STUDY OF PARAMETERS AFFECTING FRACTURE OF TITANIUM NITRIDE FILMS (TiN)

Marcos F. Odorczyk[1,*], José D. Bressan[1], Luiz C. Fontana[1]

[1]PGCEM, University of Santa Catarina State, Joinville-SC- 89219-710, Brasil

* Corresponding author: Dem6mdo@joinville.udesc.br

ABSTRACT: Present work examines theoretically the relationship between micro-cracks and failure criteria for fracture modes I and II in coating films. TiN films deposited by magnetron sputtering on substrates of steel or aluminum, with homogeneous (HMG) or functionally graded (FGM) structure were considered. The stress field in the film and substrate was generated from the Hertzian normal pressure and tangential force due to the friction from loading displacement at constant sliding velocity on the film surface. At the interface of the film and substrate, there are substantial differences among material properties. These differences, together with the film deposition conditions, can induce the formation of imperfections in the film condensation front, thus, becoming a region of potential micro-cracks formation. Stress-intensity factors at crack tip and a fracture criterion for combined rupture modes I and II in function of TiN film thickness, structure type (FGM x HMG), friction coefficient μ and substrate, were analyzed. A variance study by ANOVA has indicated that for both fracture failure mode I and II, the material factors, substrate and film structure, have higher significance than other factors analyzed. Film thickness is a significant factor, but not at the same level as material factors. Aluminium substrate with HMG coating has a higher risk level than steel substrate. FGM films reduce drastically the fracture failure risk mode I and II, when compared with HMG films,for both substrate. On FGM films, and HMG thin films over steel substrate, the mode II is more importante than the mode I, although the values are not high. For other cases, the mode I is more significative. The friction, altough is a important fator, has not the same significance level when compared with the others investigated.

Key-words: FGM, micro-cracks, TiN film, fracture criterion, combined fracture mode I and II.

1. Introduction

The use of coating films is based on the idea to combine materials with different properties, in order to obtain the benefit of both constituents. However, such differences lead to a non-continuous mechanical behavior at the interface film and substrate. To reduce this functional discontinuity, materials were developed whose properties vary gradually through the thickness direction and are called Functionally Gradade Materials (FGM). One consequence of this properties discontinuity is delamination of the film at the interface with the substrate due to load applications. This behavior depends on load factors, geometry, surface roughness and material of the film and substrate. The variation of the properties in films FGM can follow linear or exponential laws, making the transition smoother interface than the homogeneous films. Several works have been presented in this area. Shodja [1] presented a study with analytical solutions for the temperature field and stress of a tribological pair under thermomechanical loading. Odorczyk [2] presented a study with numerical solutions for the same case. The tribological pair study consists of a displacement normal force over the surface of a TiN film HMG or FGM deposited on a steel or aluminum substrate. The stress intensity factors KI and KII were analyzed in relation to the main normal and shear stresses at the interface. By analysis of variance, it was evaluated the significance of the factors friction, thickness, substrate material and film strucutre on a mixed KI/KIc and KII/KIIc criteria.

2. Methods

Titanium Nitride (TiN) is typically used in coating films due to their high elastic modulus E, low thermal conductivity *k* and low coefficient of thermal expansion α compared to steel or aluminum substrates. A normal force is applied in the form of Hertzian pressure that combined with the friction and displacement between the surfaces, generates a normal and a tangential mechanical and thermal loading, shown in Fig 1.

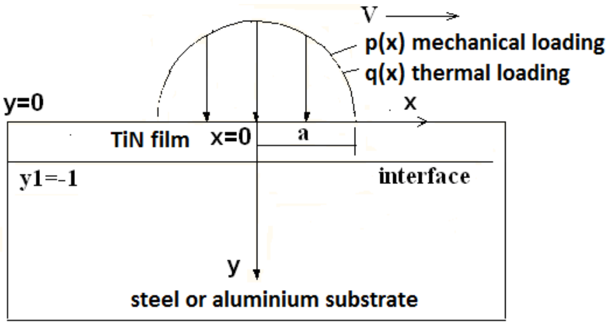


Figure 1. Tribological pair under thermomechanical loading.

