THICKNESS DEPENDENT YIELD STRENGTH OF THIN FILMS

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<u>Summary</u> Biaxial and shear loading of a thin film on an elastic substrate are modelled by a strain gradient plasticity theory. The governing equations are implemented in a finite element programme. Simulations are presented for varying ratios between the film thickness and a microstructural length scale parameter. It is showed that both yield strength and hardening are influenced by the film thickness for sufficiently small thicknesses. This is in contrast to alternative theories, which only show an influence on the hardening.

INTRODUCTION

Thin films are applied in a range of applications. Examples are microelectronic devices and surface coatings. Experiments have showed that the yield strength and hardening behaviour depend on the thickness of the film if the thickness is sufficiently small. This thickness dependence cannot be explained by standard local plasticity or viscoplasticity theories. Microstructural length scales must be taken into account. There are several ways to incorporate microstructural length scales. A number of continuum-based theories have been presented in the literature [1, 2]. Gudmundson [3] has presented a framework similar to Gurtin [4] that covers some of the other theories as special cases. A particular feature of this theory is that the structural dimension influences both the elastic range and the hardening. This is in contrast to alternative theories, which only show an influence on the hardening. The theory will be demonstrated by application to two thin film problems. A thin film on a thick elastic substrate is considered. Firstly, the film is subjected to a pure shear stress. Secondly, a prescribed biaxial strain of the film-substrate is considered. The results are compared to experiments and alternative models.

THEORETICAL MODEL

Here, only the equations for shear of a thin film on a thick elastic substrate are presented. The reader should refer to [3] for a detailed derivation of the equations for a general case. The variational principle for pure shear reads,

$$\int_{0}^{t} \left[\tau \delta \left(\frac{du}{dz} \right) + (q - \tau) \delta \gamma_{p} + m \delta \left(\frac{d\gamma_{p}}{dz} \right) \right] dz = \tau \delta u \Big|_{z=t}$$
 (1)

where τ denotes the shear stress, u the displacement in x- direction, γ_p the plastic shear, q a micro stress and m a moment stress which is conjugate to the plastic shear gradient. The film is perpendicular to the z- axis and z=0 corresponds to the film-substrate interface. The displacement and the plastic shear are assumed to vanish at the interface. If instead a plastically compliant interface is considered, the constraint of vanishing plastic shear at the interface is relaxed and an additional contribution to the variational principle results [3]. It is furthermore assumed that the moment stress m vanishes at the free surface. The constitutive law is defined by,

$$\dot{\gamma}_{p} = \dot{\gamma}_{0} \left(\frac{\Sigma}{\tau_{f}} \right)^{n} \frac{q}{\Sigma}, \qquad \frac{d\dot{\gamma}_{p}}{dz} = \frac{\dot{\gamma}_{0}}{\ell^{2}} \left(\frac{\Sigma}{\tau_{f}} \right)^{n} \frac{m}{\Sigma}, \qquad \tau = G \left(\frac{du}{dz} - \gamma_{p} \right)$$
 (2)

where

$$\Sigma^{2} = q^{2} + \frac{m^{2}}{\ell^{2}}, \quad \dot{E}^{2} = \dot{\gamma}_{p}^{2} + \ell^{2} \left(\frac{d\dot{\gamma}_{p}}{dz}\right)^{2}, \quad \tau_{f} = \tau_{s} + HE$$
 (3)

The microstructural length scale is captured by ℓ . An effective stress Σ and effective strain E are introduced. Only linear hardening, described by the hardening modulus H, is here considered. The material parameters are described by $\dot{\gamma}_0$, n, the shear modulus G and the yield stress τ_s . It is observed that the constitutive law reduces to a local viscoplastic law for vanishing plastic shear gradients. If the exponent n tends to infinity, a rate-independent plastic solution is approached. A finite element formulation of the equations (1-3) has been formulated. Simulations are presented for n=30 which should correspond to almost rate-independent plasticity. The hardening modulus H is set to G/20.

RESULTS

In Figure 1, the shear stress is presented as a function of the total average shear for varying ratios between the microstructural length scale ℓ and the film thickness t. A yield strength and hardening can be identified for each ratio. The yield strength can be defined from the shear stress where the linear elastic slope crosses the linear hardening slope. In Figure 2, the yield strength is presented as a function of ℓ/t . It is observed that the yield strength is inversely proportional to the film thickness for large thicknesses. The results are in qualitative agreement with alternative strain gradient plasticity theories and dislocation dynamics simulations [5, 6].

The governing equations for biaxial strain have a similar structure as (1-3). The external loading is in this case defined by the biaxial strain \mathcal{E}_0 , which gives an additional contribution to the integral term in (1). The right hand side of the variational principle (1) vanishes in this case, because of the free surface. Simulations have been performed for a range of thicknesses t. The results are similar to those for pure shear and they are in qualitative agreement with experiments [7, 8] and dislocation dynamics simulations [9].

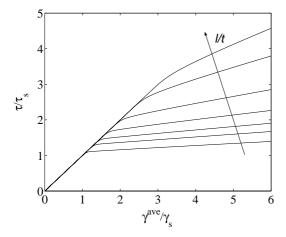


Figure 1. Normalized shear stress versus normalized average shear for varying ratios ℓ/t between microstructural length scale ℓ and film thickness t, $\ell/t = 0.082, 0.29, 0.41, 0.57, 0.82, 1.22, 1.63.$

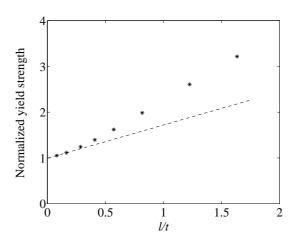


Figure 2. Normalized yield strength versus the ratio ℓ/t between microstructural length scale ℓ and film thickness t.

DISCUSSION

It has been demonstrated that the effect of increasing elastic range with decreasing structural dimension can be captured by the theory. Most of the alternative continuum based gradient plasticity models only influence the hardening behaviour. It should be noted that the present results have been obtained for a model of a plastically stiff interface. If a plastically compliant interface is considered, it turns out that small plastic deformations appear after the local yield stress criterion is satisfied. Numerical results will be presented also for this condition.

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