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The simulation of the pseudoelastic behavior for amorphous-crystalline shape memory alloys

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Abstract

The mechanical behavior and the physical properties of shape memory alloys (SMAs) considerably depend on their structural state. The current research was devoted to the amorphous-crystalline shape memory composites produced by means of the partial isothermal crystallization from melt-spun ribbons. Previous works revealed that such composites contain amorphous matrix with embedded spherical crystalline inclusions and this structure was simulated in the current study with the help of the simple nucleation and growth model. In addition, some aspects of pseudoelastic behavior of the amorphous-crystalline composites were simulated by means of finite element analysis by ANSYS FEA software. This study revealed that pseudoelastic behavior significantly depended on the volume fraction of crystalline phase in the amorphous-crystalline shape memory composite.

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Keywords: shape memory alloys, pseudoelasticity, finite element analysis, amorphous-crystalline alloys, composites

1. Introduction

The structural state of shape memory alloys has a decisive influence on their mechanical and physical properties, as well as on the shape memory effects [1,2]. It is well known that mixed amorphous-crystalline structure can be produced in the different initially amorphous alloys by means of the partial crystallization. Recently this approach was applied for the melt-spun TiNi-based shape memory alloys [3]. It appeared that crystalline phase in such

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amorphous-crystalline composites is able to undergo the martensitic transformations and therefore they should demonstrate shape memory effects [4,5]. It was shown [4] that the temperatures of direct and reverse martensitic transformations considerably depend on such factor as volume fraction of crystalline phase in amorphous-crystalline shape memory composite. Moreover, the maximal value of shape memory effect also increases with the growth of the crystalline phase content in the composite alloy [6]. Therefore, one may conclude that the volume fraction of crystalline phase may be considered as the key factor determining mechanical and physical properties of amorphous-crystalline shape memory composites. Thus, it seems interesting to simulate these composites and their properties by means of FEM analysis and such simulation is presented in the current research

2. Results and discussion

2.1. Simulation of grain growth during isothermal annealing

For the isothermal annealing of the amorphous alloy the total crystallization time depends on the annealing temperature – decrease of temperature leads to increase of time required for complete crystallization [7]. According to [7–10], during annealing of amorphous TiNi-based alloy the processes of nucleation and growth take place and the crystals grow in a close to circular shape. To simulate the microstructure of amorphous-crystalline samples, some assumptions about the kinetics of nucleation and growth were made. Previous studies [11,12] revealed that thin TiNi amorphous films undergo polymorphic crystallization, whereby the composition remains the same and only the structure is changed. Moreover, the nucleation rate as well as the grain growth rate for TiNi are virtually constant during annealing [8]. There are no accurate data about crystallization behavior of $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy, so for the current simulation, the rates of nucleation and growth were chosen from the results for TiNi alloy, as reported in [8], and these rates were equal to $0.02/m^2s$ and 0.01 m/s, respectively.

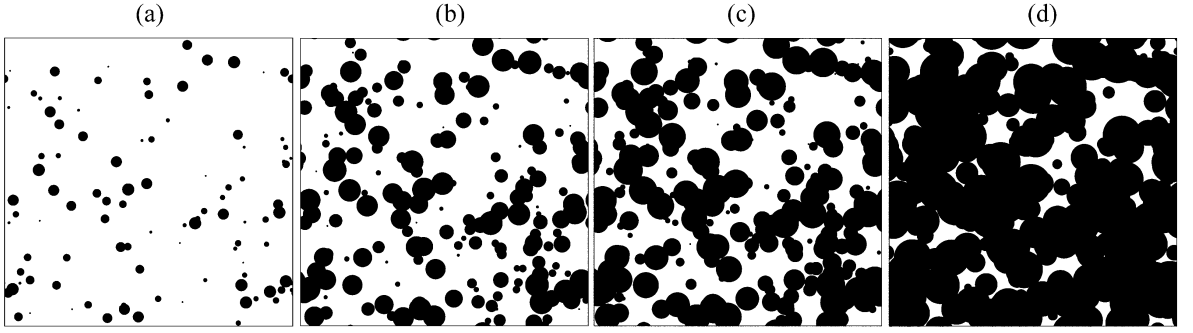

Fig. 1. The representative volume elements (RVE) for amorphous-crystalline SMA composites with (a) 5%, (b) 30%, (c) 50%, (d) 85% volume fraction of crystalline phase (size of RVE is 10x10 micron)

