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# Modeling and analysis of shear banding in metallic glasses

Vasudevan Kamasamudram\*<sup>†1</sup>, Nicolas Moes<sup>1</sup>, and Thomas Pardoen<sup>1</sup>

<sup>1</sup>Université Catholique de Louvain – Belgium

## Abstract

The inelastic behavior of metallic glasses depends on various factors such as temperature, strain rate, composition, specimen size, etc. These materials typically exhibit a macroscopically elastic-perfectly plastic behavior, with the deformation characteristics ranging from a homogeneous state at smaller strain rates to intensely localized shear banding at higher strain rates. Various studies also demonstrate a size-dependent macroscopic response, where the yield-strength and the strain to fracture depend on the specimen size. Their behavior is also known to be pressure sensitive. Thus, there has been a considerable effort towards developing models and modeling methods that effectively describe the behavior of these materials ranging from Molecular Dynamics, Kinetic Monte Carlo (KMC) methods (with rates described by Transition state theory), and Continuum models (with associative and non-associative flow rules and a possibly pressure-dependent yield function, a visco-plastic type flow rule, a gradient-enhanced model to address size effects).

The KMC methods use the rates computed from the Transition state theory to describe the inelastic behavior of the material. A sequence of random numbers are used to determine the plastic strain and the time increment at the current step, which together with equilibrium, and boundary conditions are used to evolve the system in time. However, the KMC methods exhibit time step dependency in early simulation phases. Also, many realizations of the simulations are necessary to obtain a statistically significant behavior of the system, which in turn is computationally expensive. On the other hand, the continuum methods use a constitutive model that (deterministically) describe the behavior of the material. Thus, an average behavior of the system can be directly obtained by integrating the constitutive model while enforcing the equilibrium conditions. The aim of this study is to examine the convergence of the KMC method towards the continuum methods in the limit of increasing system size.

Also, intense shear banding and the accompanied strain localization are treated by using gradient-enhanced models or by strain localization elements, where these elements are inserted between the bulk elements. In the latter technique, the thickness of shear bands are taken as a material parameter. The current study also analyzes and compares the behavior of the gradient enhanced (diffuse) models and the strain-localization (sharp) models.

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\*Speaker

<sup>†</sup>Corresponding author: vasudevan.kamasamudram@uclouvain.be