = 0.3$)

Figure 9. Multilayered coating properties for the four cases simulated. In all cases the total layer thickness is 12 μm , Load (L) = 5 N, the counter face is a rigid ball of radius 5 mm, $\nu = 0.3$ for all materials, and all surfaces are assumed to be ideally smooth. Under these conditions the maximum Hertz pressure for a homogenous body (Case 1) is $P_{Hertz} = 1.255$ GPa.

Figure 10. Predicted contact pressure distributions (along $y = 0$) for the 4 cases studied. Contact conditions and coating properties as indicated in Figure 9. Pressures have been normalized by the maximum Hertz pressure for a homogenous contact (case 1), P_{Hertz} .

Figure 11. Contours of σ_{xx} stress in the plane $y = 0$ for the 4 cases studied. Contact conditions and coating properties as indicated in Figure 10 a) Case 1 (homogenous contact); b) Case 2 (single-layered contact); c) Case 3 (two-layered contact); and d) Case 4 (four-layered contact). All stresses have been normalized by the maximum Hertz pressure for a homogenous contact (case 1), P_{Hertz} . Red lines indicate layer interfaces while the elastic modulus of each layer is also indicated in the figure.

Figure 12. Contours of σ_{xx} stress in the plane $y = 0$ for the 4 cases studied with normal and tangential surface loading. Contact conditions and coating properties as indicated in Figure 10 plus friction coefficient of 0.2. a) Case 1 (homogenous contact), b) Case 2 (single-layered contact), c) Case 3 (two-layered contact) and d) Case 4 (four-layered contact). All stresses have been normalised by the maximum Hertz pressure for a homogenous contact (Case 1), P_{Hertz} . Red lines indicate layer interfaces and the elastic modulus of each layer is also indicated in the figure.

Figure 13. Contact pressure in an example rough contact of a rigid ball and a four-layered half space with properties listed in Case 4 of Figure 9. Applied load = 5 N, ball radius = 10mm; All pressures normalized by maximum Hertz pressure for equivalent smooth homogenous contact ($P_{Hertz} = 0.79$ GPa).

Figure 14. Contours of direct stress σ_{zz} in an example rough contact of a rigid ball and a four-layered half space with properties listed in Case 4 of Figure 9. Corresponding contact pressure distribution shown in Figure 13. Applied load = 5 N, ball radius = 10mm; All stresses normalized by maximum Hertz pressure for equivalent smooth homogenous contact ($P_{Hertz} = 0.79$ GPa).

Figure 15. Contact set-up used for the study of the effects of intermediate layer properties and thickness on the sub-surface stresses in a multilayered half-space consisting of two layers and a substrate. Top layer and substrate have fixed elastic properties as indicated. Total thickness of the coating (position of the second interface) is fixed at $\eta = 1$. A uniform square pressure source of magnitude 1 GPa is applied over area $2l \times 2l$ at the origin in all cases. The elastic modulus of the 2nd layer and the position of the first interface are varied between the values indicated.

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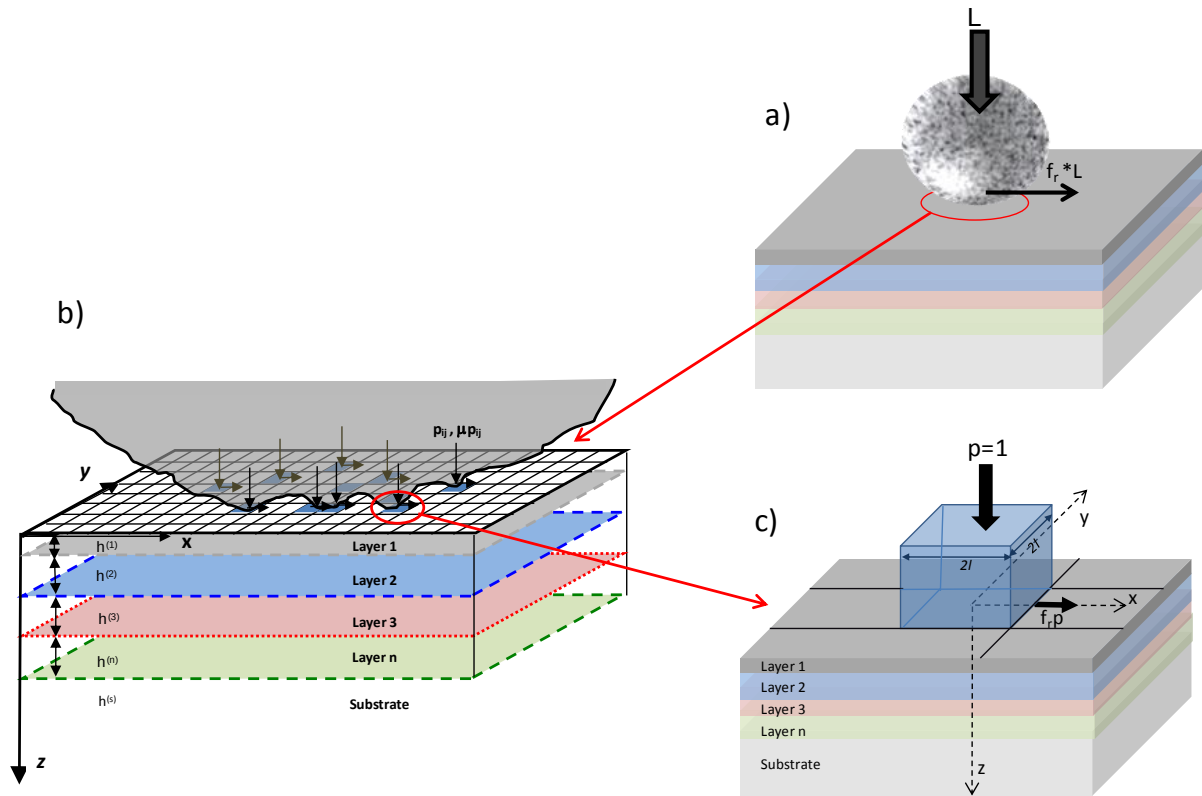


