Thin Solid Films 668 (2018) 14–22

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Crack arrest in thin metallic film stacks due to material- and residual stress inhomogeneities

D. Kozic[a,*], H.-P. Gänser[a], R. Brunner[a], D. Kiener[b], T. Antretter[c], O. Kolednik[d]

[a] Materials Center Leoben Forschung GmbH, Leoben, Austria
[b] Department Materials Physics, Montanuniversität Leoben, Austria
[c] Institute of Mechanics, Montanuniversität Leoben, Austria
[d] Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

ARTICLE INFO

Keywords:
Thin metallic films
Local crack driving force
Residual stress
Finite element modeling
Material inhomogeneity
Fracture mechanics

ABSTRACT

Miniaturized materials, in general, exhibit higher strength compared to their bulk counterparts. As a consequence, their resistance to fracture is often compromised. However, the effect of material inhomogeneities can be used to significantly improve the fracture toughness of thin film components. In this work, the material inhomogeneity effect on the crack driving force, caused by material property and residual stress variations in thin tungsten and copper stacks, is numerically investigated. To this purpose, a finite element analysis is performed using the concept of configurational forces. In this way, we are able to distinguish between the various inhomogeneity effects and draw conclusions about the effective crack driving force. It is demonstrated that the material inhomogeneity effect is not solely determined by the material property variations at the interfaces, since an important contribution emerges due to a smooth residual stress gradient within the layers. The possibility to separate the different effects represents an opportunity for cost efficient design of future reliable thin film microelectronic components.

1. Introduction

Thin metallic films are commonly used for microelectronic applications. Following the trend of miniaturization, the film thickness is consistently decreasing along with the overall device dimensions. Concurrently, the strength of a material increases if either the grain size [1–4] or the size of single-crystalline volumes [5–11] is reduced. Recent investigations deal with the interplay of internal and external dimensions [12–15], which opens the possibility of tailoring the material's strength for specific applications. However, it is very important to note that an increased strength is in most cases accompanied by a decreased fracture toughness of the materials [16].

A crack in a material starts to propagate if the crack driving force equals or exceeds the fracture toughness of the material. The crack driving force is a loading parameter for the crack and depends on the load, the crack length and the geometry of the considered body [17]. It is easy to evaluate the crack driving force in homogeneous components. For inhomogeneous components, such as thin film stacks for microelectronic devices, the material inhomogeneity effect must be taken into account.

Imagine an externally loaded layered composite with a crack that lies in the vicinity of and perpendicular to an interface (IF). Depending on the properties of the involved materials, the crack driving force at a given load can either be larger or smaller compared to that of a homogeneous material. Crack growth is facilitated in the former case and the crack tip is said to feel an anti-shielding effect due to the material inhomogeneity. In the latter case crack propagation is hindered and the crack tip experiences a shielding effect. Anti-shielding occurs if the crack is about to propagate from a material with higher Young's modulus and/or higher yield strength into a material with lower modulus and/or strength. On the contrary, shielding occurs if the crack is approaching an IF to a material with higher Young's modulus and/or higher yield strength [18,19].

Microelectronic components incorporate various small-scale materials with a diversity of material properties. For example, multi-layer stacks are fabricated with alternating soft and hard thin films [20,21]. If the layers are appropriately arranged, the shielding effect can be utilized to arrest cracks in the soft interlayers and prevent their further propagation through the structure [22,23]. Such a strategy is in some cases inspired by natural structures [24–27]. For instance, deep sea sponges have a multi-layered structure consisting of a stiff and strong bio-glass matrix which incorporates thin and soft protein interlayers

* Corresponding author.
E-mail address: darjan.kozic@mcl.at (D. Kozic).

https://doi.org/10.1016/j.tsf.2018.10.014
Received 8 March 2018; Received in revised form 2 October 2018; Accepted 8 October 2018
Available online 10 October 2018

serving as crack stoppers. In such materials the crack driving force is significantly decreased and the load necessary for further crack growth becomes very high as soon as the crack tip arrives in the soft layer. This means that the fracture toughness increases compared to a homogeneous material, without suffering a noticeable loss in stiffness or strength. The use of material property variations to improve the fracture properties of functional materials has been the topic of several investigations, see e.g. [26,28–34].