The film coating was considered isotropic, following the laws of functional gradation according to Eqs (1) and (2)

$$P_c(y_c) = P_0 e^{\beta y^M} \tag{1}$$

$$\beta = \frac{1}{y_s^M} \ln \frac{k_s}{k_0} \tag{2}$$

where P is the property studied (α, k E), the index M = 0 is for HMG and M = 1 for FGM film structure, the subscripts s, c and 0 respectively identify the values at the interface between the film and the substrate, within the film and at the surface of the coating film and y is the direction across the film. The properties of the substrates, Poisson's ratio and the thermal diffusivity of the film coating were considered constant. It is assumed that the substrate is an elastic solid homogeneous, isotropic and dimensions enough large to be considered as infinite. The normal and tangential Hertzian pressure due to mechanical loading and the friction between the sliding surfaces generates normal and shear stress and heat. The normal pressure loads p(x), shear $p_{tan}(x)$ and heat flux are defined by Eqs (3) to (5)

$$p(x) = p_0\sqrt{(1-x^2)}H(1-|x|) \tag{3}$$

$$p_{tan}(x) = p(x)\mu \tag{4}$$

$$q_p(x) = p(x)v\mu \tag{5}$$

where p_0 is the load at x = 0, H is the Heaviside function, μ is the film friction coefficient, q_p is the heat flux generated at the film surface and v is the load displacement velocity on x direction.
The flexural tensile and shear stress at film and substrate interface, responsible for failure adhesion, are defined by Eqs (6) and (7)

$$\tau_{xy(a\dim)} = \frac{\tau_{xy(\max)}}{p_0} \quad (6)$$

$$\sigma_{xx(adim)} = \frac{\sigma_{xx(\max)}}{p_0} \quad (7)$$

where $\tau_{xy(a\dim)}$ is the maximum shear stress normalized, $\tau_{xy(\max)}$ is the maximum shear stress, $\sigma_{xx(adim)}$ is the maximum flexural stress normalized, $\sigma_{xx(\max)}$ is the maximum normal stress, all at the interface. The stresses do not occur at the same point at the interface.

A variance study ANOVA presented by Odorczyk [4] indicated film thickness, friction coefficient and its interaction are factors of high significance for shear stresses. For tensile flexural stresses, material of substrate, thickness and structure and its interactions are highly significant. The velocity is not significant for both stress cases.

From the stresses calculated in Eqs.(6) and (7), were calculated the principal stresses, tensile flexural and shear for the same points. With the principal stresses, assuming the greatest stress state at the interface, were calculated values for stress intensity factors KI and KII for brittle fracture failure modes I and II.

Considering that a crack can propagate in any direction, the KI and KII parameters for the principal stress directions were investigated. It was considered a crack length of about 0.4 film thickness. The stress intensity factors KI and KII were obtained by Eq. (8)

$$\begin{Bmatrix} K_I \\ K_{II} \end{Bmatrix} = \begin{Bmatrix} \sigma \\ \tau \end{Bmatrix} \sqrt{\pi a_t} \quad (8)$$

It was adopted a mixed fracture criterion [6] considering KI and KII according to Eqs (9) and (10)

$$\left(\frac{K_I}{K_{IC}} \right)^m + \lambda \left(\frac{K_{II}}{K_{IC}} \right)^n = 1 \quad (9)$$

$$\lambda = \left(\frac{K_{IC}}{K_{IIC}} \right)^n \quad (10)$$

assuming m = n = 2.

Also, it were considered the values of fracture toughness KIc = 1 and KIIc = 2, since the present study investigates just the competition between modes of fracture I and II.

It were obtained KI and KII values for combinations of thickness, μ, type of substrate (steel and aluminum), and TiN film structure FGM x MGF. A variance study ANOVA was performed to investigate the influence of the parameters mentioned on the mixed fracture criteria shown in Eq. (9), to the main directions normal and shear. The experiment structure is shown in Table (1).

Table 1. Influence of parameters on KI/KIc and KII/KIIc.