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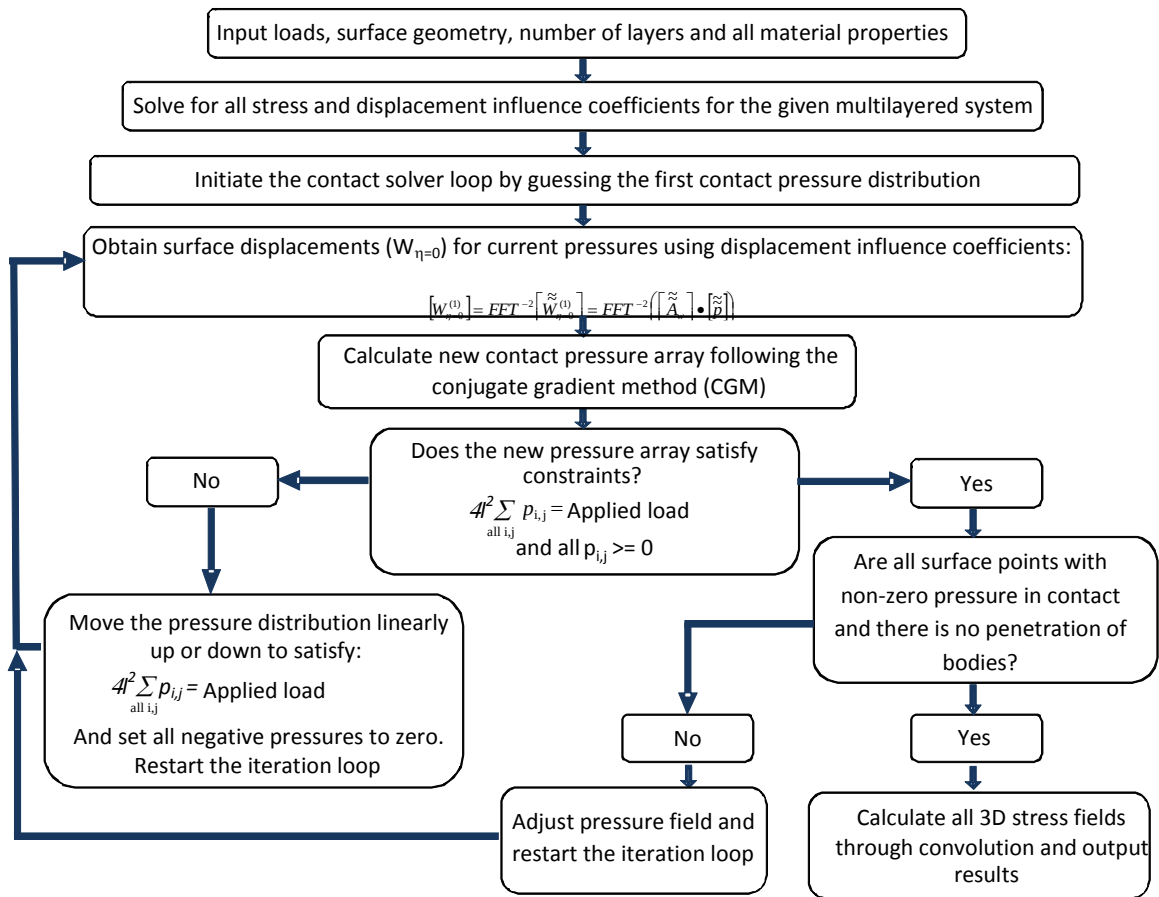


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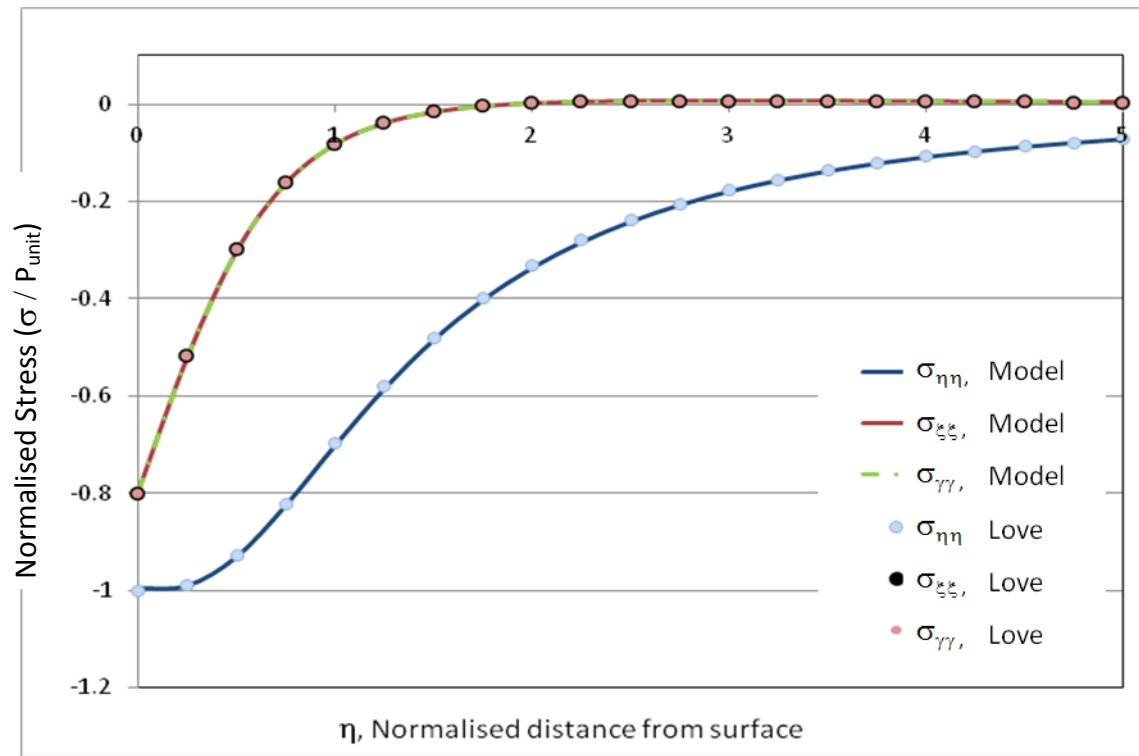