The same concept of shielding or anti-shielding can be applied for the effect of residual stresses in a body [35]. For instance, compressive residual stresses can be used to counter tensile stresses originating from external loading and have to be overcome before crack propagation is possible. Thin film components for microelectronic applications are most commonly subjected to residual stresses that emerge due to variations in the coefficient of thermal expansion or an atomic lattice spacing mismatch between the materials [36]. Several techniques that determine the residual stress state in thin films have been recently proposed: X-ray diffraction analysis [37–39], focused ion beam milling in combination with digital image correlation [40–43] and the Ion beam Layer Removal (ILR) method [44]. Experimental and computational results have shown that residual stresses can strongly influence the fracture behavior of materials [45–50]. Therefore, it is important to understand the influence of residual stresses on the crack driving force in multi-layered structures.

In this work, we investigate the influence of material inhomogeneities on the crack driving force in thin film stacks with an alternating arrangement of copper (Cu) and tungsten (W) layers deposited on a silicon (Si) wafer. It will be shown that the precise knowledge of the local material behavior as well as the magnitude and the distribution of residual stresses in a stack are important to appropriately calculate the crack driving force.

2. Evaluation of the crack driving force

2.1. Configurational forces and the J-integral

The configurational force concept is based on the ideas of Eshelby [51] and was expanded by Gurtin [52] and Maugin [53]. Configurational forces (CFs) describe the behavior of defects in materials without making any assumptions about the constitutive behavior of the materials. From a thermodynamics point of view, a CF tries to push a defect into a configuration where the total potential energy of the system has its minimum. In general, a CF vector **f** can be determined at each point in a body as

$$\mathbf{f} = -\nabla \cdot (\phi \mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{S}) \tag{1}$$

which is the divergence of the expression in parentheses, the so-called configurational stress tensor. In Eq. (1), ϕ is the strain energy density and **I** denotes the unity tensor. $\mathbf{F}^{\mathrm{T}}$ and **S** represent the transposed deformation gradient and 1st Piola-Kirchhoff stress tensor, respectively. The CF vector becomes non-zero only at positions of a defect in the body [18,54].

If we consider a two-dimensional homogeneous elastic body with a sharp crack, a CF vector $\mathbf{f}_{\mathrm{tip}}$ emerges at the crack tip. The projection of $\mathbf{f}_{\mathrm{tip}}$ in the crack extension direction gives the crack driving force

$$J_{\mathrm{tip}} = -\mathbf{e} \cdot \mathbf{f}_{\mathrm{tip}} \tag{2}$$

where **e** is the unit vector in crack propagation direction. If the body is externally loaded the crack driving force is equal to $J_{\mathrm{tip}} = J_{\mathrm{far}}$, where J_{far} is the far-field J-integral, which can be understood as the driving force induced by the external load in the body.

For simple cases, such as monotonic loading conditions and/or homogeneous materials, the J-integral calculated with the CF concept is equivalent to the conventional J-integral proposed by Rice in 1968 [55]. The conventional J-integral has been used as a loading parameter for cracks in the regime of elastic-plastic fracture mechanics. However,