SUBSTRACT MATERIAL	AL(-1)						STEEL (+1)					
FILM STRUCTURE	FGM (-1)			HMG (+1)			FGM (-1)			HMG (+1)		
THICKNESS	0,5	1	2	0,5	1	2	0,5	1	2	0,5	1	2
FRICTION	0,05	0,25	0,50	0,05	0,25	0,50	0,05	0,25	0,50	0,05	0,25	0,50

3. Results

The variance study ANOVA results are show in Figs. (2) and (3). The values in Italic have high significance.

ANOVA; Var.:KI/KIc; R^2 =0,89576; R Adj=0,77198 Experiment with 2 factors at 2 levels combined with 2 factors at 3 levels, 36 runs ; MS Residual=0,4254813					
Factors	SS	df	MS	F (fisher)	p
(1)Substrate (L)	14,42	1	14,42	***33,88***	***0,000026***
(2)Film structure (L)	16,68	1	16,68	***39,21***	***0,000011***
(3)Film thickness (L+Q)	3,27	2	1,63	***3,84***	***0,043463***
(4) µ Friction coef (L+Q)	0,64	2	0,32	0,75	0,488018
Interaction 1 x 2	14,35	1	14,35	***33,73***	***0,000027***
Interaction 1 x 3	3,70	2	1,85	***4,35***	***0,030995***
Interaction 1 x 4	0,67	2	0,34	0,79	0,470006
Interaction 2 x 3	3,29	2	1,65	***3,87***	***0,042603***
Interaction 2 x 4	0,65	2	0,32	0,76	0,483810
Interaction 3 x 4	0,83	4	0,21	0,49	0,745476
Error	6,81	16	0,46		
Total SS	65,31				

Figure 2. ANOVA results for KI/KIc.

ANOVA; Var.:KII/KIIc; R^2 =0,89293; R Adj=0,76579 Experiment with 2 factors at 2 levels combined with 2 factors at 3 levels, 36 runs ; MS Residual=0,0210749					
Factors	SS	df	MS	F (fisher)	p
(1)Substrate (L)	0,67	1	0,67	***31,83***	***0,000037***
(2)Film structure (L)	0,80	1	0,80	***38,16***	***0,000013***
(3)Film thickness (L+Q)	0,21	2	0,10	***4,89***	***0,021926***
(4) µ Friction coef (L+Q)	0,04	2	0,02	0,91	0,421088
Interaction 1 x 2	0,60	1	0,60	***28,49***	***0,000067***
Interaction 1 x 3	0,18	2	0,09	***4,31***	***0,031890***
Interaction 1 x 4	0,04	2	0,02	1,02	0,381568
Interaction 2 x 3	0,17	2	0,08	***4,17***	***0,034908***
Interaction 2 x 4	0,04	2	0,02	0,97	0,398810
Interaction 3 x 4	0,05	4	0,01	0,60	0,670521
Error	0,34	16	0,02		
Total SS	3,15				

Figure 3. ANOVA results for KII/KIIc

The results on Fig.(2) and (3) shows that the film structure (FGM x HMG) and his interactions, followed by the substrate material, are the most important factors to prevent fracture failure, on mode I and II. The film thickness is a significant factor, but lower (about 10 times) than the material factors significance. The friction is not significant for mode I and II. On Fig. (4), it is possible to compare the significance of the factors and their interactions.

