Simulation for Additive Manufacturing
11^{th}–13^{th} October 2017
Munich, Germany

Phase-field model for microstructural evolution during metallic glass formation

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Key Words: *Phase-field model, Glass formation, Amorphous metal, Bulk metallic glass, Nucleation*

Introduction

Bulk metallic glasses (BMGs) is a promising novel class of materials with remarkable mechanical and magnetic properties in comparison to conventional metallic materials. Attributes such as high strength, high resilience, high corrosion resistance and excellent soft magnetic properties makes them suitable for a wide range of engineering applications [6]. Synthesizing BMGs can be a cumbersome task that typically requires high cooling rates, which implies limitations on component size and complexity when produced with conventional casting [6]. The layer by layer approach utilized in additive manufacturing (AM) enables the possibility to maintain high cooling rates and serves as a promising alternative to casting with the capability to produce BMG components without geometric limitations [4]. However, components manufactured by AM undergo severe heating and cooling during processing, which affects the final properties of the component. The processing steps have a strong influence on the microstructual evolution of the material and the processing parameters needs to be tuned accordingly. Understanding and being able to predict the microstructural evolution during glass formation is therefore of fundamental importance in order to succesfully produce BMG components through additive manufacturing. In the present work, a computational modeling framework for glass formation is presented. It is based on the phase-field description and has been developed to capture the thermodynamic and kinetic interplay that causes the phenomena of glass formation.

Modeling approach

Bulk metallic glasses are commonly synthesized through rapid cooling of an alloy melt in order to achieve substantial undercooling of its liquid state. The rapid cooling causes a reduction in the atomic mobility of the melt, implying reduced kinetics that limits the long range atomic rearrangements required for crystallization. In other words, crystallization is bypassed, causing the atoms to ”freeze” in an amorphous atomic configuration at a temperature referred as the glass transition temperature [6]. To simulate this behaviour, a phase-field model has been developed to predict the process of crystalline

nucleation from an undercooled liquid melt. The model parameters are adapted to experimental data for the BMG alloy AMZ4 ($Zr_{59.3}Cu_{28.8}Al_{10.4}Nb_{1.5}$) [3]. The evolution equation is implemented and solved by utilizing the finite volume PDE solver FiPy [2] with a fully implicit backward Euler time-stepping scheme.

Phase-field model

The phase-field method uses a scalar order parameter $\phi(\mathbf{x}, t)$ to describe the inhomogeneous distribution of the phases present in the material [5]. The order parameter is continuous in time t and space $\mathbf{x}$ and has the value $\phi = 0$ or $\phi = 1$ in each of the two bulk phases. The transition between the phases is described by the symmetric polynomial $g(\phi)$ and the assymetric polynomial $p(\phi)$ and are used to define the free energy density of the bulk phases as

$$f(\phi, T) = W g(\phi) - \frac{\Delta G^{L-S}(T)}{V_m} p(\phi) \tag{1}$$

where W is the energy activation barrier, $\Delta G^{L-S}(T)$ is the difference in Gibbs free energy separating the two states and V_m is the molar volume. By substituting Eq. (1) into Allen-Cahn's equation [5], the evolution equation for $\phi(\mathbf{x}, t)$ becomes

$$\frac{\partial \phi}{\partial t} = M_\phi(T) \left[\epsilon_\phi^2 \nabla^2 \phi - W \frac{dg(\phi)}{d\phi} + \frac{\Delta G^{L-S}(T)}{V_m} \frac{dp(\phi)}{d\phi} \right] + \eta(\mathbf{x}, t) \tag{2}$$

where ϵ_ϕ is the gradient energy coefficient and $M_\phi(T)$ is the mobility of the interface, assumed to be dependent on temperature as a representation of the kinetic slowdown observed during glass formation. The last term in Eq. (2) is a statistical thermal noise [1], chosen to satisfy $\langle \eta(\mathbf{x}, t) \rangle = 0$ and $\langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = 2 M_\phi k_B T \delta(\mathbf{x} - \mathbf{x}') \delta(t - t')$, where the primes denote a position and time different from the unprimed variables and k_B is the Boltzmann constant.

Acknowledgements

The SSF-project Additive Manufacturing - Development of Process and Materials, is acknowledged.

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