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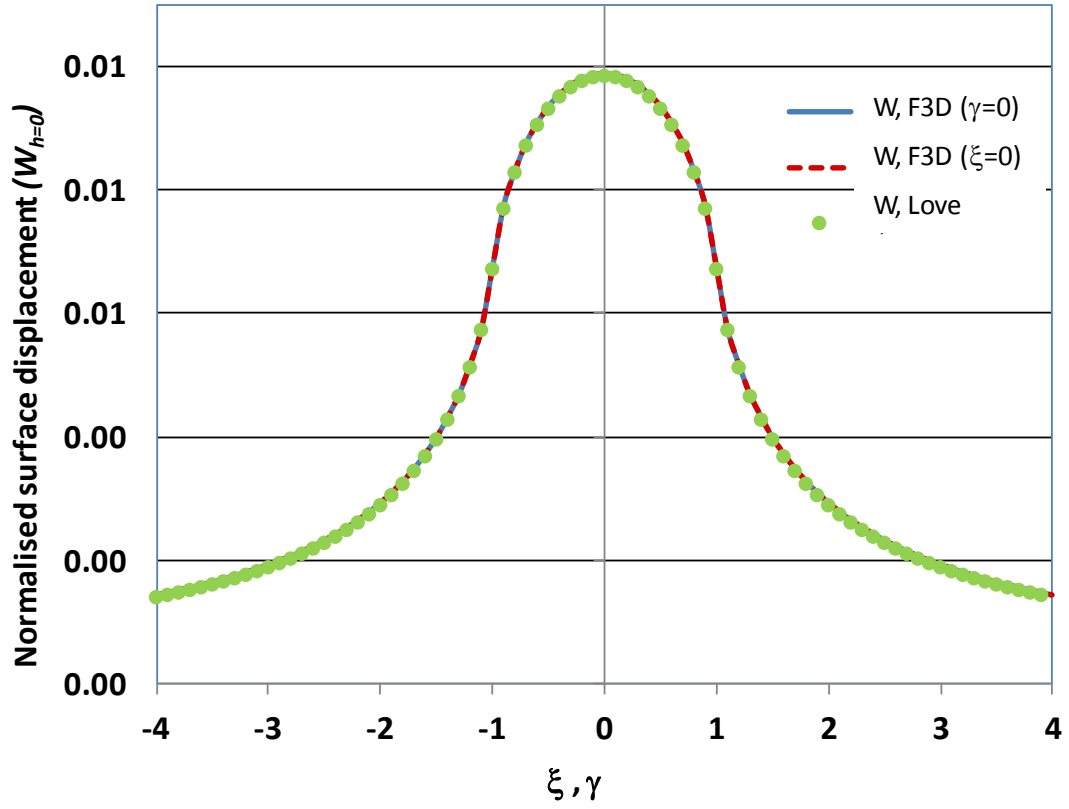


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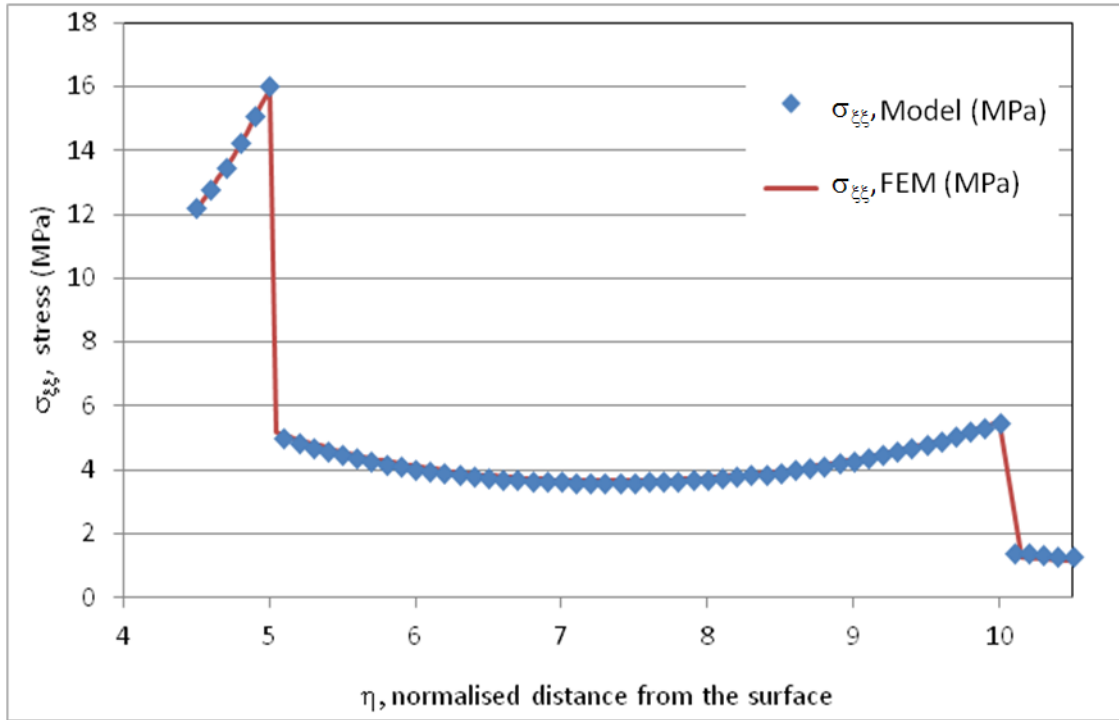


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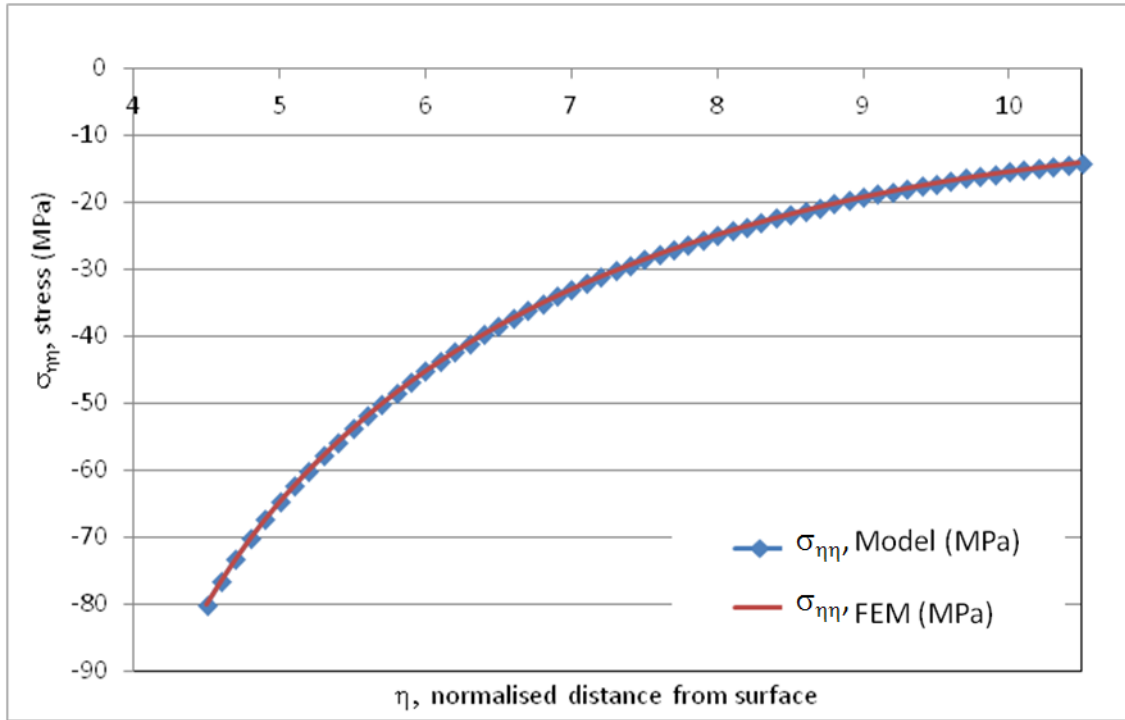


