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STUDY OF INTRINSIC AND EXTRINSIC SIZE EFFECTS ON SHEAR BANDS IN METALLIC GLASSES

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Summary In the present contribution intrinsic and extrinsic size effects on the shear band propagation behavior in metallic glasses are studied. To this end, a thermodynamically consistent finite strain viscoplasticity model is formulated. The strongly coupled and highly nonlinear system of field equations consisting of deformation, free volume and plastic strain field, is implemented into the finite element method, resulting in a non-local model formulation. The results show that the proposed continuum plasticity model is well suited to predict stable or delayed shear localization process with decreasing sample size. With an underlying microstructure, the material behavior in metallic glasses can be significantly influenced, as demonstrated numerically in this contribution on the basis of porous structures.

INTRODUCTION

Despite their superb mechanical property combinations [1], their significantly flawed ductility at room temperature bounds application of metallic glasses with homogeneous structure [2]. Various strategies to remedy this lack of ductility include predeformation, synthesizing composite materials reinforced with a secondary crystalline phase or introduction of soft glass-glass interfaces or pores. All these seemingly different strategies aim at proliferation of shear bands through *extrinsic* stress concentrators instead of a single catastrophic one. It is also known that reducing the sample size in the sub-micron range, experimental observations indicate that the shear localization process is delayed or even suppressed [3], i.e., *smaller is stronger*. Mathematical modeling allows clarification of the interplay between *intrinsic* and *extrinsic* length scales by allowing try outs which are mostly not accessible to experiments, see, e.g., [4, 5, 6] for numerical notch and defect sensitivity investigations. In this work we elaborate further in this direction and report on our recent findings which demonstrate the influence and use of *intrinsic* and *extrinsic* size effects in the amorphous metals making use of a gradient dependent continuum plasticity [7, 8] and various specimen size and geometries and loading scenarios.

MODEL FORMULATION

The material model is formulated in the framework of continuum thermodynamics and rate variational methods. The metallic glass consists of atoms of different sizes. This leads to a free volume ξ inside the material which determines the inelastic deformation. The free volume generation $\dot{\xi} = \zeta\,\dot{\gamma} + \dot{\xi}_{\mathrm{m}}$ is either induced by plastic shearing (i.e., plastic strain γ) or other mechanisms (i.e., diffusion, hydrostatic pressure or structural relaxation) which are accounted for by ξ_m. ζ denotes the free-volume creation factor which accounts for the tension-compression asymmetry, characteristic for metallic glasses. In [9] it is demonstrated that a von Mises-type plastic yield criterion and flow rule most accurately describes the plastic yield and flow behavior of metallic glasses. As shown elsewhere [8], application of rate variational methods leads to the flow rule the evolution equation for the free-volume generation as

$$\dot{\xi}_{\mathrm{m}} = \left[v_m \frac{s_{\xi 1}}{s_{\xi 3}}\right] \mathrm{Div}(\nabla\xi) - \frac{v_m}{s_{\xi 3}}\left[\bar{p} + s_{\xi 2}\left[\xi - \xi_{\mathrm{T}}\right]\right], \quad \dot{\gamma} = \dot{\gamma}_0 \left[\frac{f^p}{c}\right]^{1/a}, \tag{1}$$

where $f^p := \bar{\tau} - \zeta\left[\bar{p} + s_{\xi 2}\left[\xi - \xi_{\mathrm{T}}\right]\right] + \zeta\, s_{\xi 1}\,\mathrm{Div}(\nabla\xi)$. $s_{\xi 2}$ is a material constant representing the defect-free energy coefficient, ξ_{T} denotes the fully annealed free volume, $s_{\xi 1}$ the gradient free energy coefficient where its value depends on the material lengthscale l, $\dot{\gamma}_0$ the reference strain (shearing) rate, a the strain-rate sensitivity parameter of the material, c the intrinsic resistance, v_m a frequency-like term and $s_{\xi 3}$ a material constant representing the resistance to free-volume generation due to mechanisms other than plastic shearing. Also $\bar{p} = -\frac{1}{3}\mathrm{tr}(\boldsymbol{M})$ is the hydrostatic pressure and $\bar{\tau} := \sqrt{\frac{1}{2}}|\mathrm{dev}(\boldsymbol{M})|$ the equivalent shear stress in terms of the Mandel stress tensor $\boldsymbol{M}$. Following [7], the model is completed by the evolution equation for the cohesion $\dot{c} = c\,\frac{k\,\dot{\varepsilon}}{\cosh\left(\frac{\dot{\xi}}{f_\star}\right)}$ with the initial resistance $c(0) = c_0$, the dimensionless fitting constant k and the characteristic frequency $f_\star$. This strongly coupled and highly nonlinear system of equations is solved by different numerical implementation schemes including implicit and explicit gradient computations leading to similar numerical results.