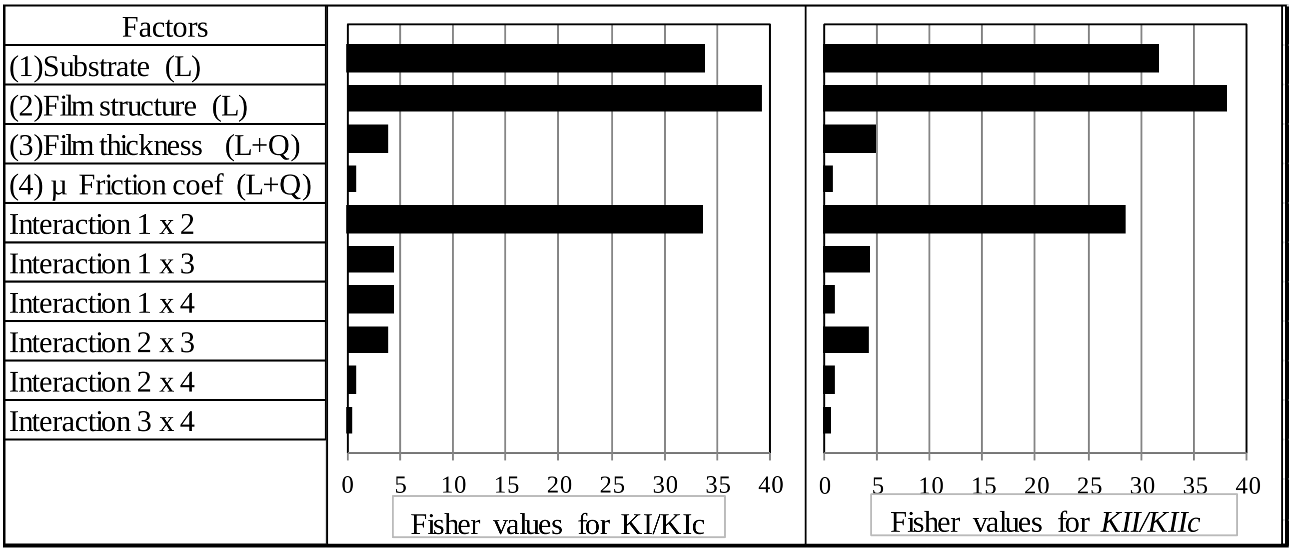
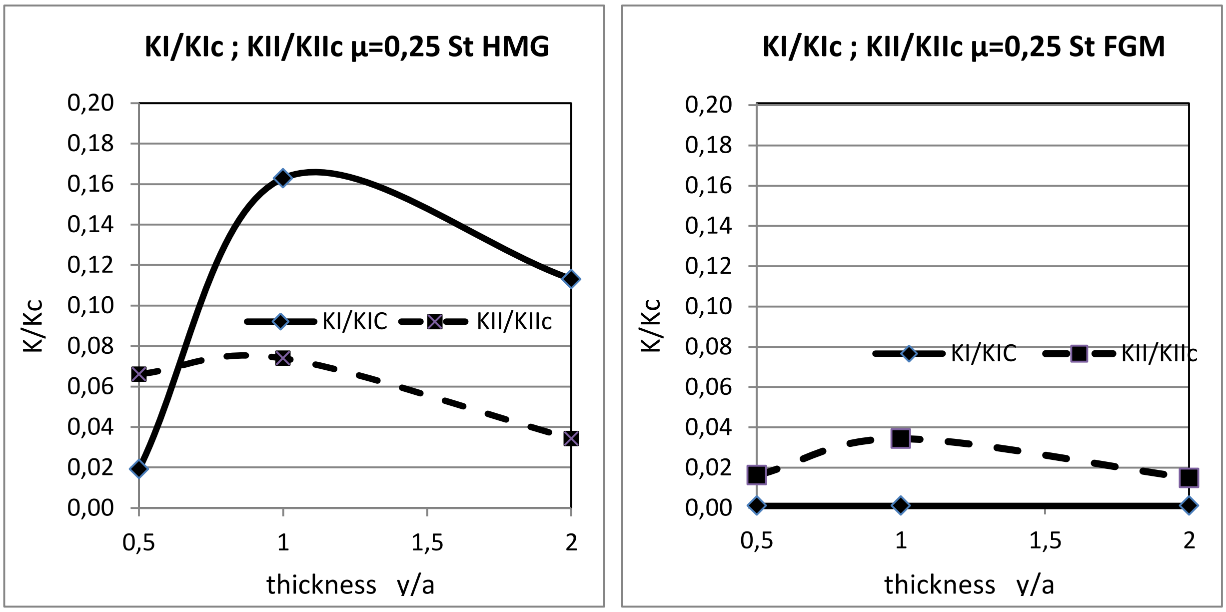


Figura 4. Fisher distribution values of influence factors on KI/KIc and KII/KIIc modes.