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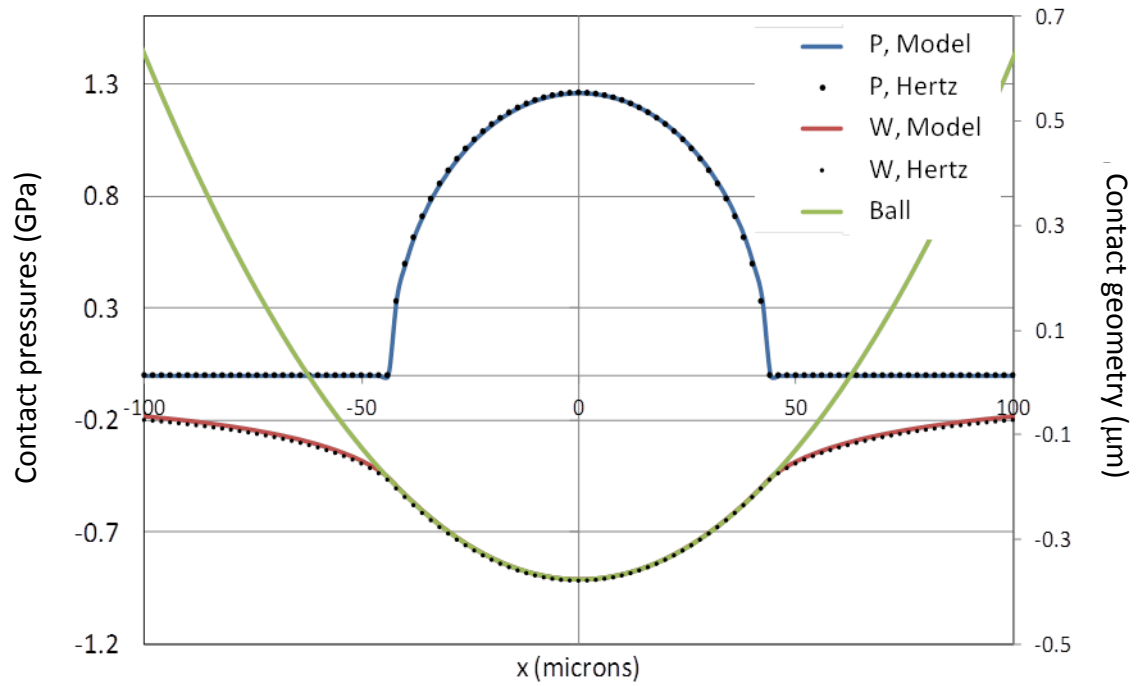


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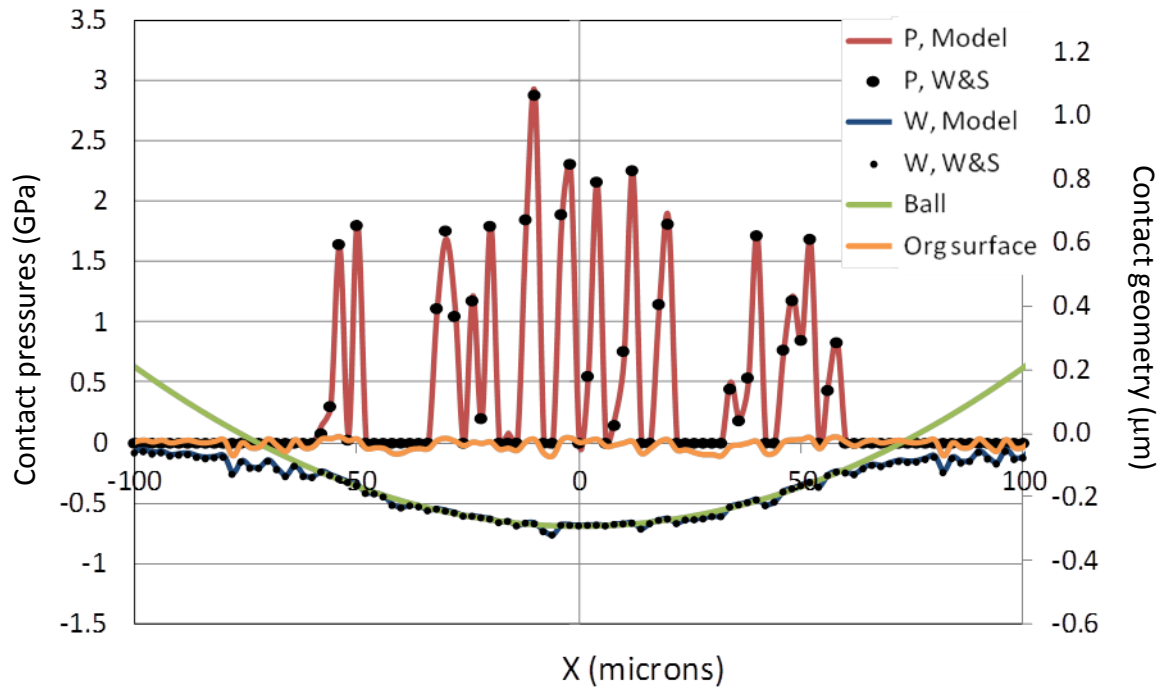