Special software to simulate the nucleation and growth processes during crystallization was developed on the python computer language. Considering the previous assumptions about crystallization process, by means of developed software, the several representative volumes (RVE) of amorphous-crystalline composites were generated for the different steps of crystallization process (Fig. 1). Comparison of generated RVEs with some TEM results, recently published in [13], reveals the significant similarity between simulated and observed structures. Moreover, according to Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory, the nucleation and growth process can be described by means of the equation $\Phi = 1 - \exp(-kt^n)$ here Φ is the fraction of the crystallized materials, k is a temperature-dependent rate constant and n is the so-called Avrami coefficient [14]. In order to estimate Avrami constant for proposed simulation and check validity of developed software, the dependence of the volume fraction of crystalline phase on the annealing time was approximated by JMAK equation. The calculated value is equal to 2.98 and this value is in a good agreement with the case of two-dimension polymorphic crystallization with constant nucleation and growth rates [15].

2.2. Simulation of the amorphous-crystalline SMA composites pseudoelastic behavior

One of the most prominent properties of shape memory alloys is their ability to recover large inelastic deformation by means of the pseudoelasticity caused by the stress-induced martensitic transformation [1]. In the case of amorphous-crystalline SMA composites only crystalline phase are able to undergo martensitic transformations while amorphous part of composite may act as the elastic matrix. In order to study the pseudoelastic behavior, generated on the previous step amorphous-crystalline composites with different volume fraction of crystalline phase were subjected to uniaxial tension by means of ANSYS FEA software package. The cyclic boundary conditions were postulated on the borders of RVE and the tension force were applied along the horizontal direction. Simulation was performed under assumption of 2D plane strain state and material constants were chosen on the base of the previous tensile experiments for totally amorphous and crystalline $Ti_{40.7}Hf_{9.5}Ni_{44.8}Cu_5$ alloy, which undergo B2↔B19' transformation in crystalline state [16]. Young modulus for amorphous and crystalline phases were 26 GPa and 18 GPa, respectively. The phenomenological model of Auricchio [17] was used to describe the pseudoelastic behavior and the chosen material constants for crystalline phase are shown on Fig. 2(a). This model takes in account stress-induced forward and reverse martensitic transformations, which leads to pseudoelastic behavior of shape memory alloys, but it is not able to capture the plastic strain, which may lead to the degradation of the mechanical properties of amorphous-crystalline shape memory composites. In order to carry out FE analysis, simulated RVEs were divided on about 100000 elements each (exact number of elements depended on RVE). To provide more accurate results the mesh was finer in the proximity of amorphous-crystalline interfaces and the resulted mesh was checked in order to avoid highly distorted elements.