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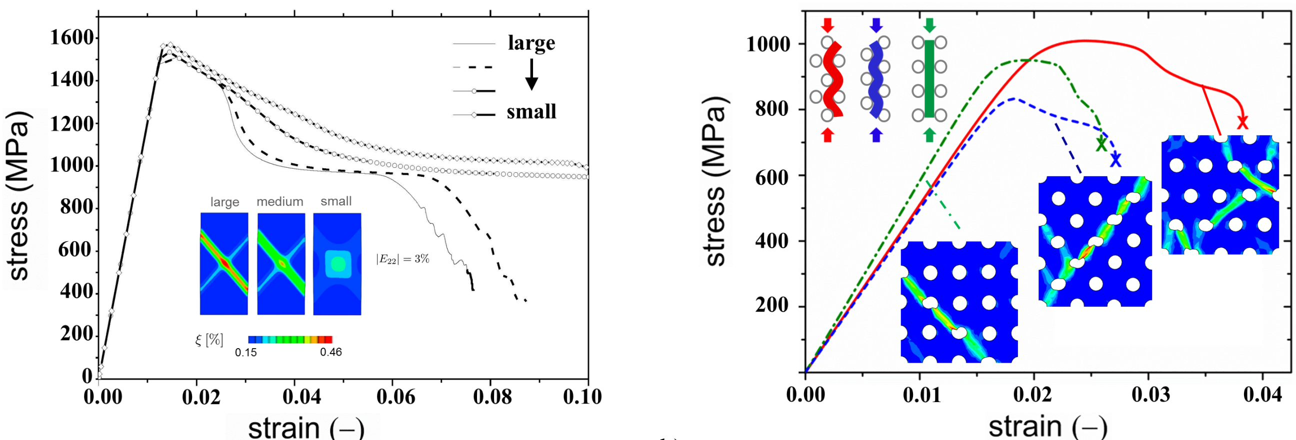
RESULTS

The numerical examples in the following illustrate the shear localization process in submicron metallic glasses and porous heterostructures at room temperature. The first example is an investigation on a rectangular specimen loaded in compression. The shear band is triggered by a local imperfection placed near the center. The stress-strain behavior as well as the spatial distribution of the free volume for different samples sizes is shown in Figure 1a. The numerical results show that the shear localization process is delayed or even suppressed with decreasing sample size. These results indicate that the failure mode changes from fragmentation (catastrophic failure) for large bulk metallic glasses to shear fracture which is in agreement with experimental observations [10].



a) b)

Figure 1: a) Stress-strain responses and spatial distributions of free volume at 3% strain for different specimen sizes ($20\,\mathrm{nm}$ - $1\,\mu\mathrm{m}$) illustrating the delay in shear localization and fracture process due to the sample size effect. b) Influence of pore configuration on the mechanical behavior of metallic glass samples of same size [11]. Enhanced mechanical properties (larger plastic deformation) are achieved for AB stacking configuration with specific lateral pore spacing distance (red curve). The shear band distribution is based on the free volume illustrated for the different microstructures.

Additionally, the effect of an underlying microstructure by introducing randomly or regularly distributed pores is displayed in Figure 1b. The results highlight the importance of the microstructure, here in particular the pore configuration. An appropriate arrangement of the pores and spacing ratio to internal lengthscale, intrinsic size effects can be used to enhance the material properties. The results indicate that shear localization is interrupted by the pore configuration with AB stacking configuration with specific lateral pore spacing distance.

It is clearly demonstrated that the proposed model captures the different size effects in metallic glasses. In contrast to bulk metallic glasses, where a catastrophic localization process is observed, a decreasing sample size as well as a specific microstructure stabilize, delay and even suppress shear localization process. This insight can be used for the design of such samples for certain applications. Additional results, including a variation of the overall porosity, diameter to spacing ratio of the pores, the influence of crystalline nanoprecipitates rather than pores and comparison to experimental observations will be presented and discussed during the conference.

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