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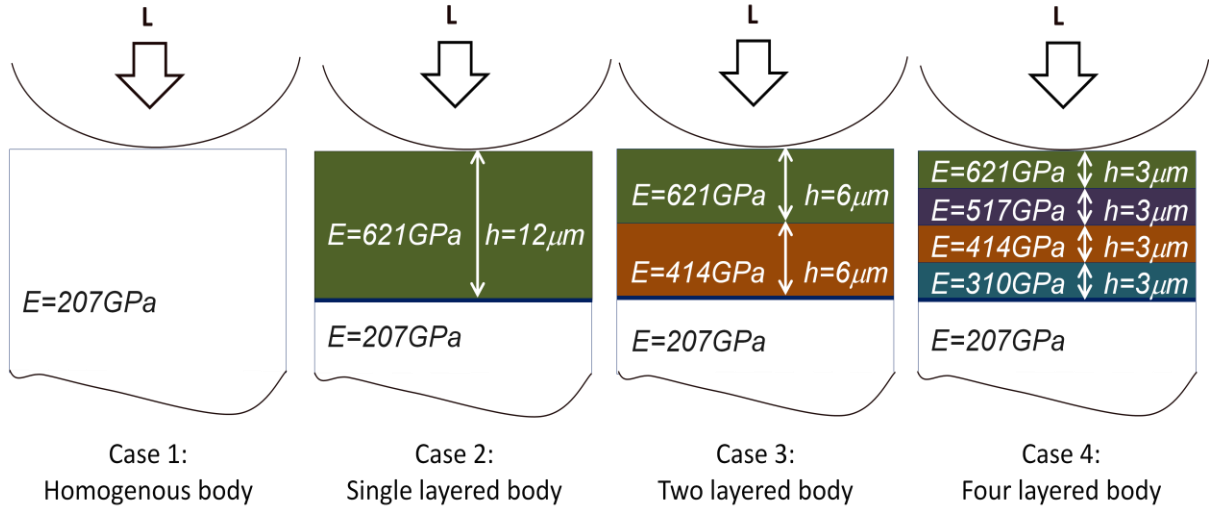


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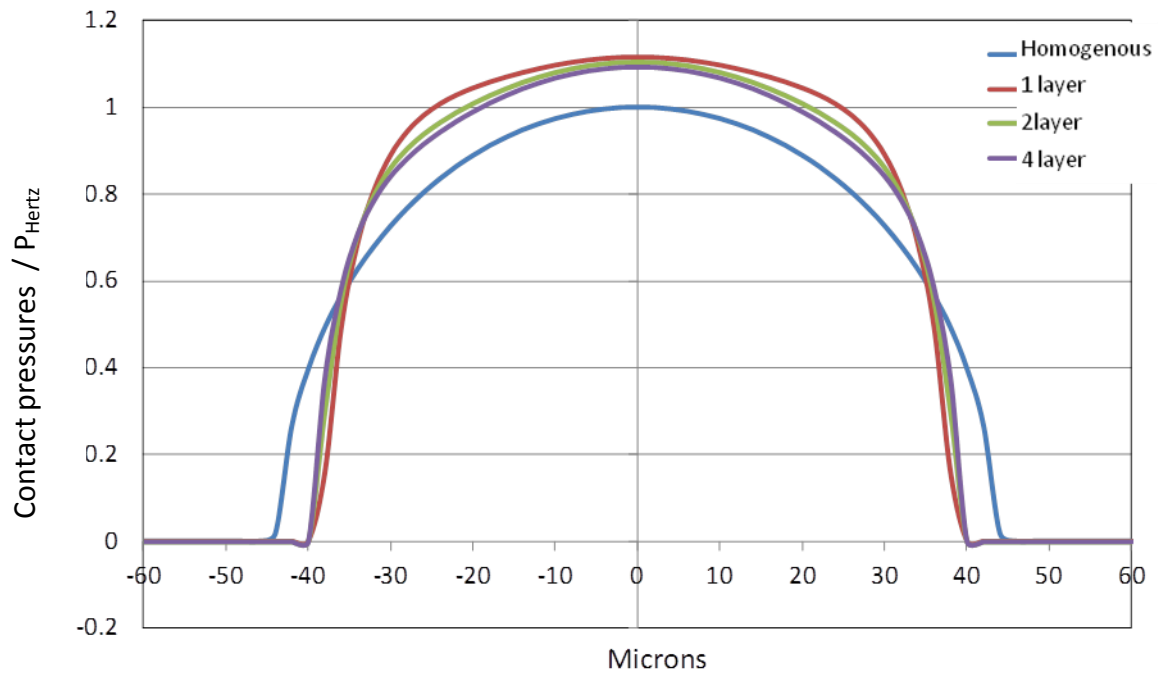


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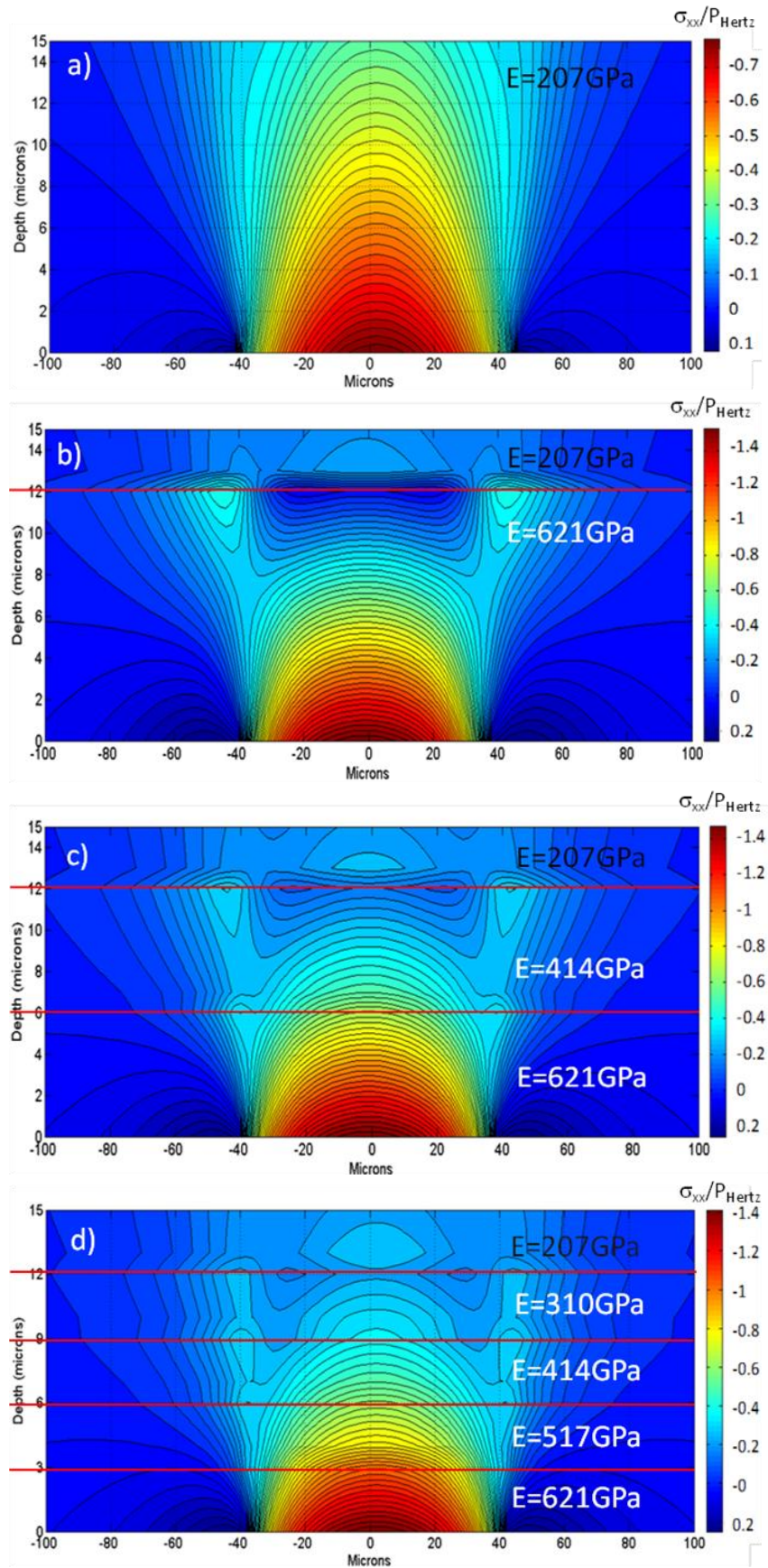


