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Modelling the elastic properties of bi-continuous composite microstructures captured with TriBeam serial-sectioning

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ABSTRACT

The elastic and physical properties of a tungsten-copper (W-Cu) bi-continuous composite were predicted from microstructural data captured using TriBeam serial sectioning. The reconstructed 3D volume was converted into a Finite Element (FE) mesh. The minimum representative volume elements (RVEs) required for calculating phase volume fraction, Young's modulus and Poisson's ratio were determined. The predicted volume fraction of Cu and Young's modulus were found to be within 2.6%, and 3.6% of the respective experimentally determined values. The minimum RVE size is found to be dependent on the material property. The variability in the required RVE size must be considered for material properties of W-Cu and similar bi-continuous composite microstructures.

1. Introduction

In many engineering applications, the requirements for critical system components cannot be met by any single material or alloy. Future aerospace and energy technologies will require functional materials that can effectively manage and dissipate temperatures greater than 2000 °C and that can retain structural integrity over long thermal exposures [1,2]. Heterogeneous, composite-microstructure materials have been shown to withstand these extreme environments, as they provide favourable properties from their constituent phases.

Copper-infiltrated-tungsten (W-Cu) bi-continuous metal-matrix composite (MMC) materials have been shown to perform well in high-temperature applications. Optimization of the W-Cu microstructure is required in order to improve the high - temperature properties of this material. Computational modelling and simulation have been used in conjunction with mechanical testing and characterisation to tailor the specific material properties of W-Cu and similar heterogeneous materials.

The prediction of the physical and mechanical properties from three-dimensional (3D) microstructural representations of bi-continuous W-Cu composites has previously been limited to functionally graded models [3] and continuous fibre-reinforced set-ups [4]. Recently, two-dimensional (2D) models created using the Voronoi tessellation technique [5] have been used to generate virtual bi-continuous W-Cu microstructures. However, 2D stress states generated using finite element (FE) analysis cannot be directly compared to the experimentally measured properties in W-Cu and other composites [6].

Finite element simulations using idealised, 2D microstructures under plane strain conditions have been performed elsewhere [7,8]. In these simulations, a simple representation of the microstructure consisting of a unit cell with a single circular void inside a square elastic-plastic medium was used, which allowed for the study of void interaction effects. The model was further simplified by treating one quarter of the cell and by applying periodic boundary conditions.

The unit cell could also be approximated through the FE analysis of axisymmetric cylindrical unit cells, as proposed by Tvergaard [9]. Both the 2D plane strain and axisymmetric unit cell techniques

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have been used extensively to analyse the mechanical response of particle-reinforced composites (PRCs) [10–13]. These simplified 2D unit cell methods have provided computationally inexpensive insight into the deformation behaviour of materials, however they ignore microstructural complexities such as phase connectivity and non-uniform particle distributions in PRCs, which significantly affect the deformation behaviour [6,14]. Recently, Chen et al. [15] have addressed this issue in a voxel-based, discrete, computational model for both bi-continuous and particulate composites and have produced successful results for the dependence of bulk and shear moduli on volume fraction.

Modelling efforts that are based on 3D microstructure-based FE simulations, are able to capture the alignment, aspect ratio, and distribution of the particles. Particle stresses, localised damage and debonding mechanisms have been studied using simulations that approximate the reinforcement phase of PRCs as perfect spheres [16–20].

Characterisations of 3D microstructure for input to FE simulations have been performed using non-destructive techniques such as X-ray micro-tomography [21–23]. However, dense materials such as tungsten have a high mass attenuation coefficient, making microstructural characterisation impractical with low-energy X-ray micro-tomography systems. Neutron micro-tomography is also not a viable option, because the technique currently lacks the spatial resolution to characterise the fine-grained microstructures present in W-Cu composites [24]. Mechanical polishing-based, serial sectioning techniques have been used to characterise 3D microstructures [25,26] and in a recent approach [27], a 3D microstructure was developed from statistical analysis of a single 2D microstructure from a scanning electron microscope image. However, these approaches require significant time, financial investment, and careful polishing routines for composites containing phases with non-uniform hardness.

