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Experimental and modelling characterisation of residual stresses in cylindrical samples of rapidly cooled bulk metallic glass

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ABSTRACT

Quench processing is widely used in industry to impart the desired structural and mechanical properties by controlling microstructure and compositional gradients, e.g. to obtain supersaturated solid solutions in aluminium alloys, or to achieve martensitic hardening in steels. Rapid cooling, also referred to as quenching or tempering, is also the principal production route for bulk metallic glasses that exhibit high hardness and strength due to their amorphous structure that precludes plastic deformation by easy crystal slip. Importantly, rapid cooling is accompanied by the creation of residual stresses that also have a strong effect on the deformation behaviour. The present study aims to obtain insight into the residual stresses in cylindrical samples of Zr-based bulk metallic glass (BMG) by combining analytical modelling of thermal and mechanical problems with experimental measurements using Focused Ion Beam–Digital Image Correlation (FIB-DIC) ring-core milling. The results show good agreement between the two approaches, providing improved confidence in the validity of the two approaches considered here.

1. Introduction

The present short note contains the derivation of the family of explicit closed form solutions in the theory of thermal diffusivity and theory of elasticity that describe the stress states associated with transient problems in heat conduction and stress analysis. Problems of this kind often arise in the studies of materials, e.g. when considering quenching of structural components as part of primary manufacturing or heat treatment, or in the context of the analysis of internal stresses and damage in lithium ion battery electrodes [1].

The study of residual stresses arising as a consequence of thermomechanical processing has a long history that goes back to the 18th century work of Gabriel Lamé on the internal stresses in hollow and composite cylinders [2]. The most straightforward case of residual stress generated in a composite cylinder due to the mismatch in the coefficient of thermal expansion can be treated within the framework of elasticity. A circular dissimilar inclusion represents the simplest case of an ellipsoidal inclusion that was later generalised by Jock Eshelby in his famous general treatment presented almost a century later [3].

A series of treatments that combine Lamé axisymmetric treatment with plastic yielding appeared in the second half of the 20th century, e.g. [4]. These approaches allow the prediction of residual stresses that arise as a consequence of yielding under reversed thermo-mechanical loading. Inverse problem formulations have also been proposed aimed at extracting material yield strength from the measurement of residual stresses [5].

A problem of particular interest in materials processing concerns rapid cooling (quenching) that is a heat treatment often necessary to control material microstructure and residual stress, e.g. in glass tempering operations. In this study we present a combined theoretical and experimental evaluation of the residual stresses within rapidly cooled bulk metallic glass (BMG) cylinders. Bulk metallic glasses possess an unusual combination of properties that makes them attractive for a range of applications. As with many other glassy materials, BMG's can fail by brittle fracture [6]. Therefore, the residual stress state in samples of BMG plays an important contributing role in determining their structural integrity [7]. The purpose of this study is to chart the way towards reliable evaluation of residual stresses in BMG samples at the micro-scale resolution.

2. Theory

The construction of the solution for residual stress in a rapidly cooled glass cylinder consists of two sequential steps. First step is the solution of the transient thermal conduction problem that allows the determination of inelastic strains (eigenstrains) 'frozen in' at this stage. The eigenstrain distribution obtained from the thermal problem solution is

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then incorporated into the continuum mechanics equations to derive the final residual stress state.

2.1. Power law approximants for transient thermal diffusion within a cylinder

Consider a cylindrical object of radius a initially maintained at the normalised temperature $\theta = 1$ throughout its volume.

At time zero, the temperature is reduced to $\theta = 0$ at its surface, and maintained at that level afterwards. The time-dependent temperature distribution within the cylinder is governed by the 2D transient diffusion equation:

$$\frac{\partial\theta}{\partial t} = \alpha\nabla^2\theta, \tag{1}$$

where $\alpha = \kappa/\rho c_p$ is thermal diffusivity expressed through the combination of thermal conductivity κ, density ρ and heat capacity c_p of the body. In the axi-symmetric case considered here the Eq. (1) simplifies to

$$\frac{1}{\alpha}\frac{\partial\theta}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta}{\partial r}\right). \tag{2}$$

The solution is sought by the method of separation of variables, assuming.

$$\theta(r,t) = R(r)T(t). \tag{3}$$

Substitution into Eq. (2) gives the variable separable form:

$$\frac{1}{\alpha}\frac{T'}{T} = \frac{R''}{R} + \frac{1}{r}\frac{R'}{R} = -\lambda^2 \tag{4}$$

The time-dependent part of the solution is given by:

$$T = \exp\left(-\lambda^2\alpha t\right), \tag{5}$$

where the choice of $-\lambda^2$ as the constant is justified by the requirement that the temperature must not become infinitely large with time.