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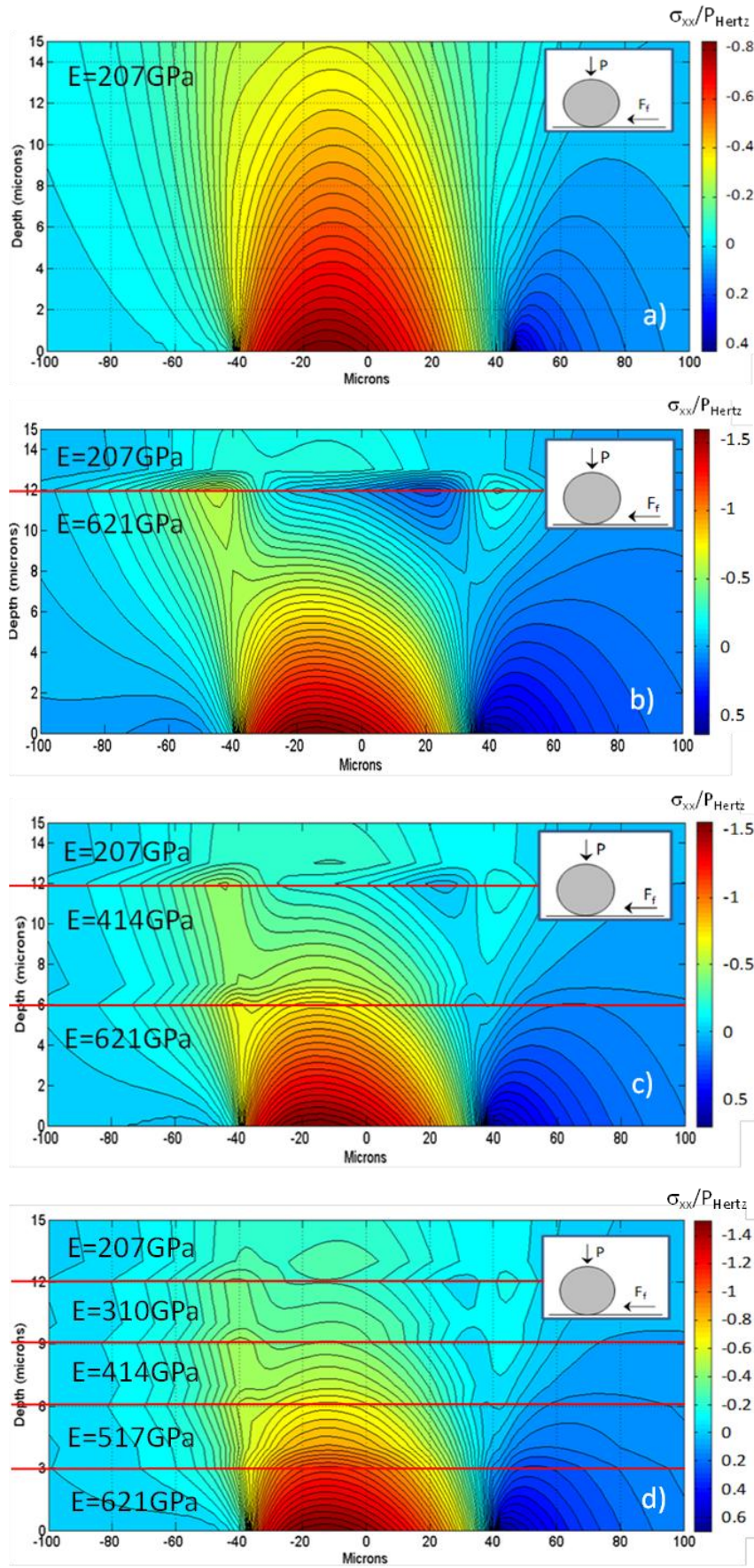


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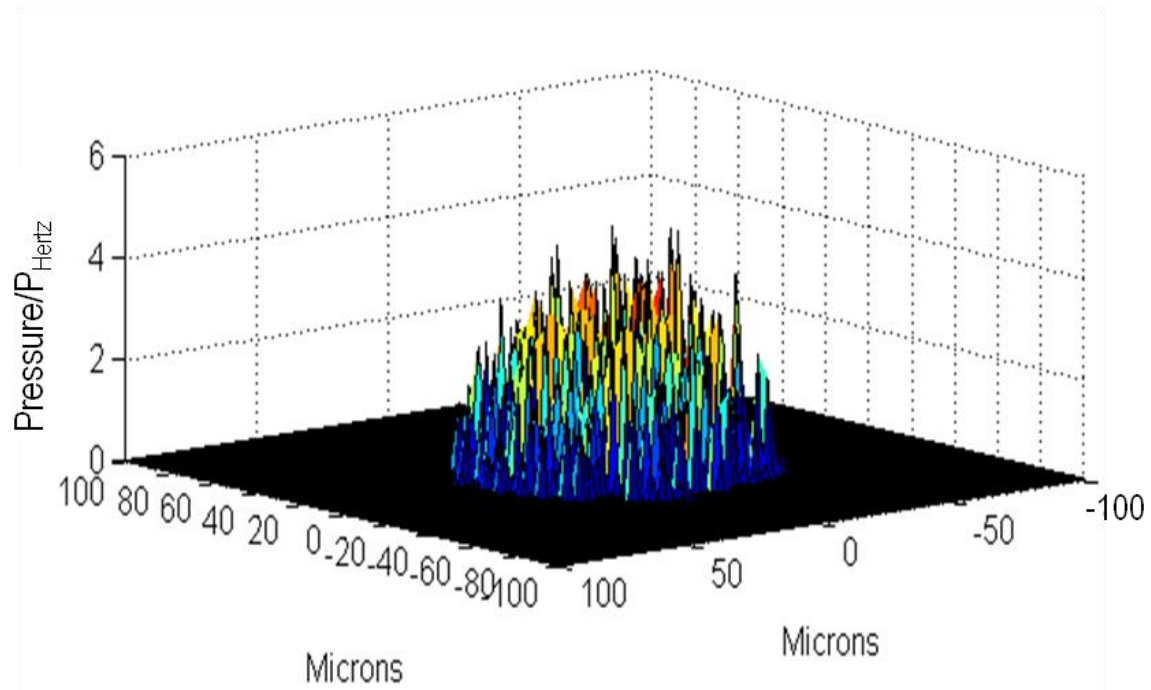


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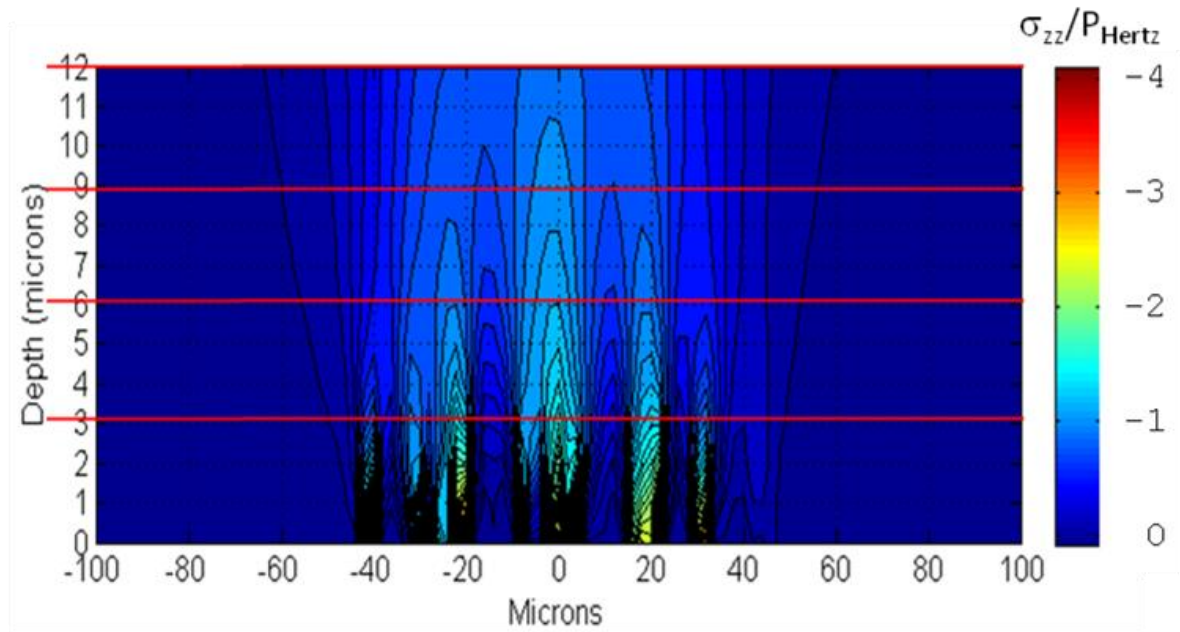


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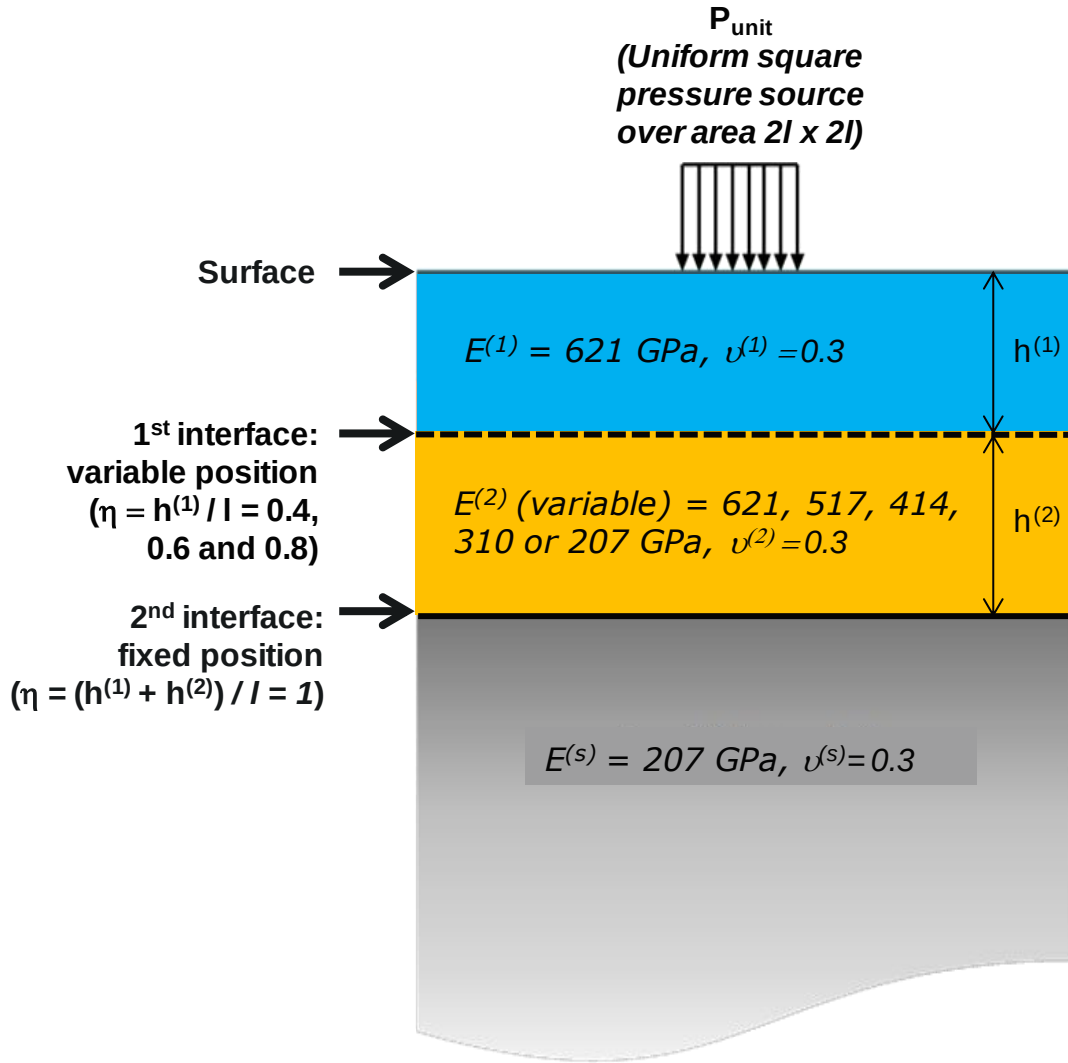


