ORIGINAL RESEARCH PAPER Characterising of internal stresses in duplex coating by FEM

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The internal stresses in a duplex coating involving a prequenched layer are believed to change if it is exposed to thermal loading. To characterise the internal stresses in such a duplex coating, a gradient model of finite element method is set up. The initial stress within the substrate developed in as quenching and the internal stresses due to the tempering of the prequenched layer (TPQL) in such a duplex coating are calculated. The synthetical internal stresses in coating can be estimated by superposing uniform initial stresses developed during plating. The results indicate that the residual tensile stresses due to fabrication in coating will be decreased greatly, or even synthetical compressive internal stresses may arise in the coating.

Keywords: Internal stresses, Duplex coating, Thermal loading, FEM

Introduction

Duplex coating is widely used, where the pretreatment layer is expected to provide a reinforced support for the hard coating.¹ However, the pretreatment layer will degrade if the structure is exposed to thermal loading;² a typical case is the tempering of prequenched layer (TPQL). This seems to restrict the application of the duplex coating in thermal circumstances. Nevertheless, accompanied with the degradation of the prequenched layer, an internal stress state of benefit may develop in coating because the prequenched layer will contract due to being tempered by thermal loading. As one can image, this bulk contraction will be constrained with the coating and thus compressive stresses will develop in coating. Such compressive stresses may partly counteract the tensile stresses in coating generated with plating, or even introduce a state of residual compressive stresses within the coating. This compressive stress is believed to be useful to improving the fatigue performance of the coating.3

In this study, the bulk dilation and contraction with phase transformation are simulated with a lineal elastic FEM model. A gradient model is used to involve the gradient of the volume fraction of martensite in the prequenched layer, which decreases from the surface to the interior of the substrate. First, initial stresses arising in the substrate during as quenching are simulated. Then, the changes of internal stresses due to TPQL are achieved numerically. Finally, the synthetical internal stresses in the substrate or the coating can be estimated by superposing the stress due to TPQL and the respective initial stresses developed during as quenching or plating.

Sketch of duplex coating

Consider that the substrate of the example material, say low carbon alloy steel 30CrNi2MoVA, is surface quenched first. This induces a gradient layer, in which the volume fractions of martensite decrease gradually from the surface. This gradient of volume fractions of martensite will induce graded volume dilation in macroscopy and hence, a specified initial stress within the substrate should arise. For the sake of simplification, a linear function of depth from the surface is assumed for the volume dilation coefficient as

$$\varepsilon_{y}^{q} = 2\overline{\varepsilon^{q}}(1 + y/t_{q}) \tag{1}$$

where ε_y^q represents the volume dilation coefficient of the quenched layer, which varies linearly with the depth from the surface, $\overline{\varepsilon^q}$ denotes the average volume dilation of the quenched layer with a specific non-negative value, y the depth from the surface with a negative magnitude for the substrate according to the present coordinates and t_q the maximum depth of the quenched layer. The rectangular Cartesian coordinates are set up as shown in Figs. 1 and 2. It can be noted that the coating should not be there at present. Thus, it can be found that the maximum volume dilation will occur on the top surface of the substrate.

Subsequently, chromium is plated on the prequenched layer. This plating procedure always introduce uniform residual tensile stresses within the coating, which range from 0.1 to 1 GPa responding to different plating parameters. The sketch of this duplex coating is shown in Fig. 1. If this duplex coating is exposed to thermal loads, the tempering of the prequenched layer will be induced. The bulk contraction of the prequenched layer is constrained with the coating, which will lead to the redistribution of the internal stresses in the coating. Again, the volume contraction coefficient of the prequenched layer is assumed as

$$\varepsilon_{\rm v}^{\rm t} = 2\varepsilon^{\rm t}(1+y/t_{\rm q}) \tag{2}$$

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1 Schematic of duplex coating

where ε_y^t represents the volume dilation coefficient of the quenched layer, which varies linearly with the depth from the surface, $\overline{\varepsilon^t}$ denotes the average volume dilation of the quenched layer with a non-positive value in comparison with $\overline{\varepsilon^q}$ in equation (1), *y* the depth from the surface and t_q the maximum depth of the pre-quenched layer. Again, for convenience, another assumption is adopted that the volume dilation developed in as quenching will be counteracted completely by the volume contraction during tempering, that is

