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A Novel Multi-scale Modelling Approach for Determining the Bulk Properties of Difficult-to-Characterise Composites

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A multi-scale modelling approach is presented for determining the bulk properties of copper-infiltrated Tungsten (W-Cu). A three-dimensional (3D) data-set of the W-Cu microstructure was generated using a novel serial-sectioning instrument. The image data were then reconstructed into a 3D Finite Element (FE) mesh. This made it possible to determine the bulk properties of W-Cu by simulating a representative volume of the microstructure.

1. Introduction

In many of today's cutting-edge engineering applications, the demand placed on the critical components of a system cannot be met by any single material or alloy. Future aerospace and energy technologies will require materials that can effectively manage and dissipate ultra-high temperatures (2000°C and higher), while retaining high thermo-mechanical strength over long time domains [1]. However, long lead times and high financial costs are typical during the development and certification stages of such materials [2].

Recent advances in microstructural imaging techniques, multi-scale computational modelling, and high-performance computing, have led to a drive towards implementing these methods into material development and certification processes. The ultimate objective is the reduction of experimentation costs and lead times required to bring ultra-high temperature materials to commercial applications. These computational techniques require significant financial investment and time to develop expertise. More importantly, accurate image-processing and FE meshing of the material microstructure are critical for numerically correct results, and require best-practice techniques to control [3].

In addition, the 3D microstructure of some materials is difficult to characterise (DTC) using traditional x-ray tomography (μCT) techniques. X-ray absorption makes the characterisation of highly dense materials (e.g. tungsten) impractical with low-energy μCT. Neutron tomography is currently not an alternative as it lacks the resolution to characterise fine-grained microstructures (Fig. 1) [4].

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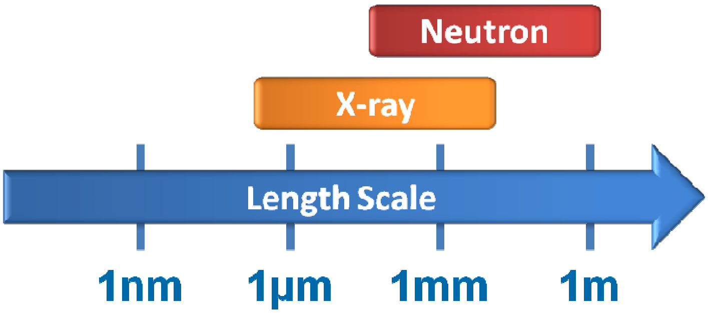

Fig. 1: Resolutions of x-ray and neutron tomographic techniques

The following research presents a technique for characterising microstructural data and generating FE meshes for determining the bulk mechanical properties of DTC composite microstructures. The 3D microstructural data of W-Cu, a candidate material for high-temperature applications, were generated using serial-sectioning and image-processing techniques. The image data were then reconstructed into a 3D FE mesh using iso2mesh (i2m), an open-source meshing library traditionally used in medical applications [5]. A mesh-sensitivity study was conducted on this microstructure using i2m, and compared against Simpleware (SIP), a commercial mesh generator, via the Finite Element Method (FEM).

2. Methodology

A sample of W-Cu (15wt% Cu) was obtained from Plansee, a manufacturer of high-performance, refractory-metal components [6]. The material was created using the infiltration technique. The exact infiltration process and its parameters for this sample are propriety to Plansee and not known for this investigation. A typical infiltration process to create W-Cu composites of 98-99% density is outlined in the literature [7]. To obtain the 3D dataset of the W-Cu microstructure, the use of non-destructive techniques, such as low-energy x-ray or neutron tomography, is currently impractical. However, destructive techniques (i.e., serial-sectioning) whereby material is removed and images are taken to build the 3D dataset are a viable alternative. For this investigation, the sample was placed in a new serial sectioning device called the TriBeam [8], which combines a femtosecond laser with a Focused Ion Beam (FIB) and a Scanning Electron Microscope (SEM). This allows for the fast acquisition of 3D microstructural data sets.

The TriBeam uses a femtosecond laser to ablate the top surface of the sample at 250 nm intervals. Between each interval or ‘slice’, the sample is tilted so that the ablated surface is normal to the electron beam. A two-dimensional (2D) secondary-electron image is then collected from the recently ablated sample surface. The process is continued to produce a stack of secondary electron images through the sample thickness. On completion of the data collection, further image processing was required to characterise accurately the microstructure before FE meshing and simulation. Individual images in the stack were aligned to correct for any planar displacement during sample rotation towards the electron beam. Image filters were used to remove image artefacts, and to define clearly the separate copper and tungsten material phases. The modified image stack was then converted into a black/white (i.e. binary) image. Fig. 2a shows a 25µm x 25µm x 25µm sample stack of W-Cu (with 15% wt Cu), that was used for further analysis.

The image stack was imported into Matlab as a 3D image array. Iso2mesh was used to convert the 3D image array into an all-tetrahedron mesh (Fig. 2b). Simpleware meshes were generated using its proprietary mesh algorithm and graphical user interface. The meshes were then imported into Abaqus 6.11-1 for Finite Element Analysis (FEA) simulations. The tungsten Young's modulus and Poission's ratio used for the simulations were 408.0 GPa and 0.28, respectively [9]. The copper Young's modulus and Poission's ratio used for the simulations were 129.8 GPa and 0.34, respectively [9]. Periodic (i.e., symmetry) boundary conditions are applied to fix the model in 3D space. A known, compressive displacement is applied to the model to obtain the reaction force and displacement output. Hooke's law is then used to determine the Young's modulus.