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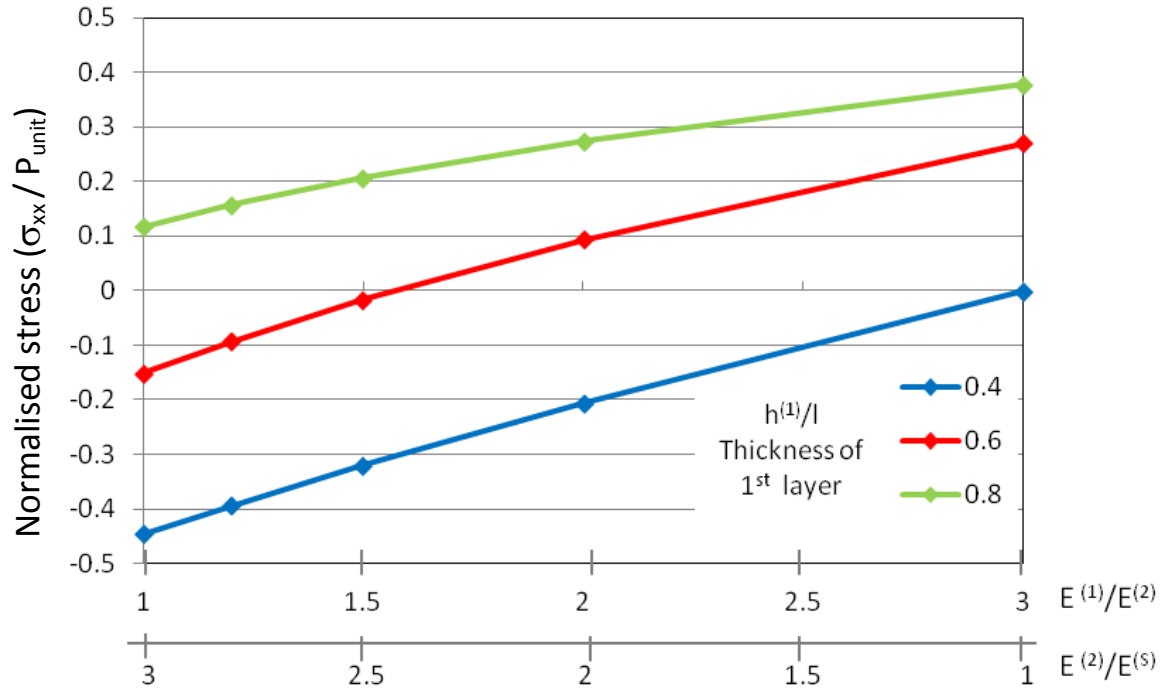


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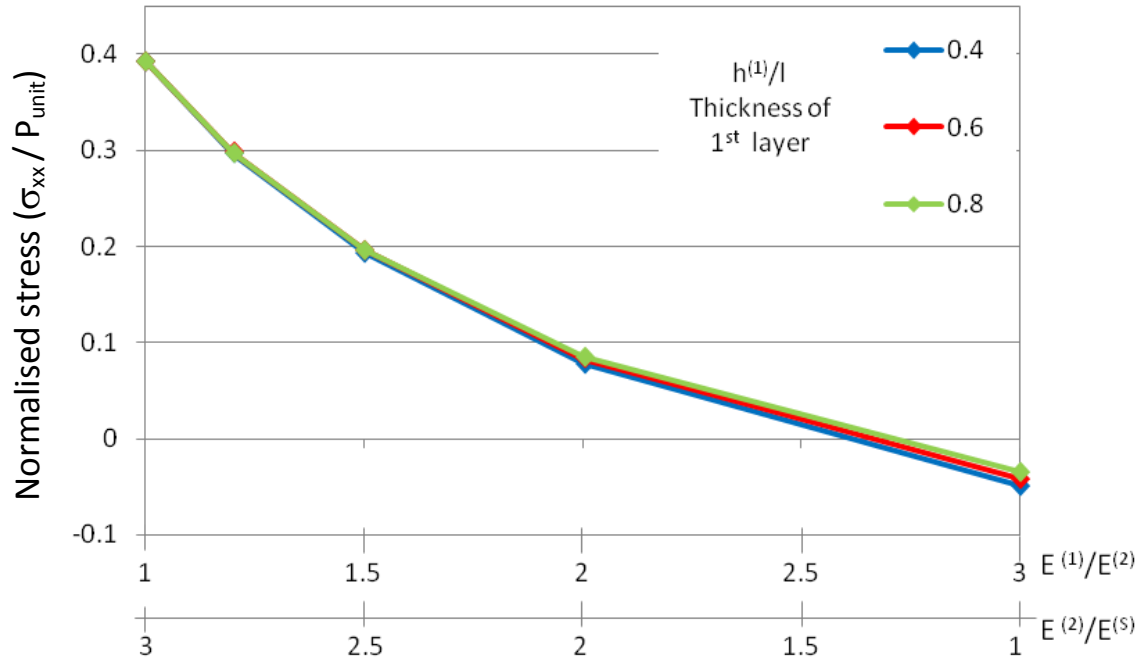


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