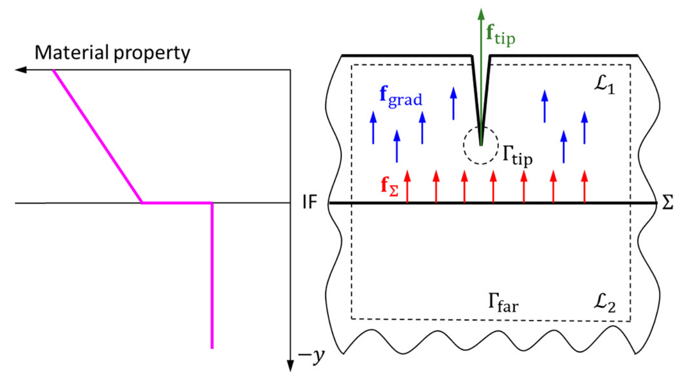

Fig. 1. Schematic distribution of configurational forces (CFs) in a two-layer component. The variation of material property, e.g. Young's modulus E, is shown on the left. CFs $\mathbf{f}_\Sigma$ are induced at the interface Σ due to the jump of E. CFs $\mathbf{f}_{\mathrm{grad}}$ are generated in layer $\mathscr{L}_1$ caused by the smooth E-variation. No CFs are present inside layer $\mathscr{L}_2$, since E = const. A single CF $\mathbf{f}_{\mathrm{tip}}$ emerges from the crack tip.

it has its limitations when applied for cases where non-proportional loading conditions prevail and, especially, for inhomogeneous materials, as pointed out in [18,54,56]. For the latter case where the J-integral becomes path dependent, the CF concept is very suitable for the determination of the crack driving force. This is described in the following section.

2.2. Evaluation of the material inhomogeneity effects

In a specimen where two material layers, $\mathscr{L}_1$ and $\mathscr{L}_2$, are separated by a sharp IF Σ, as sketched in Fig. 1 the material properties, e.g. the Young's modulus E, exhibit a jump at the IF, as depicted on the left side of Fig. 1. Due to this jump CFs are generated at the IF, given by the relation [19].

$$\mathbf{f}_\Sigma = -([\![\phi]\!]\,\mathbf{I} - [\![\mathbf{F}^{\mathrm{T}}]\!]\langle \mathbf{S}\rangle)\mathbf{n} \tag{3}$$

In Eq. (3), $[\![q]\!] = (q^+ - q^-)$ denotes a jump of a quantity at the IF and **n** is the unit normal vector to the IF. $\langle q\rangle = (q^+ + q^-)/2$ represents the average of q across the interface.

Additionally, a smooth material property variation can be present *inside* of a layer, e.g. in layer $\mathscr{L}_1$. This gradient results in the formation of bulk CFs, given by [19].

$$\mathbf{f}_{\mathrm{grad}} = -\nabla_{\mathbf{x}}\phi(\mathbf{F},\mathbf{x}) \tag{4}$$

The strain energy density ϕ in Eq. (4) depends on the reference coordinate $\mathbf{x} = \mathbf{x}(x,y,z)$ and $\nabla_{\mathbf{x}}$ denotes the explicit gradient in the reference frame. For the example of a gradient in Young's modulus E in y-direction as shown in Fig. 1, $\mathbf{f}_{\mathrm{grad}}$ has only a y-component given by $f_{\mathrm{grad},y} = \frac{\partial\phi}{\partial E}\frac{\partial E}{\partial y}$.

The CF vector emerging at the crack tip $\mathbf{f}_{\mathrm{tip}}$ and, therefore, the magnitude of the crack driving force, see Eq. (2), are strongly affected by the CFs induced at the IF and in the bulk. This effect is quantified by two terms [19]:

An *interface inhomogeneity term* C^{IF}, corresponding to the sum of all CFs $\mathbf{f}_\Sigma$ that are generated at the sharp IF Σ

$$C^{\mathrm{IF}} = -\mathbf{e} \cdot \int_\Sigma \mathbf{f}_\Sigma dl \tag{5}$$

A *gradient term* C^{GRAD}, corresponding to the sum of all CFs $\mathbf{f}_{\mathrm{grad}}$ inside of a material layer $\mathscr{L}$

$$C^{\mathrm{GRAD}} = -\mathbf{e} \cdot \int_{\mathscr{L}} \mathbf{f}_{\mathrm{grad}}\, dA \tag{6}$$

The sum of all inhomogeneity effects in the body,

$$C_{\mathrm{inh}} = C^{\mathrm{IF}} + C^{\mathrm{GRAD}} \tag{7}$$