Effect of dilatation on the elasto-plastic response of bulk metallic glasses under indentation

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ABSTRACT

Unlike metals, elasto-plastic response of bulk metallic glasses (BMGs) follows closely that of granular materials through pressure dependent (or normal stress) yield locus and shear stress induced material dilatation. While on a micro-structural level, material dilatation is responsible for stress-softening and formation of localized shear band, its influence on the macro-scale flow and deformation is largely unknown. In this work, we systematically analyze the effect of material dilatation on the gross indentation response of Zr-based BMG via finite element simulation. The strengthening/softening effect of load-depth response and corresponding stress-strain profiles are presented in light of differences in elastic-plastic regimes under common indenters. Through comparison of the numerical predictions with existing experimental data, we draw conclusions to guide the selection of a suitable dilatation parameter for accurately predicting the gross response of BMGs.

INTRODUCTION

Bulk metallic glasses (BMGs) have gained considerable scientific and practical importance due to their unique combinations of mechanical properties [1]. This has opened up new avenues for their structural applications [2] and hence greater need for understanding the mechanical response of BMGs at different length scales, and for developing accurate predictive capabilities. On a macro-scale level, it is now commonly agreed that their plastic yield condition is better predicted using the pressure sensitive (or normal stress sensitive) yield criteria such as the Drucker-Prager (or the Mohr-Coulomb) model [3]. However, the flow rule or the plastic flow condition beyond yield is not clearly agreed upon and is the focus of the current study. We systematically investigate the effect of different plastic flow conditions for the Drucker-Prager (DP) yield criteria. Specifically, we focus on the effect of variation in dilatation angle on the gross indentation response of BMGs through numerical simulation and compare the predictions with existing experimental data to guide the selection of a suitable material parameter.

FINITE ELEMENT AND THE MATERIAL MODEL

Conical (apex angle of 90° and 140.6°) and pyramidal indentation (Berkovich and Vickers indenter) analysis was performed using the general-purpose FEM package ABAQUS Standard (SIMULIA, Providence, RI, USA). Axisymmetric two-dimensional mesh was used for conical indentation, while a full three-dimensional mesh was used for pyramidal indentation, with the mesh size being optimized for result accuracy. For all cases, at least 10 to 15 elements were in contact with the indenter at full indentation depth. A typical mesh for the axisymmetric case is shown in Figure 1a.
The extended DP material model of ABAQUS was used for BMGs, where the yield function \( f \) and the flow rule \( g \) is given by equations (1) and (2) below and is shown in Figure 1b. The p-q space is related to the stress invariants space, where \( p \) relates to the first invariant of principal stress, and \( q \) relates to the second invariant of deviatoric shear stress. The material parameters include the material friction angle \( \beta \), the cohesive strength \( d \), and the dilatation angle \( \psi \).

\[
\begin{align*}
  f(p,q) &= q - p \tan(\beta) - d = 0 \\
  g &= q - p \tan(\psi) 
\end{align*}
\]

The dilatation angle determines the inclination of plastic flow from the shear stress direction \( q \) (see Figure 1b). The associative (or the normality) flow rule assumes a flow direction normal to the yield function, as indicated by the dashed arrow in the figure, whereby \( \psi = \beta \). Non-associative flow rule on the other hand allows for an independent representation of the plastic flow and is indicated by the solid arrow in the figure. Here, material parameters for Zr-based BMG were taken from literature [3] corresponding to non-associated DP model, with the dilatation angle being varied as percentage of \( \beta \) from 0% to 100%, where 100% corresponds to associated flow condition.

Figure 1: (a) Typical finite element mesh for the axisymmetric indentation with the inset showing refined mesh close to indentation (b) Drucker-Prager yield function in p-q space. The material parameters \( \beta \) and \( d \) represent the material friction angle and cohesion, respectively. The dilatation angle is given by \( \psi \), where \( \psi = \beta \) represents the normality or the associative flow condition.

RESULTS AND DISCUSSION

The results are discussed in light of typical plastic flow fields below common indenters, as shown in Figure 2, where the equivalent plastic strains (PEEQ) for the sharp conical (90°) and the Berkovich indenters is shown under similar indentation load of 10 N. The plastic field demarcation zones are based on work by Giannakopoulos and Suresh [4], where PEEQ > 29% denotes the cutting zone where intense rigid plasticity flow is expected. For the sharp conical indenter, the cutting zone completely surrounds the indenter and reaches the free surface outside the indentation ring, while for the Berkovich indenter, this zone lies close to the indentation tip. The overall plasticity zone is confined to a much smaller zone for the 90° cone (< 2h, where h is
the indentation depth) as compared to Berkovich case (>5\(h\)). The profile for the other indenters considered here (conical 140.6\(^0\) and vickers) follow similar trends as for the Berkovich case. The load-depth and material pile-up response will be affected by the plastic zones of indentation and hence will guide the interpretation of the results that follow.