The TriBeam system [28,29] was used to section and capture high-resolution SEM images of the W-Cu composite microstructures. The TriBeam consists of a femtosecond laser coupled with a FIB-SEM microscope for fast and automated 3D dataset acquisition with multiple imaging modalities, as described in more detail elsewhere [29]. Using this technique, material volume elements of several hundred microns on edge were gathered, with a sub-micron sectioning resolution and material removal rates four to five orders of magnitude faster than those of a gallium focused ion beam (FIB).

Without accurate microstructural information, the minimum representative volume element (RVE) (i.e., the smallest volume of microstructure in which simulations can be made to statistically represent the macroscopic properties of the composite), for W-Cu and similar bi-continuous composites, cannot be determined accurately. While modelling a larger, more conservative RVE size will better represent the composite statistically, it comes at the cost of increased computational time and resources. An optimally defined RVE allows for the evaluation of simulations at optimal time, permitting higher degrees of freedom in the FE simulation (i.e., the investigation of non-linear effects such as plasticity, damage and de-bonding of material phases).

The minimum RVE size is dependent on the specific material property of interest. Previous research has quantified this variability in RVE size for physical, mechanical, thermal and electrical properties of a material [28,30–32]. While considerable work has been conducted on determining these properties, RVE analysis of the Poission's ratio in composite microstructures, has not been extensively studied [33–35]. In addition, experimental techniques for evaluating the Poisson's ratio of composites are scarce and complex when compared with those for other mechanical properties. These techniques include uniaxial tensile testing [36,37], bulge testing [38,39], X-ray diffraction [40,41], resonance testing [42] and micro-bending techniques [43]. These limitations persist, despite Poission's ratio being an important material property used in the design of mechanical and thermo-mechanical components. Therefore, development of computational approaches for determining this property is essential for the overall improvement of material design processes.

In this investigation, serial sectioning via the Tribeam system using femtosecond laser ablation was used to capture the microstructural information in W-Cu composites. SEM images captured during serial sectioning were segmented into constituent W and Cu phases and then aligned into binarized image stacks. The final datasets were then converted into 3D meshes that were used for finite element analysis (FEA) to simulate compressive strain. The volume fraction of Cu, Young's modulus and Poisson's ratio of the material were determined for the collected 3D datasets and the RVE sizes for these material properties are discussed.

2. Methodology and material

2.1. Tungsten-Copper composite (W-Cu)

W-Cu is a two-phase, bi-continuous, metal-matrix composite consisting of a tungsten (W) matrix phase and a copper (Cu) reinforcement phase. Additionally, W and Cu have different atomic crystal structures (W and Cu being BCC and FCC, respectively), large atomic radii difference of >20%, and significantly different electro-negativities (W = 2.36 and Cu = 1.9), thus violating the Hume-Rothery rules [44,45] and making them virtually immiscible. An exception to immiscibility exists when W and Cu powders undergo high-energy ball milling. In this case, dissolution of a small amount of Cu into W has been observed [46,47].

W-Cu composites are generally fabricated by Cu infiltration into porous W. This process involves compacting and pre-sintering W powder at approximately 1300 °C. The pre-sintered blocks are submerged in molten Cu at approximately 1400 °C to fill the pore space between the W grains. Typically, 1–2% of residual porosity is found in W-Cu composites [48–50]. Other processes exist to produce thin W-Cu films such as plasma spraying [51] and electron-beam physical vapour deposition [52].

The high electrical and thermal conductivities of Cu, combined with the high melting point (3422 °C) and low vapour pressure of W, have led to W-Cu being widely used in technologies such as electrical contacts, welding electrodes and as tools for electro-discharge machining [53–56]. For short time periods, until the Cu is completely consumed, W-Cu composites are able to withstand extreme temperature loading via Cu ablatively cooling the W structure. At high temperatures, the Cu melts and vaporises, extracting heat from the system and passively cooling the W matrix, keeping it at a temperature no more than the boiling point of the Cu (about 2550 °C). When the Cu reservoirs are empty, the composite becomes susceptible to high-temperature degradation and failure of the W matrix will occur as the temperature of the material can then increase above the boiling point of Cu [56,57].

For this investigation, literature values for the Cu volume fraction and Young's modulus of W-Cu with 10 wt% Cu, produced by Plansee [58], were used for validating the simulations based on the TriBeam tomography W-Cu datasets. Table 1 shows these data.

2.2. Capturing the microstructure with TriBeam serial sectioning

A full description of the TriBeam sectioning methodology for the W-Cu sample is available elsewhere [28]. A summary of this work is presented as follows: