Numerical modeling of high temperature fracture of metallic composites

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Abstract. Mechanical properties of materials are strongly affected by increasing temperature, showing behaviors that could cause failure as creep. This article provides a brief theoretical description about fracture of materials, deepening on creep and intergranular creep. Some parameters as creep strain, strain rate, time to failure and displacement of the crack tip of a metallic glass selected at high temperature were studied. This paper shows a computer numerical model that permits establish mechanical behavior of a metal composite material Zr₅₂.₅Cu₁₈Ni₁₄.₅Al₁₀Ti₅, bulk metallic glass. In the presence of cracking when the material is subjected to temperatures exceeding 30% of the melt temperature of material. The results obtained by computer simulation show correlation with the results about the behavior of the material viewed through the creep test. From the results we conclude that the mechanical properties of the material generally do not undergo major changes at high temperatures. However, at temperatures greater than 650°C, the effect of the application of stress during creep entails failures in this kind of material.

1. Introduction
At low temperatures metallic material is strained only if the stress state at a point reaches the yield stress of the material. However, at high temperatures plastic strain is developed with the application during some period of lower levels of stress than yield stress [1]. This process called Creep is developed in crystalline and non-crystalline materials and involves some strain mechanisms mainly involving movement of dislocations in the material [2]. The main aim of this research is to evaluate stress, creep strain, strain rate, and displacement of the crack tip a metal composite material Zr₅₂.₅Cu₁₈Ni₁₄.₅Al₁₀Ti₅, bulk metallic glass.

2. Computational implementation
In this article for the construction of the mesh tetrahedral elements were used, because this type of elements coupled better to the geometry near to the tip of the crack, compared with hexahedral elements of similar sizes. On the tip of the crack mesh refinement was performed, this refinement has the shape of circular rings, which permits to find more realistic values around the tip of the crack. All algorithms used in the mesh are available in the software Comsol Multiphysics, that was used to resolve the state of the stress in each node. Table 1 presents the material properties used in the simulation. Some of these properties has been extracted from Shakur et al. [3], and others has been taken from the materials properties database of the software. Interactions and the type of material used as second phase in the composite material was not considered because it generates higher computational complexity. Similarly, this model...
differs from CTOD (crack tip opening displacement) due the simulation developed in this study represents a condition of plastic strain at high temperature, adversely to CTOD method that requires the plasticity remains in a small zone in the front of the crack tip.

Table 1. Properties of the material model used in the simulation.

| Mechanical properties                      | Value   | Units    |
|-------------------------------------------|---------|----------|
| Elasticity module in X axis               | 200000  | N/mm²    |
| Poisson coefficient in XY                 | 0.29    | ~        |
| Stiffness module in XY                    | 77000   | N/mm²    |
| Mass density                              | 7900    | kg/m³    |
| Yield stress in X                         | 420.51  | N/mm²    |
| Elastic limit                             | 351.57  | N/mm²    |
| Thermal expansion coefficient in X        | 1.5e-005| K⁻¹      |
| Thermal conductivity in X                 | 47      | W/(m·K)  |
| Specific Heat                             | 420     | J/(kg·K) |

2.1. Thermal-elastic model

Computational model is focused in the analysis of stress and strain behavior of the material under study as shows the Equation 1, which relates the external force $F$ applied on the volume of material $V$ with the variation in the time of the rate of deformation and the internal stresses $\sigma$ into the the bulk material.

$$\rho \frac{\partial^2 [u]}{\partial t^2} - \nabla \cdot \sigma = F \cdot V \tag{1}$$

Equation 2 is the general heat conduction equation in the cracked plate coupled with the thermal-elastic deformation gradient. In this equation $\rho_o$ and $C_p$ are the density of the material and the specific heat at constant pressure of the material, respectively. Similarly, the term $K$ is the conductivity of the material and the heat transfer during deformation $Q$ is coupled with the term for the variation of the thermal deformation in the material under constant external stress applied.

$$\rho_o C_p \frac{dT}{dt} = \nabla \cdot (K \nabla T) + Q - T_o \left( \frac{\partial \epsilon}{\partial T} \right)|_{\epsilon} \tag{2}$$

Nabarro-Herring high temperature fracture theory is given in the Equation 3, which shows the relation between the nodal displacements and the temperature in the node when the domain is discretized in the single edge crack plate.

$$\epsilon_{NH} = \frac{1}{2} \left[ (\nabla \cdot u)^T + \nabla \cdot u \right] \tag{3}$$

3. Results and analysis

The displacement of the crack tip was established based on the computational simulation and is shown in Figure 1(a) in which is noted as this parameter varies as a time function measured in hours at different temperatures for the same condition of remote stress applied over cracked flat plate. From the results shown in Figure 1(a) can be established that under stress $\sigma = 0.5 \sigma_y$ at temperatures of 600°C and 650°C presents the highest values of displacement for the crack.
tip in function of the time due to at this temperature the material flows more readily than to lower temperatures. Figure 1(b) illustrates the behavior of the level of applied stress and the time required for breaking the cracked metallic material. From the Figure 1(b) can be inferred that for a established value of stress applied on the cracked plate at a higher temperature, the material reaches the most unfavorable condition; because for a given level of stress, the material require less time to reach additional cracking of the plate.

**Figure 1.** (a) Crack tip displacement and (b) Stress level $\sigma_{xx}$ in front of the crack tip ($\theta = 0$) as a time function.

Temperatures near 600°C present load conditions more unfavorable, the analysis was developed to establish the strain behavior due action of stress and temperature on the material. Thus, Figure 2(a) illustrates the behavior of the creep strain of the crack tip at a specific temperature (600°C) and stress values of $\sigma = 0.5\sigma_y$, $\sigma = 0.75\sigma_y$ y $\sigma = 0.95\sigma_y$. Based on these results can be established that at this temperature and higher applied stress the highest values for the creep strain of the crack tip are reached. Moreover, Figure 2(b) shows the strain rate of the crack tip as a function of the temperature with respect to the applied stress. In Figure 2(b) is observed than higher temperature a higher strain rate is obtained for several remote stresses applied on the cracked material.
Figure 2. (a) Strain as a time function for several stress levels and (b) Strain rate as a function of material temperature.

4. Conclusion

This study presented a finite element method that has been implemented based closely on the Nabarro-Herring high temperature fracture theory [2]. The implementation is able to evaluate CTOD (crack tip opening displacement), stress, creep strain and creep strain rate directly without any requirement for aditional calculations for 3D simulations. Results shows convergency between experimental results established in the literature, [4] and the results obtained through FEM method. However is evident that more refinement in the FEM model must be established as those present in a XBEM implementation which presents more accuracy than FEM method on the evaluation of mechanical parameters. Nevertheless XBEM present higher complexity in the computational implementation for that reason FEM could be used as a first estimation for these parameters used in dimensioning and desing of mechanical systems involving composite materials.

References

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