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# Residual stresses and distortion in additively manufactured compositionally graded and dissimilar joints

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## ABSTRACT

Additively manufactured compositionally graded joints are potentially attractive to minimize abrupt changes in residual stresses and distortion of dissimilar alloy joints. Performance of these graded joints depends on the residual stresses and distortion governed by the transient temperature field during additive manufacturing and local mechanical properties of the joint. Here we develop, validate and utilize a thermo-mechanical model to provide a definitive way to additively manufacture sound graded joints for minimizing abrupt changes in residual stresses and distortion of the dissimilar joints. This model calculates residual stresses and distortion from accurate temperature fields calculated using a well-tested heat transfer and fluid flow model and temperature dependent alloy properties estimated by thermodynamic calculations. Both graded and dissimilar joints of 2.25Cr-1Mo steel to alloy 800H and Ti-6Al-4V to 800H, fabricated using laser-assisted powder based direct energy deposition process are examined. It is found that the sharp changes in residual stresses in dissimilar joints between Ti-6Al-4V and 800H can be effectively minimized by fabricating a graded joint between them. Although the magnitudes of residual stresses in Ti-6Al-4V to 800H joint are higher than that in 2.25Cr-1Mo steel to 800H joint, the former is less susceptible to warping, buckling and delamination due to the high room temperature yield strength of the Ti-6Al-4V substrate.

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## 1. Introduction

Dissimilar metal joints are used in aerospace, nuclear power generation, marine and automobile industries [1,2]. However, dissimilar joints often fail because of the distortion and high gradient of residual stresses generated due to the sharp changes in chemical composition and properties across the joint interface [2–5]. These difficulties can be minimized by the development of compositionally graded transition joints where the variations of chemical composition and properties occur smoothly across the joint over a large distance [6,7]. Additive manufacturing (AM) is a practical choice to fabricate compositionally graded transition joints by adding materials of varying compositions in a layer-by-layer manner [8-12]. AM has already been used to fabricate transition joints between stainless steels and nickel base superalloys for nuclear applications [10,11] and between titanium alloys and iron-nickel alloys for aerospace applications [12]. However, additively manufactured compositionally graded components also encounter residual stres-

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https://doi.org/10.1016/j.commatsci.2017.11.026 0927-0256/© 2017 Elsevier B.V. All rights reserved. ses and distortion because of the spatially non-uniform and transient temperature field during the process. Depending on the local room temperature yield strength of the graded components, these residual stresses and distortion may result in premature fatigue failure, delamination, warping and buckling. Therefore, accurate estimations of residual stresses and distortion are necessary for both dissimilar and graded joints to fabricate sound compositionally graded components by AM for minimizing abrupt change in residual stresses and distortion of the dissimilar joints.

There are two main differences in residual stresses and distortion between compositionally graded and single alloy components. First, the evolution of residual stresses depends on the cooling process of the component at the end of the deposition. In graded components, the difference in the thermo-physical properties between the two end alloys governs the cooling process and thus the evolution of the residual stresses and distortion. Second, susceptibilities to warping, buckling and delamination depend not only on the magnitudes of the residual stresses but also on the local room temperature yield strength of the graded component. Since, the yield strength varies spatially in many compositionally graded components, two regions with the same magnitude of residual stresses







can have different susceptibilities to delamination, buckling and warping.

Experimental measurements of residual stresses and distortion of AM components are time consuming and expensive [13]. These measurements also depend on sample preparation, shape and size of the components and accuracy of the experimental methods such as X-ray or neutron diffraction [14–16]. For both compositionally graded and dissimilar metal joints, use of non-destructive measurement techniques are restricted by the limited availability of strain free lattice spacing for all compositions [4,17]. A recourse is to calculate residual stresses and distortion in all locations of the component using numerical models. However, most of the existing numerical models of AM residual stresses neglect the convective flow of liquid metal inside the molten pool that often dominates the heat transfer during AM [18]. This simplification may result in inaccuracy in temperature field calculations. [19] and as a result, residual stresses and strain calculated based on such inaccurate temperatures can become unreliable [18]. Another difficulty in these calculations is the limited availability of the temperature dependent thermo-physical and mechanical properties data for different alloy compositions used in the graded components [20]. In the literature, thermodynamic calculations have been done to estimate the alloy properties for graded joints between titanium alloys, nickel base superalloys and steels [11,12]. However, so far the estimated properties have not been used to calculate residual stresses and distortion of the compositionally graded transition joints. Because of the challenges mentioned above, literature on the estimation of residual stresses and distortion of additively manufactured compositionally graded components is scarce.