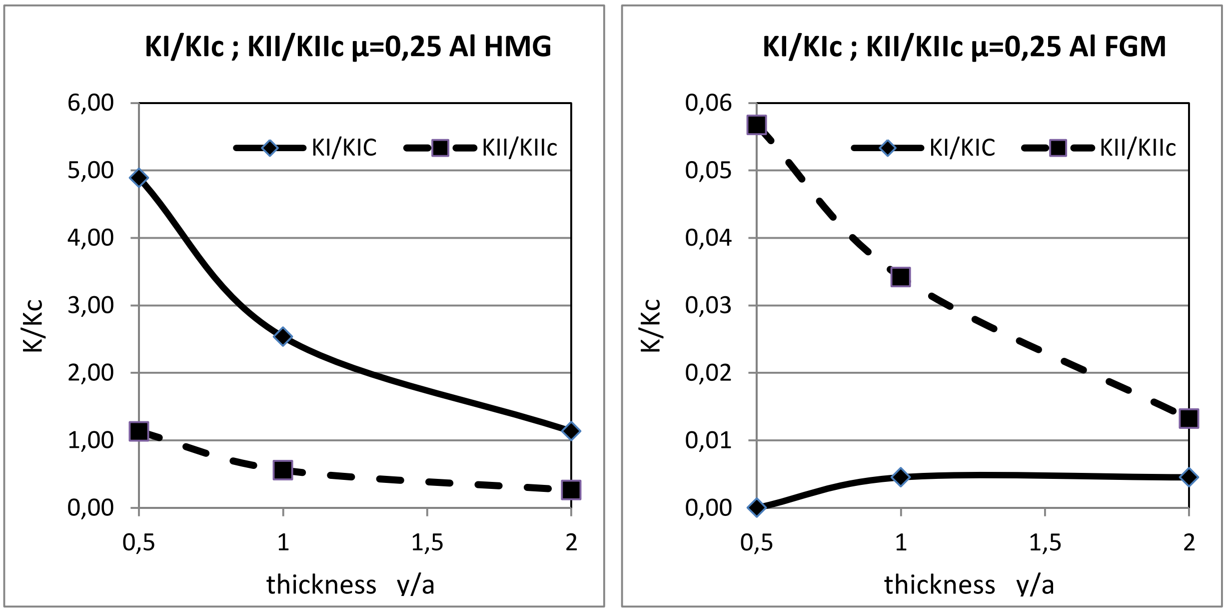
The results of KI/KIc and KII/KIIc obtained by Eq.(9) corresponding to the principal directions, for µ=0.25, for film thickness thin, medium, large, for TiN film FGM and HMG over steel and aluminium substrate, are shown in Fig. (5a), (5b), (6a), (6b).



(a) (b)

Figure 5. KI/KIc and KII/KIIc for µ=0.25 Steel, (a) TiN HMG, (b) TiN FGM.

In Fig. (5) is possible to see that for TiN film HMG over steel substrate, the fracture mode I is more important than the mode II, except for thin films, although these values for thin films are not high when compared with other film thickness. For TiN film FGM over steel substrate, the mode of fracture II is more important than the mode I for all thickness, although the values are not high when compared with TiN HMG steel cases.



(a) (b)

Figure 6. KI/KIc and KII/KIIc for μ=0.25 and aluminium: (a) TiN HMG, (b) TiN FGM.

In Fig. (6) is possible to see that for TiN film HMG over aluminium substrate, the fracture mode I is more importante than the mode II and the values are significativelly higher compared with TiN steel cases. For TiN film FGM over aluminium substrate, the mode of fracture II is more important than the mode I, although the values are not high compared with TiN HMG Al and similar to TiN FGM steel cases.

4. Conclusions

From the theoretical analysis using ANOVA variance study to investigate the influence of factors such as friction, thickness, substrate material and film structure and the relationship between micro-cracks and failure criteria for fracture modes I and II in coating films, the following conclusions can be drawn.

For both fracture failure modes I and II, the material factors, substrate and film structure, have higher significance than other factors analyzed. Film thickness is a significant factor, but not at the same level as material factors. Aluminium substrate with homogeneous structure, HMG, coating has a higher risk level than steel substrate. The functionally graded structure, FGM, films reduce drastically the fracture failure risk mode I and II, when compared with HMG films, for both substrate. On FGM films, and HMG thin films over steel substrate, the mode II is more important than the mode I, although the values are not high. For other cases, the mode I is more significant. The friction, altough is an important factor, has not the same significance level when compared with the others investigated.

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