$$\overline{\varepsilon^{t}} = -\overline{\varepsilon^{q}} \tag{3}$$

For this assumption, the present computation results should only apply to the cases when the complete or nearly complete tempering organisation can be achieved. As for the material considered at present, the low carbon alloy steel 30CrNi2MoVA, the tempering conditions meeting this requirement can be summarised as: heated up to $\sim 480^{\circ}$ C and hold for 5–6 h, latter on cooled down in furnace to under 330°C and then cooled in air.⁶ It is noteworthy that herein, the isotropic assumption is adopted for the coating and the substrate respectively.

FEM model and results

The structure is modelled with three layers as shown in Fig. 1, including substrate, quenched layer and coating, and a finite element analysis (FEA) model is set up as shown in Fig. 2, where t_c (=0.15 mm), t_q (=0.15 mm)

 \mathbf{Y} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V}

2 Finite element analysis model



3 Initial stress in substrate after as quenching and internal stress σ_{xx} due to TPQL

and t_s (=5 mm) represent the thicknesses of coating, quenched layer and substrate, and w (=4 mm) the width of the specimen. The mechanical behaviours of the substrate and the coating are assumed to be linear elastic. The material parameters used in this study are listed in Table 1, where *E* and *v* represent the elasticity modulus and the Poisson's ratios. The elasticity of the prequenched layer is assumed to be identical to that of the origin substrate in this study, although it may be changed lightly by heat treatment. It is treated as a plane strain problem and as for the symmetry of the structure and loading, only half of the specimen is modelled.

Of the models shown in Figs. 1 and 2, the coating should be imaginarily removed from the model to understand the process of computing the stress of the substrate after quenching. To actualise the non-uniform volume dilation, a method, so called virtual temperature field, is adopted to exert a grade temperature field along the Y direction on the nodes of the substrate. That is, eigenstrain due to phase transformation is substituted by thermal strain and the latter can be realised conveniently in FEM. The grade temperature field T(y) can be expressed as

$$T(y) = 2(1 + y/t_q)$$
 (4)

when $-t_q < y < 0$, otherwise

$$T(y)=0$$

Thus, the grade volume dilation or contraction, corresponding to equations (1) and (2), is simulated conveniently with

$$\varepsilon_{\rm v} = \alpha T(y) \tag{5}$$

where α represents the virtual thermal expansion coefficient of the material of substrate, which in magnitude is equal to $\overline{\epsilon^q}$. With symmetry boundary conditions being used at the left side of the model in Fig. 2 (without coating), the stress distribution along the Y direction of the substrate can be obtained as depicted in the curve No. 1 in Fig. 3, which indicates a state of compressive stress varying linearly with y within the

Table 1 Material parameters⁴

	<i>E</i> , Pa	υ	
Coating	300×10^9 200×10^9	0·2	
Subsilate	200 x 10	0.3	



4 σ_{xx} in coating due to TPQL

quenched layer in comparison to that of tensile stress outside the quenched layer.

To calculate the stresses in the coating with the TPQL, the finite element analysis (FEA) model as shown in Fig. 2 is again utilised with the coating being perfectly bonded to the substrate. Similarly, the method of virtual temperature field is adopted to simulate the volume contraction of the prequenched layer and the symmetry condition is defined at left sides of both the coating and the substrate. After the computation, the initial stress of the substrate from the previous results should be superposed to obtain the final stress of the substrate.

The internal stresses originating from the TPQL are attained as shown in Figs. 3–6. For normalisation, let

$$\overline{\sigma} = \overline{E}\overline{\varepsilon} \tag{6}$$

where $\overline{E} = E_c E_s / (E_c + E_s)$ and the eigenstrain $\overline{\varepsilon} = \overline{\varepsilon^q} = -\overline{\varepsilon^t}$ corresponding to the average linear dilation of the quenched layer during phase transformation. E_c and E_s represent the Young's modulus of coating and substrate respectively.