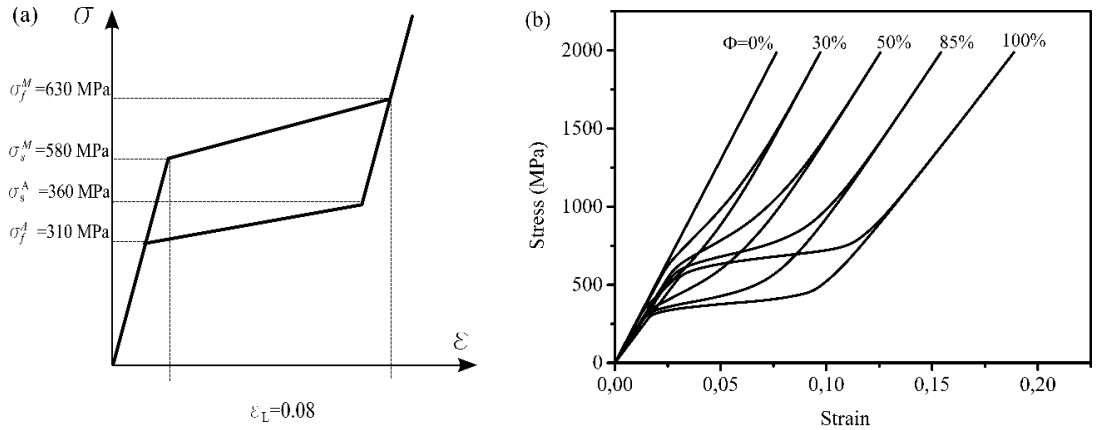

Fig. 2. Material constants for Auricchio model (a) and calculated strain-stress curves, obtained during loading-unloading cycle for RVE with different volume fraction of crystalline phase (b).

Fig. 2(b) represents the stress-strain curves, obtained during FEM analysis of several amorphous-crystalline SMA composites with different volume fraction of the crystalline phase. As one may see, the pseudoelastic plateau is observed on each curve (obviously except completely amorphous sample), but the extent of this plateau considerably depends on the content of the crystalline phase. Also, one should pay attention that stress of the start of the direct martensitic transformation remains virtually the same for each SMA composite, while the stress, which corresponds to the finish of the direct transformation, increases with the decrease of the volume fraction of crystalline phase. Therefore, in the case of amorphous-crystalline composites one may potentially reach higher stress than in crystalline counterpart. It is also easy to see, that the area of the hysteresis loop is proportional to the volume fraction of crystalline phase. From the one hand, the reducing of the material amount, which is able to undergo transformation, decreases the value of the maximal recoverable strain, but from the other hand, it also leads to the decreasing of the area of hysteresis loop. According to [18], for high frequency devices it is critical to reduce the

area of the hysteresis loop to reach stable performance in the range of many cycles. Therefore, according to performed simulation, the amorphous-crystalline SMA composites potentially can find some application in the field of, for instance, microelectromechanical systems, where the small dimensions and high stability are required.

Despite the fact that developed software allows to simulate nucleation and growth processes for 3D case as well as for 2D case, it is clear that 2D FE simulation cannot completely capture the complexity of mechanical behavior of amorphous-crystalline composites. Firstly, applied Auricchio model is quite simple phenomenological model, and it can describe only pseudoelastic behavior and it does not pay much attention to internal microstructure of amorphous-crystalline composites. Also, considering extension of used approach from 2D case to 3D case, it should be mentioned that not only 3D model, accurately describing mechanical response of crystalline phase should be chosen, but also correct boundary condition should be applied on the faces of RVE. It becomes even more difficult, considering that such amorphous-crystalline alloys are usually produced in the form of thin ribbons or foils, so the boundary conditions in the third direction become very important for the simulation.

3. Conclusions

Considering the results of the proposed simulation, it should be noticed that applied SMA pseudoelastic model is not able to describe full range of unique mechanical properties of shape memory alloys and the temperature dependences of material constants, so the implementation of the more complex SMA model is one of the main aim of the ongoing studies, which results will be published elsewhere. Nevertheless, the following conclusions can be drawn from the current research:

- Basing on the simple nucleation and growth model, the representative volumes for amorphous-crystalline shape memory composites with different volume fraction of crystalline phase can be generated;
- The simulation of the mechanical behavior of the amorphous-crystalline SMA composites by means of FEM and the Auricchio SMA model allows one to calculate the macroscopic pseudoelastic stress-strain curves;
- The finish stress of the direct transformation as well as the area of pseudoelastic hysteresis loop considerably depends on the volume fraction of crystalline phase in amorphous-crystalline shape memory composites.

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