![Figure 2: Typical plastic zones under indentation for presssure sensitive material with no dilatation with (a) sharp conical indentation of 90\(^0\), and (b) Berkovich indenter. The zones are demarcated based on Giannakopoulos and Suresh [4] where PEEQ>29\% indicates cutting zones with rigid plastic response. The response of the sharp conical indenter is distinctly different from others in that rigid-plasticity completely surrounds the indenter and reaches the surface of indentation.](image)

The indentation load-depth profile provides valuable information for the mechanical response of the surface and is commonly used to extract the elasto-plastic material parameters. Hence it is important to study the influence of dilatation parameter on the P-h curve and is shown in Figure 3a, where the results are plotted for the sharp conical and the Berkovich indenter with no (0\%), low (10\%) and full (100\%) dilatation. As can been seen in the figure, there is a stiffening of the load-depth response with increase in dilatation for both the indenters, with the results showing low sensitivity to dilatation angle \(\leq 10\%\). Overall, the normalized load increases by 10\% to 20\% for the associated flow condition compared with corresponding case with no dilatation, the higher value being observed in the 90\(^0\) cone. The pile-up response shows similar trend of increasing value with increasing dilatation, with the pile-up being higher by a factor of 2 for 90\(^0\) conical indenter.

These effects and the differences in behavior between the indenters can be explained via the localized compressive nature of indentation and through the differences in plastic flow fields below different indenters. The increase in the dilatation angle causes an increase in the amount of material flow, which in turn is resisted by the relatively stiffer elastic core outside the plasticity zone and hence leading to the stiffening of the load-depth response. The pile-up response on the other hand is affected by the nature of plastic flow closer to the indenter. Since the cutting zone completely surrounds the sharp conical indenter, it shows a much higher pile-up and also increased sensitivity of the pile-up value to the material dilatation angle.

The above differences in the load-depth and pile-up response with dilatation angle can have important implications for property extraction and hardness prediction of BMGs. Based on direct density measurements of BMGs, the overall volume reduction for the material is typically low and is of the order of 0.15-0.25\% [1]. Hence BMGs show low gross dilatation effects unlike
other granular materials. Thus with associative flow rule assumed in numerical predictions, the fitting of the load-depth curve to experimental response may lead to gross error in property estimation and/or over prediction of the material pile-up. This likely discrepancy in experimental and numerical results with associated flow analysis is supported by the work by Kervyn et al [5], where the associated flow analysis resulted in over prediction of the pile-up response numerically as compared to their experimental results. Additionally, as shown in Figure 4, the shear rings observed experimentally [3] can be matched using low or zero dilatation (figure 4a), while the associative flow conditions predicts a more diffused surface effect (see Figure 4b).

Figure 3: (a) Load depth response with and without associative flow rule for sharp conical and Berkovich indenters. Clearly, associative flow rule has significant stiffening effect on the P-h curve with the influence being more prominent for sharp conical indenter.

Figure 4: Effective Von mises stress on the surface of the material for Berkovich indenter for material with (a) zero dilatation, and (b) associative flow rule. The associative flow rule predicts a diffused surface plasticity, while with zero dilatation, the results follows closely the shear bands rings observed experimentally.
SUMMARY AND CONCLUSION

Using finite element analysis of indentation, the influence of dilatation parameter on the numerical prediction of pressure-sensitive BMGs is investigated and the results are discussed in light of experimental data for Zr-based BMGs. We have shown that careful attention to the flow rule is required to answer some of the discrepancies currently present in literature in terms of matching the experimental results to numerical prediction. Overall, a low or zero dilatation is preferred, given the low level of dilatation in experiments. Associated flow condition is clearly not accurate for BMGs as it can lead to as high as 20% stiffer load-depth response and increase in pile-up by a factor of 2. It is also important to note here while simple models such as DP can incorporate gross dilatation effects, sophisticated material models such as the elastic-viscoplastic model of Anand and Su [7] can more accurately predict the frictional and dilatant mechanism of plastic flow of BMGs. However, in spite of these limitations, these simple models will continue to play an important role for BMG modeling given their ability to capture the gross mechanical response, ease of use, and availability in most commercial FE codes.

Finally, we should also note that continuum mechanics based FEM simulations including the sophisticated constitutive models do not include atomistic level details and related smaller scale mechanics. For understanding detailed atomistic level mechanisms, finer scale modeling/simulations should be pursued.

REFERENCES