

Numerical Prediction of Effective Functional Behavior of Mg-NiTi Strut-Architected Interpenetrating Phase Composites

Shahzaib Ilyas, Marwan El-Rich, Mohamad Khalil, Wael Zaki

Abstract

Improving both stiffness and strength and damping capability in metals is critical, but it is a challenging task since both qualities conflict with each other. This study conducted a numerical study to investigate the effective mechanical behavior of Mg-NiTi composites with bi-continuous interpenetrating phase architecture. An in-house UMAT subroutine constitutive model is utilized to incorporate functional behaviors of the superelastic NiTi SMA phase. These smart architected IPCs are modelled as RVEs where a unit-cell method is used to reduce the computational cost, while the functional behavior of the complete composite is assessed using the volumetric homogenization technique under periodic boundary conditions. The composite exhibits a unique combination of mechanical properties with improved stiffness and excellent strain recovery behavior that is unexpected from magnesium material and its alloys. The effective elastic stiffnesses are influenced by reinforcement morphology, which varies monotonically with NiTi SMA concentration. Moreover, Mg-NiTi IPCs exhibit an exponential strain recovery behavior, with the concentration of NiTi indicating good damping capability without compromising the stiffness of the magnesium material. Moreover, the power-law fitting parameters predict stretching-dominated behavior for each loading state. These exceptional responses highlight the potential of such smart composites for structural, including vibration absorption, and biomedical, including implants.

Key words: Shape Memory Alloys, Smart Materials, Interpenetrating Phase Composites, Finite Element Analysis, Lattice Structures.

1 INTRODUCTION

Nitinol (NiTi) is a well-known intermetallic shape memory alloy (SMA) that can exhibit both shape memory and superelastic functional properties. The functional response of NiTi SMAs

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is due to their capacity to undergo thermos-mechanically induced microstructural solid-phase transitions [1-3]. Contrarily, magnesium and its alloys are distinguished from other metallic materials by their high specific strength and stiffness, which are strength and stiffness normalized by density [4, 5]. Mg has superior damping qualities, outperforming most metals due to its ease of twinning, dislocation mobility, and weak dislocation pinning at defects or impurities [6-8].

The applications, however, associated with magnesium are limited by their poor strength at both ambient and increased temperatures, as well as lesser ductility when compared to steels and aluminium alloys. Strengthening magnesium while retaining its high damping capability remains a challenge, as conventional strengthening methods frequently degrade damping performance [2, 6, 9]. Furthermore, like other engineered materials, magnesium alloys and composites cannot restore their original shape and mechanical integrity after inelastic deformation or damage. Achieving shape memory or self-recovery in Mg-based materials might increase their endurance, which can allow for the creation of smart materials with sophisticated functions that could have potential advantages for biomedical and vibration-damping applications [7].

To overcome this restriction related to magnesium and its alloys, we numerically investigated and characterized the mechanical properties of interpenetrating phase composites (IPCs) with dual-phase bi-continuous architecture, where NiTi SMA is modelled with strut lattice as reinforcement phase, while magnesium is the matrix phase. These Mg-NiTi IPCs can provide high strength, attributed to the superelastic nature of NiTi and larger strain recovery due to the SME of NiTi SMA without compromising the lightweight and damping properties of Pure Mg. Furthermore, preserving the structural integrity and continuity of the NiTi material inside the composite can boost strength efficiency and strain recovery during unloading [7].

This study presents a proof-of-concept for quantitatively analyzing the functional behavior (elastic moduli, strain recovery, and phase transformation) of NiTi-reinforced IPCs under various loading conditions. To incorporate NiTi SMA, an in-house built Fortran subroutine is used in the finite element program *Abaqus*, while the Mg phase material data is obtained from the literature. In this article, Section 2 will focus on the material and methodology, with an emphasis on the 3D CAD design of the composite, the constitutive model for NiTi SMA, and the effective homogenization technique. The results and discussion will be presented in Section 3, followed by the conclusion in Section 4.