Figure 3 depicted the stress σ_{xx} along the path perpendicular to the surface of the specimen due to TPQL, for which the horizontal location is x=0, i.e. the centre of the specimen. Herein, the curve No. 1 represents the stress of the substrate after quenching, No. 2 the stress of the specimen without considering the initial stress of the substrate and No. 3 the superposition of Nos. 1 and 2. That is, the curve No. 3 in Fig. 3 denotes the stress of the specimen due to TPQL. It indicates that a state of compressive internal stress arises within the coating. However, different from the stress state of a prequenched specimen with free surface after







6 σ_{yy} in coating due to TPQL

tempering, a slightly tensile stress state arises within the prequenched layer. This is partly due to the constraint effect of the relatively hard coating on the contraction of the substrate and partly due to the assumption that the complete tempering organisation can be achieved, i.e. that the volume dilation developed in as quenching will be counteracted completely by the volume contraction during tempering, as introduced in the above section.

Figures 4–6 depicted the stress within the coating due to TPQL, in which the curves (y=0 and $y=150 \mu m$) represent the stress states at the locations of the interface and the surface of the coating respectively. The curves ($y=50 \mu m$ and $y=100 \mu m$) represent the stress states at the locations of 50 and 100 μm from the interface.

Figure 4 shows the stress σ_{xx} in coating, where the four curves represent the stress state of the coating at four depths. It is indicated that within the boundary region, 10% of the width W from the free edge, there is a non-uniform state of the stress σ_{xx} . The stress σ_{xx} of y=0 has a non-zero value at the free edge, which shows a singularity due to the jump of materials across the interface.⁵ The absolute values of stress σ_{xx} for y=50, 100 and 150 µm increase from zero at the free edge to a stable level, and there is an almost uniform compression state away from the edge.

Assuming that the initial stress in the coating developed during plating is uniform, say it is σ_0 , then the synthetical internal stresses can be attained as the superposition of the internal stress due to TPQL and σ_0 , i.e. the synthetical internal stresses in the X direction should be $\sigma_{xx} + \sigma_0$. For instance, if $\bar{\epsilon} = 1\%$ and $\sigma_0 = 1000$ MPa, the σ_{xx} is about -1400 MPa away from the free edge and thus, the synthetical internal stresses in the X direction is about -400 MPa. This indicates that a synthetical compressive internal stress may arise in the coating although the initial stress developed in coating after plating is of large tensile stress.

Figure 5 shows the stress σ_{xy} in coating. The results show that the in-plane shear stress σ_{xy} vanishes far away from the free edge and the concentration of the shear stress arises near the free edge. It is evident that the shear stress should decrease with the decrease of the distance from the surface. The shear stress at $y=150 \mu m$, i.e. the surface of coating, is zero.

Figure 6 shows the stress σ_{yy} in coating. It can be found that σ_{yy} is almost zero away from the free edge. A complex state arises near the free edge, which is generally known as edge effect.

Conclusions

To characterise the internal stresses in a duplex coating with a prequenched layer, a gradient FEM model is set up to compute the initial stresses developed in the substrate after as quenching and the internal stresses due to the TPQL.

The synthetical internal stresses in the substrate and the coating have been estimated by superposing the stress due to TPQL and the respective initial stresses developed during as quenching or plating.

A state of compressive internal stress arises within the coating due to the TPQL, therefore a synthetical compressive internal stress may arise in the coating although the initial stress developed in coating after plating is of large tensile stress.

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References

- 1. T. Bell, H. Dong and Y. Sun: *Tribol. Int.*, 1998, 31, 127.
- K. Zhang, C.-W. Wu, Y. Hu and G.-N. Chen: Solid State Phenom., 2006, 118, 243.
- 3. E. Uhlmann and K. Klein: Surf. Coat. Technol., 2000, 131, 448.
- 4. Z. X. Zhang: 'Handbook of enginery metal materials', (in Chinese); 1989, Beijing, Weapon Industry Press.
- 5. V. L. Hein and F. Erdogan: Int. J. Fract. Mech., 1971, 7, 317.
- 6. Z. Liu, Z. J. Wu, J. Z. Wu and Y. Zhang: 'Numerical simulation on the heat treatment process' (in Chinese); 1996, Beijing, Science Press.