The spatially varying part satisfies the equation

$$rR'' + R' + \lambda^2 rR = 0. \tag{6}$$

and the solution has the form

$$R(r) = CJ_0(\lambda r). \tag{7}$$

Here $J_0(\lambda r)$ is the Bessel function of zero order chosen to ensure that temperature remains finite and continuous at $r = 0$.

The values of parameter λ are found from the requirement that at the boundary $r = a$ the normalised concentration must be zero. Hence

$$J_0(\lambda_n a) = 0, \text{and } \lambda_n a \text{ are the roots of } J_0. \tag{8}$$

The general solution is assembled in the form

$$\theta(r,t) = \sum_{n=1}^{\infty} C_n J_0(\lambda_n r)\exp\left(-\alpha\lambda_n^2 t\right). \tag{9}$$

At time $t = 0$ the expression in Eq. (9) must satisfy:

$$\theta(r,0) = \sum_{n=1}^{\infty} C_n J_0(\lambda_n r) = 1. \tag{10}$$

Using orthogonality relation for Bessel functions to enforce boundary conditions, and re-assembling, the final solution is found in the form:

$$\theta(r,t) = 2\sum_{n=1}^{\infty}\frac{J_0(\lambda_n r)}{(\lambda_n a)J_1(\lambda_n a)}\exp\left(-\alpha\lambda_n^2 t\right). \tag{11}$$

Introducing notation $\xi_n = \lambda_n a$, and normalised variables $\rho = r/a$, $\tau = \alpha t/a^2$, the above solution can be re-written in dimensionless form as:

$$\theta(\rho,\tau) = 2\sum_{n=1}^{\infty}\frac{J_0(\xi_n\rho)}{\xi_n J_1(\xi_n)}\exp\left(-\xi_n^2\tau\right). \tag{12}$$

Consider the temperature profiles corresponding to the solution expressed by Eq. (12) and illustrated by continuous curves in Fig. 1 for selected values of normalised time $\tau = \alpha t/a^2$. Throughout the process of transient diffusion the temperature distribution can be approximated well by a power law function, $\theta(r) = 1-(r/a)^m$. The suitability of this approximation is supported by the consideration that small inhomogeneities of material and diffusivity are likely to cause concentration variations comparable or in excess of the difference between the full solution Eq. (12) and power law approximants. Hence, subsequent elasticity analyses are built on the basis of this power law assumption.

The value of m must be chosen suitably to obtain good agreement. The approximate relationship between the power law parameter m and the normalised diffusion time τ obtained by least squares fitting illustrated in Fig. 1(g) is given by:

$$m = 0.36\tau^{-0.66}. \tag{13}$$

In summary, the solution of the transient diffusion equation as a function of time and radial position within the sphere can be expressed to good approximation in the form of the concentration varying as a power law expressed in the form:

$$\theta(\rho,\tau) = 1 - \rho^{0.36\tau^{-0.66}}. \tag{14}$$

The solution persists until the solute concentration at the centre of the sphere begins to differ significantly from the initial value. This occurs at the normalised time of $\tau \cong 0.05$, when $\theta(0) = 0.987$, i.e. decreases by ~1.3%.

It is worth highlighting here briefly the significance of formula (Eq. (14)) that presents a closed form, non-series expression for the temperature within a cylinder subjected to cooling (tempering or quenching) as a function of time and coordinate. This form of expression allows ready inversion. For example, the normalised time needed for the temperature at half-radius of the cylinder to be decreased by one tenth of the maximum value is expressed by the compact relation:

$$0.1 = (0.5)^{0.36\tau^{-0.66}} \tag{15}$$

Its inversion gives the following simple result:

$$\tau \approx 0.0345. \tag{16}$$

For normalised times exceeding $\tau = 0.05$, similar approximate descriptions can be elaborated if the following temperature profile is assumed

$$\theta(\rho,\tau) = \Theta(1-\rho^m), \tag{17}$$

where Θ denotes the temperature at the centre. The power law exponent m varies between the value of **2.6** at $\tau = 0.05$ and **1.6** at $\tau = 0.2$, and for practical purposes can be fixed at this value for all $\tau \geq 0.2$. A satisfactory approximation for the central temperature value Θ at all