2 METHODOLOGY AND MATERIAL

2.1 DESIGN OF STRUT LATTICE AND ITS COMPLEMENTARY PHASE

The dual-phase strut-architected IPCs considered in this study are modelled, discretized, and numerically analysed using modern software. First, the unit cell for the Kelvin-cell (K) strut architecture unit-cell model for strut architecture is created using *nTopology* software. The process starts with the creation of an implicit body, followed by surface meshing with a feature size of 0.2 mm. Then the second phase is created by using a Boolean operation where the K-stut lattice is subtracted from a dense cube, resulting in a second porous phase. This method

allows the development of cellular structures with exact control over both geometric aspects and material distribution. Figure 1(a)-(c) illustrates the K-strut phase, its complementary structure, and the complete K-IPC. The interconnectivity pattern of the K-strut with IPC can be visualized in Figure 1(d). The interconnectivity pattern between the strut and its complementary phase significantly influences the overall effective response of the composite and varies from one topology to another.

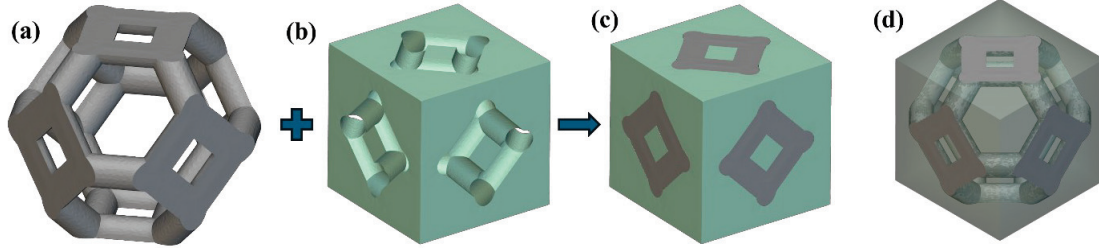


Figure 1: 3D CAD model of the K-strut interpenetrating phase composite (IPC): (a) Kelvin-cell (K) strut lattice structure, (b) corresponding secondary phase of the composite, (c) complete K-strut architected IPC, and (d) IPC with transparent secondary phase to visualize the interconnectivity of the architected phase within the composite.

2.2 THE ZM MODEL FOR NITI SMA

A user-defined subroutine material model [2, 10, 11] has been used that includes the constitutive relationships for NiTi SMA by integrating a time-discrete version to describe the dense NiTi material characteristics. Within the frame of the ZM model, the stress-strain behaviours of NiTi are addressed as follows:

$$\boldsymbol{\sigma} = \mathbf{K} : (\boldsymbol{\varepsilon} - z\boldsymbol{\varepsilon}_{tr}) \quad (1)$$

Where $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{K}$ is the equivalent stiffness of NiTi, $\boldsymbol{\varepsilon}$ is the total applied strain, z is the volume fraction of martensite, and $\boldsymbol{\varepsilon}_{tr}$ is the local inelastic strain due to detwinning and reorientation of the martensitic phase. The equivalent stiffness $\mathbf{K}$ is given in terms of the elastic stiffnesses of austenite ($\mathbf{K}_A$) and martensite ($\mathbf{K}_M$) that are mathematically correlated:

$$\mathbf{K} = [z\mathbf{K}_M^{-1} + (1 - z)\mathbf{K}_A^{-1}]^{-1}. \quad (2)$$

The validation of the ZM NiTi SMA numerical model with experimental data has been performed in preceding work [2, 11], which makes a reliable choice for investigating the behaviors of the NiTi SMA core of the IPC samples considered in this work. Furthermore, the UMAT model requires fourteen input material parameters defining the loading-unloading stress-strain behavior for dense non-linear NiTi and is listed in Table 1. These dense NiTi material parameters are derived from experimental tests cited by Zaki and Momin [2]. Meanwhile, the dense material parameters for the second pure Mg phase material are sourced from the literature [12], with a Young's modulus of 31.06 MPa and a Poisson's ratio of 0.33, respectively.