Here, we calculate, for the first time, the residual stresses and distortion of compositionally graded joints as well as dissimilar joints of (a) 2.25Cr-1Mo steel to an iron-nickel alloy (800H) and (b) a titanium alloy (Ti-6Al-4V) to 800H, fabricated using laser assisted powder based direct energy deposition process. In these graded joints, alloy composition changes with layers along the build height direction. A thermo-mechanical model is used to calculate residual stresses and distortion from the transient temperature field accurately estimated using a heat transfer and fluid flow model that considers the effects of convective flow of liquid metal. The temperature and composition dependent thermo-physical and mechanical properties are estimated by thermodynamic calculations using a commercial program, JMatPro<sup>®</sup>. This program calculates different alloy properties for a specified temperature range based on the chemical composition of the alloy. The thermomechanical model is rigorously tested and validated against independent experimental data. The spatial variation of the residual stresses and distortion for the two types of graded joints is compared based on their alloy properties, transient temperature fields and molten pool dimensions. The relative advantages of fabricating graded joints over dissimilar joints for minimizing the abrupt changes in residual stresses and distortion are examined for the two types of joints.

#### 2. Theoretical investigation

#### 2.1. Modeling assumptions

The calculations of the residual stresses and distortion are performed in two steps. First, a well-tested three-dimensional heat transfer and fluid flow model [21–23] is used to calculate transient temperature fields. Second, based on the calculated temperature fields, residual stresses and distortion are predicted using a commercial finite element analysis (FEA) code, Abaqus<sup>®</sup> [24]. The following simplified assumptions are made in both the heat transfer and fluid flow model and the FEA mechanical model.

- (1) Densities of the solid and liquid alloys are considered as temperature independent.
- (2) The surfaces of the deposited layers are assumed to be flat.
- (3) The effects of strains induced by solid-state phase transformation and creep are neglected to make the calculations tractable.
- (4) Each layer is assigned to a pre-defined composition and the effect of dilution due to re-melting of the substrate or previous layers on the layer composition is not considered.

# 2.2. Thermodynamic calculations for alloy properties

Temperature and composition dependent thermo-physical and mechanical properties of alloys are needed for the heat transfer and fluid flow calculations as well as the finite element based mechanical model. During the fabrication of compositionally graded joints, the mixing of chemistries often leads to high alloving element concentrations. Local chemical compositions can extend into regions where experimental property data are not available and approximations such as simplified phase diagrams, stressstrain plots and dilute alloy properties are not applicable. An alternative for determining important material properties is through numerical modeling based on elemental mixing interactions. [Mat-Pro<sup>®</sup> is a thermodynamic program designed for materials processing applications that models important alloy properties such as equilibrium phases, phase transformations, thermo-physical properties and mechanical behavior [25]. The CALculation of PHAse Diagrams (CALPHAD) method, which is widely established in the literature [26], is used to determine phase fractions and compositions for a given alloy concentration and temperature or temperature range.

The modeling of thermo-physical and mechanical properties using JMatPro<sup>®</sup> involves the following sequential steps. First, the equilibrium fraction of phases is determined through the minimization of the total Gibbs energy method using thermodynamic excess functions to account for the mixing of elements. The property, *P*, of interest for each phase is expressed as [27],

$$P = \sum_{i} x_{i} P_{i}^{0} + \sum_{i} \sum_{j>1} x_{i} x_{j} \sum_{\nu} \Omega_{ij}^{\nu} (x_{i} - x_{j})^{\nu}$$
(1)

where  $P_i^0$  is the property of the phase in the pure element,  $\Omega_{ij}^{\nu}$  is a binary interaction parameter between elements *i* and *j* dependent on an integer, *v*. *x<sub>i</sub>* and *x<sub>j</sub>* are the mole fractions of *i* and *j* in the phase, respectively. The effects of temperature on the property of a phase are taken into account through both  $P_i^0$  and  $\Omega_{ij}^{\nu}$ , which are function of temperature. The total property of the alloy is then determined from the phase fractions and properties of each phase using the general law of mixtures [28]. The use of this type of model allows for the approximation of both thermo-physical and mechanical properties as functions of composition and temperature and accounts for effects of multi-phase microstructure. The thermo-physical and mechanical properties are provided in Tables 1–5 and in Supplementary document.

#### 2.3. Governing equations and boundary conditions

Detailed description of the thermo-mechanical model is available in a previous publication [18]. For completeness, a few salient features of the model are provided as follows. The heat transfer and fluid flow model solves the equations of conservation of mass, momentum and energy [29], as given below, respectively.

$$\frac{\partial \left(\rho \, u_i\right)}{\partial x_i} = 0 \tag{2}$$

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