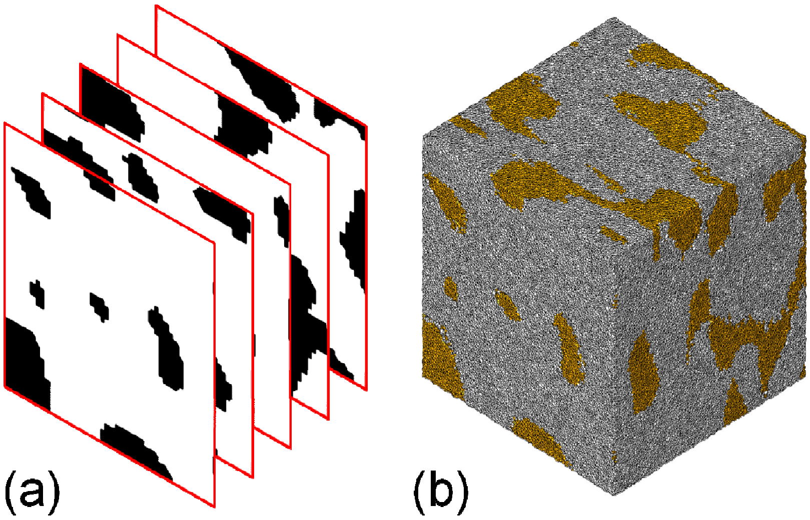

Fig. 2: (a) Binarised microstructure showing Tungsten (white) and Copper (black) phases. (b) Microstructure converted into a FE mesh.

3. Results & Discussion

Fig. 3 shows the average Young's modulus comparison between the Simpleware and iso2mesh meshing techniques at different levels of mesh refinement. For the Simpleware result, as the model size increases, there is a slight drop in the Young's modulus value. This shows a small, yet present amount of mesh sensitivity in the model as the model size is increased from 800,000 to 1.6 million elements. The change in result is less than 0.5% between coarse- and fine-mesh results, indicating Simpleware's capability in accurately capturing the microstructure at its most-coarse mesh generation settings.

The iso2mesh result shows a similar relationship between Young's modulus and mesh refinement, with less than a 0.5% change between coarse- and fine-mesh results. An exception exists however, when the iso2mesh models use coarse meshes (i.e., 800,000 to 1 million elements). In this region the Young's modulus result peaks at approximately 1 million elements before dropping in value. This small change is possibly due to how iso2mesh approximates the microstructure at coarse mesh values. The effect however is negligible and disappears when the mesh density is increased.

Table 1 shows a summary of the most coarse (800,000 elements approx.) and most fine (6.5 million elements approx.) Simpleware (SIP) and iso2mesh (i2m) mesh results, and compares them with analytical and literature-based results. The theoretical result was calculated using the rule of mixtures [10]. The coarse and fine results of both mesh techniques are within 0.2% of the official result for W-Cu (15wt% Cu) in Plansee literature, indicating the robustness of the multi-scale modelling approach. A 7% variation between the FE results and theory is also observed. However, the rule of mixtures is an ideal calculation and does not consider factors such as material morphology, which can significantly affect material properties.

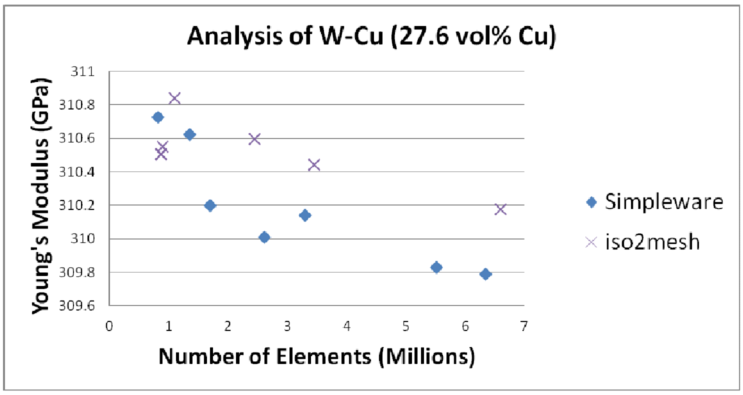

Fig. 3: Average Young's modulus comparison between the Simpleware and iso2mesh techniques.

W-Cu Result	Young's modulus (GPa)
Theory	331.20
Plansee [6]	310.00
i2m (Coarse)	310.51
i2m (Fine)	310.18
SIP (Coarse)	310.73
SIP (Fine)	309.59

Table 1: Summary of Simpleware and iso2mesh results.

4. Conclusion

The variations of results were found to be less the 0.5% at different mesh densities for both meshing techniques. This indicates that both iso2mesh and Simpleware are capable of calculating the bulk mechanical properties of microstructures at reasonably coarse mesh densities. This would be ideal for the simulation of larger samples, such as would be required for representative volume-element studies. Future research is currently investigating this. Both mesh techniques generated mechanical properties within 7% and 0.2% of the theoretical and literature-based results, respectively. While further research is required, iso2mesh has shown significant capability as an open-source alternative for low-cost pre-processing of complex material microstructures.

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