Table 1: Dense material parameters for superelastic NiTi SMA phase [2]

NiTi SMA Parameter Values			
E_A	61,500 MPa	a	6.89 MPa
E_M	24,000 MPa	b	6.9 MPa
ν	0.3	ε^o	0.04
γ	110 MPa	G	4.66 MPa
α	2,750 MPa	β	5,500 MPa
$\xi_{\sigma E}$	0.4381 MPa/°C	k	2.49 MPa
A_f^o	40 °C	-	-

2.3 FINITE ELEMENT MODELLING AND EFFECTIVE HOMOGENIZATION TECHNIQUE

Both the K-strut and its second phase are meshed with 3D 10-noded tetrahedral elements in *Altair Hypermesh*, which is equivalent to C3D10 in *Abaqus* v16.3 software. The average number of mesh elements is approximately 120,000, with an element size of 0.2 mm in each case. An effective mesh convergence has been found when the number of elements is greater than 50,000 for single-unit cell lattice structures [13]. Furthermore, tetrahedral mesh optimization is performed in *Hypermesh* to further enhance the mesh quality and eliminate unwanted elements that could lead to stress concentrations. The finite element pre-processing is carried out in *Abaqus* v2022. Finite element analyses are carried out in *Abaqus* v2022 under displacement-controlled loadings. The perfect “tie” constraint inhibits the relative motion between the two phases.

The finite element simulations are conducted on a high-performance computing (HPC) facility provided by Khalifa University, where 30 cores are utilized on a single node on the high-performance workstation. Additionally, to reduce the computational cost, the representative volume element (RVE) approach [13] with a single unit-cell method under the influence of periodic boundary conditions is a verified approach reported in various literature [14, 15]. The unit-cell size of the IPC is 1 mm × 1 mm × 1 mm, and the volumetric fraction of NiTi SMA in the IPC ranges from 15% to 40%, with increments at 15%, 20%, 25%, 35%, and 40%. Furthermore, the homogenization technique extracts the effective response of the complete structure from the RVE, where the effective stress is evaluated by using the following correlation:

$$\bar{\sigma} = \frac{\int_A dF}{\int_A dA} = \sum_i^N F_i^R \quad (3)$$

Where $\bar{\sigma}$ represents the effective stress (uniaxial, hydrostatic, or shear) that depends on the loading circumstances, N represents the total number of nodes on which displacement is applied, and A and V represents the geometric parameters with cross-sectional area and volume,

respectively. Here, F_i^R corresponds to the average reaction force, which was computed on the faces where the displacement is applied and then divided by the cross-sectional area A to extract the effective stress of the IPCs.

To compute the evolution of martensite during the phase transformation of NiTi SMA lattice phases, the effective martensite volumetric fraction (z^*) is computed, that arises from a solution-dependent variable (SDV1) from the ZM UMAT subroutine model, providing the phase transformation of TPMS/strut SMA functional phase. The z^* is computed from the following relationship:

$$z^* = \frac{1}{V} \int_V z \, dV \quad (4)$$

2.4 ANALYTICAL BOUNDS FOR ELASTIC STIFFNESS

The effective elastic properties for strut-architected TPMS-IPCs are estimated with two well-known analytical models that include Weiner, alternatively known as Ruess and Voigt [16], and Hashin–Shtrikman [17]. Weiner bounds are a consequence of solving the boundary value problem of a random medium while assuming a homogeneous material, and can be represented as:

$$\sum_{m=1}^n \left(\frac{\phi_m}{E_m} \right)^{-1} \leq E^* \leq \sum_{m=1}^n \phi_m E_m \quad (5)$$

Where ϕ_m is the volumetric fraction of the strut and its second phase, E_m corresponds to the Young's modulus of dense NiTi and Mg materials and E^* is the effective stiffness (uniaxial, shear, and hydrostatic) of the complete composite. As dual-phase IPCs are considered in this study, this provides $n = 2$. On the other hand, Hashin–Shtrikman (HS) bounds are tighter and more accurate than the rule of mixture, and the governing relations for the bounds are presented in [16].

3 RESULTS AND DISCUSSIONS

Starting with the elastic behaviour of the composite, Figure 2 presents the effective elastic moduli (uniaxial, shear, and hydrostatic) of all NiTi SMA strut-architected IPCs for three loading conditions against the volumetric fraction of reinforcement material. To offer a comparative assessment, the effective elastic characteristics are normalized against the dense stiffness of NiTi SMA. This will provide an improvement in the stiffness of the composite with the inclusion of NiTi material within the composite. The overall elastic stiffness results in an increase in elastic stiffness with increasing volumetric fraction of NiTi for all loads. Among analytical bounds, Weiner perfectly predicts and bounds the effective moduli where the response is almost in the middle of the bounds, except during hydrostatic loads. The hydrostatic modulus (Figure 2(c)) for Mg-NiTi IPCs is more closely aligned with the Weiner lower bound, especially at higher volumetric fractions. Contrarily, regarding HS bounds, the model overpredicts the effective response of the IPCs during the hydrostatic loading case. This indicates that the HS limitations are inadequate for predicting the effective response of Mg-

NiTi IPC during hydrostatic loading conditions. Furthermore, the composite exhibited comparatively softer behaviour during hydrostatic loading as indicated by the effective moduli that are closer to the lower bound. Thus, such a combination of materials is suggested to apply in the case of uniaxial and shear loading scenarios.

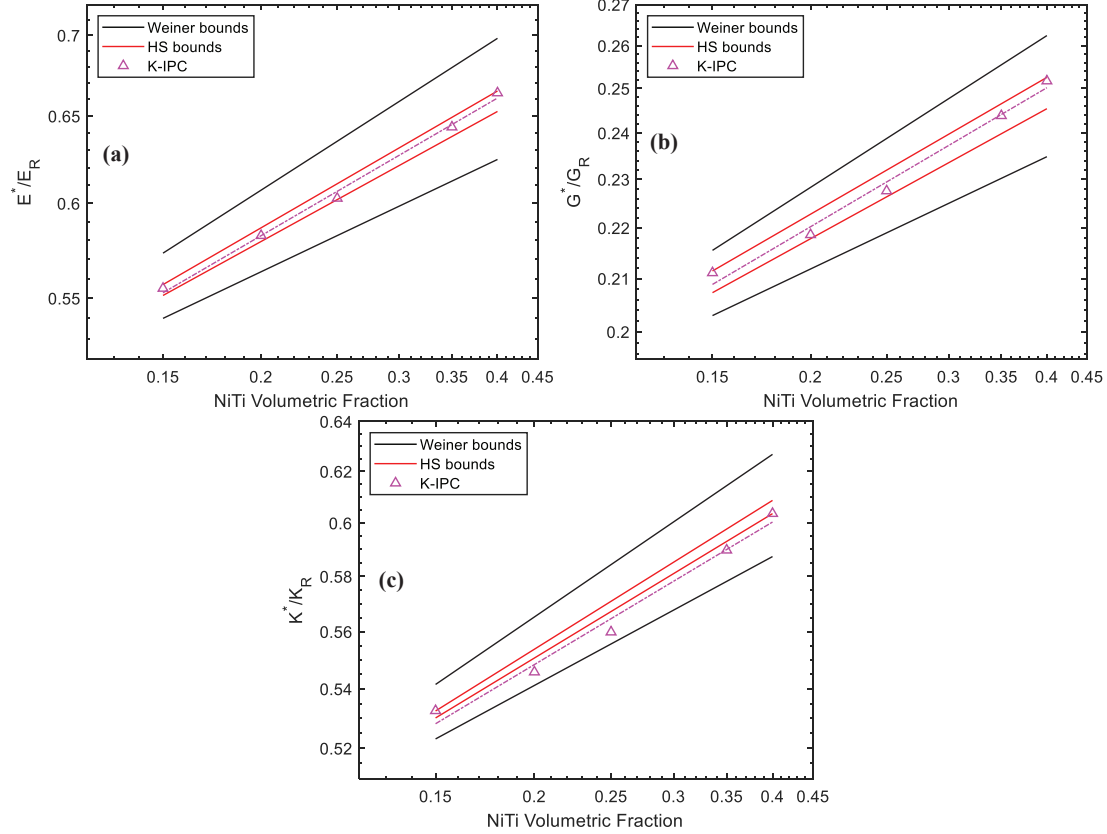


Figure 2: Influence of volumetric fraction of NiTi microstructure on the effective normalized elastic stiffnesses for Mg-NiTi IPCs: (a) uniaxial, (b) shear, and (c) hydrostatic

The phase transformation of NiTi SMA lattice structure within IPCs corresponds to the austenite-to-martensite shifting of the SMA with the application of load. This phase transformation is studied by analysing the change in martensite concentration that corresponds to the martensite volumetric fraction (z^*) with the application of an applied uniaxial load and presented in Figure 3(a). It was observed that an increase in NiTi concentration results in a steeper slope in the z^* -strain curve during the austenite-to-martensite transition zone, indicating a faster and more abrupt phase transition from austenite to martensite. For instance, the 40% NiTi strut lattice exhibits a steeper and more abrupt transition than the 15% or even 20% variants. Moreover, Figure 3(b) presents the effective strain recovery for Mg-NiTi IPC, which shows an exponentially increasing trend in recovering the overall strain with increasing concentration of NiTi material within the composite. This can be attributed to the shape memory

effect of NiTi material that returns the maximum possible amount of strain during unloading of the composite. This is the primary advantage for Mg and its alloys to integrate with NiTi SMA, which will not only enhance the damping capability but also without compromising the strength of the magnesium.

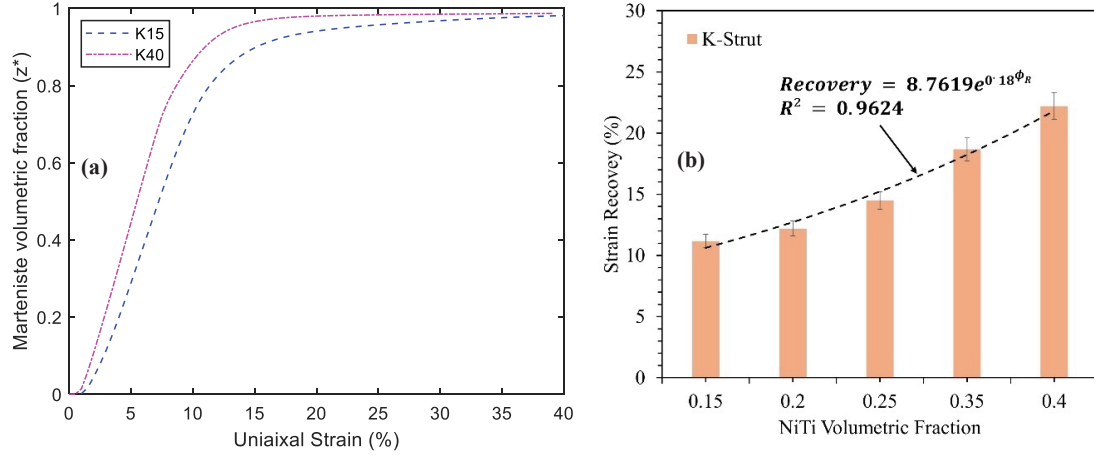


Figure 3: Influence of volumetric fraction on (a) Effective martensite volumetric fraction (z^*) with respect to uniaxial load, and (b) strain recovery behavior for Mg-NiTi IPCs

Figure 4 presents the contour plots illustrating the austenite-to-martensite transformation in a K-strut lattice structure under uniaxial loading. The blue color represents the austenite phase, the red color highlights the martensite phase, and the intermediate colors indicate the transition zone from austenite to martensite.

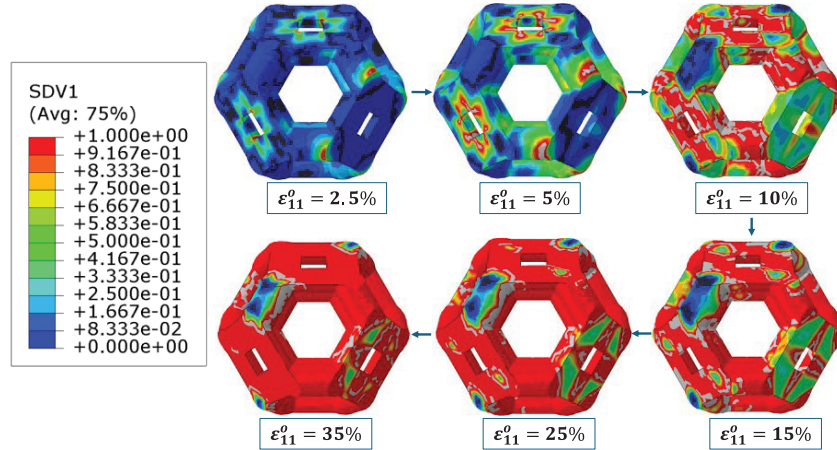


Figure 4: Austenite-to-Martensite phase transformation contours of K-strut NiTi SMA phase against uniaxial strain.

At lower strains, the transformation initiates at the corners of the strut lattice, making them critical zones during phase transformation. This is followed by a transformation in the strut

arms, which are bounded by the Mg secondary phase. Notably, the interface region between the Mg and NiTi phases experiences higher stress, which triggers the phase transformation and facilitates its propagation throughout the structure. The von Mises stress contours are presented in Figure 5, which indicates high stress regions around the strut lattice, especially at the corners. These high-stress regions indicate regions across struts that are prone to crack initiation and debonding.

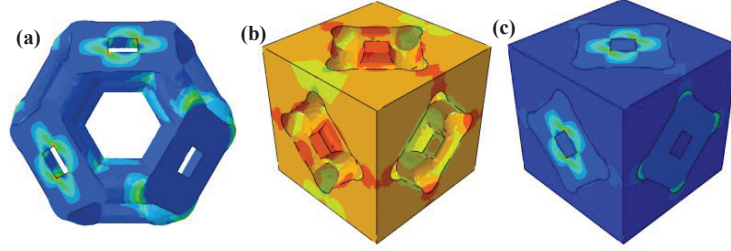


Figure 5: von-Mises contours: (a) NiTi Kelvin cell foam, (b) Mg complementary phase, and (c) Mg-NiTi IPC at 20% volumetric fraction of NiTi material.

Table 2 indicates the power-law fitting parameters that describe the deformation mechanism of the K-Strut IPC, indicating a stretching-dominated response ($n = 1$) across all loading scenarios. The primary reason for this is that the Kelvin cell strut lattice structure is symmetric in all three perpendicular directions, exhibiting strong resistance to bending, which drives the overall effective response to be stretching-dominated rather than bending-dominated. Furthermore, the exponential strain recovery, driven by the NiTi phase change, emphasizes the critical role of strain recovery in increasing the stiffness and functional behaviour of the composites.

Table 2: Fitting parameters for elastic moduli and strain recovery for Mg-NiTi IPC.

K-Strut IPC	Elastic modulus, E^* [MPa]		Shear modulus, G^* [MPa]		Bulk modulus, K^* [MPa]		Strain Recovery (%)	
Expression	$\left \frac{E^*}{E_R}\right = a\phi_R^n + \frac{E_M}{E_R}$		$\left \frac{G^*}{E_R}\right = a\phi_R^n + \frac{G_M}{E_R}$		$\left \frac{K^*}{E_R}\right = a\phi_R^n + \frac{K_M}{E_R}$		$ae^{n\phi_R}$	
Fitting parameters	a	n	a	n	a	n	a	n
Values	0.4401	1.1089	0.1696	1.0988	0.2959	1.0931	8.7619	0.18

4 CONCLUSIONS

In summary, this study numerically investigates the functional behaviour of dual-phase interpenetrating phase composites (IPCs) where the reinforcement phase comprises of smart nitinol (NiTi) core that is embedded in elastoplastic magnesium as the second phase. K-strut lattices are considered here to model the NiTi SMA reinforcement phase, where a UMAT subroutine model is used to incorporate the constitutive model for the SMA phase. A representative volume element (RVE) with a unit-cell method is used, where periodic boundary

conditions and effective homogenization techniques are employed to analyze the functional behavior of IPCs.

- The effective performance of the composite provides improvement in elastic stiffness and displays exponential strain recovery, making them suitable for vibration absorption and biomedical applications.
- Integrating NiTi SMA with magnesium significantly enhances the effective stiffness of the composite.
- Regarding analytical bounds, Weiner analytical model perfectly predicts and bounds the stiffness of the composite. However, the Hashin–Shtrikman (HS) bound is tighter than Weiner and overpredicts the effective properties during hydrostatic loads.
- The volumetric fraction of NiTi SMA significantly influences the phase transformation behavior of the lattice structure.
- The effective strain recovery for Mg-NiTi IPC exhibits exceptional results, showing an exponentially increasing trend with the concentration of NiTi. This behavior can be attributed to the shape memory effect of NiTi material and is not expected from magnesium alone.
- The power-law fitting parameters indicate a stretching-dominated response across all loading scenarios, primarily due to the Kelvin cell architecture's high bending resistance.

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