Computational Materials Science 84 (2014) 318–326

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Mechanism of plastic damage and fracture of a particulate tungsten-reinforced copper composite: A microstructure-based finite element study

Alessandro Zivelonghi [1], Jeong-Ha You *

Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, 85748 Garching, Germany

ARTICLE INFO

Article history:
Received 28 June 2013
Received in revised form 4 October 2013
Accepted 19 November 2013
Available online 9 January 2014

Keywords:
Microstructure-based finite element analysis
Tungsten–copper composite
Plasma-facing component
Heat sink material
Plastic damage
Fracture

ABSTRACT

Tungsten particle-reinforced copper composites offer a unique combination of conductivity and strength for high-temperature heat sink applications. Particulate tungsten reinforcement leads to a strong enhancement of strength below 300 °C while the ductility is significantly decreased on the other hand. Above 500 °C, the reinforcing effect disappears completely and the ductility is further reduced. The composite exhibits a considerable scattering in the tensile elongation.

The aim of this computational study is to understand the deformation and fracture behavior of the composite on the basis of its microstructure. To this end, we employed a microstructure-based finite element analysis using a dedicated micrograph mapping tool OOF. The material parameters required for damage modeling were calibrated by fitting the simulated tensile curve into the measured one.

A simulation of tensile loading case at 300 °C revealed the characteristic development of plastic strain localization forming a narrow deformation band. Such a localized plastic yield pattern occurs as a result of von-Mises stress concentration in this band. Hydrostatic tensile stress is also concentrated in the same band leading to initiation and accumulation of ductile damage and finally to cracking. The scattering in the final rupture strain is shown to be a consequence of the random microstructure. The local configuration of the phase morphology turns out to play an important role in triggering the strain localization.

The pronounced impact of test temperature on yield stress and rupture strain is attributed to the presence of thermal stress produced by thermal expansion mismatch upon heating.

1. Introduction

The heat sink of the plasma-facing components in a nuclear fusion reactor plays an important role in the power exhaust of the facility. Since the plasma-facing component is a high-heat-flux component to be subjected to surface heat loads up to 20 MW/m^2, mechanical stability as well as heat removal capacity at an elevated operation temperature is a crucial requirement. Since the heat sink is operated as a pressurized nuclear component, a heat sink material has to possess sufficient strength and toughness to fulfill the structural design criteria. One of the hitherto most preferred heat sink materials for a water-cooled high-heat-flux component is precipitation-hardened Cu1CrZr alloy.

For enhancing the mechanical performance at higher temperatures, various kinds of tungsten–copper (W–Cu) composites have been considered as candidate heat sink materials [1–5]. The combination of hard and refractory W reinforcement with ductile and highly conductive Cu matrix enables one to achieve the essential requirements on the properties, which otherwise can hardly be met in a monolithic material.

Recently, a novel W–Cu composite material was successfully developed based on the vacuum melt infiltration technique by the authors and the partners of Fraunhofer Institute of Applied Materials [6]. This composite consists of particulate W reinforcements and Cu alloy matrix. In their work, precipitation-hardened Cu1CrZr alloy was used as matrix material in order to enhance the high-temperature strength. In conventional W–Cu composites pure Cu has been usually used, but it suffers from significant thermal softening at elevated temperatures. In this study, we consider a specific composite composition with W volume fraction of 30%.

The effect of the particulate W reinforcement on the mechanical behavior of the composite seems rather ambivalent. The observed general trend of tensile stress–strain curves shows that the rupture strength is increased in comparison to the Cu1CrZr alloy whereas the elongation is considerably decreased. However, both effects disappear completely at high temperatures (>500 °C). Another feature is that the composite material exhibits a notable scattering in

---

* Corresponding author. Tel.: +49 (0)89 3299 1373; fax: +49 (0)89 3299 1212.
E-mail addresses: a.zivelonghi@2-g.it (A. Zivelonghi), you@ipp.mpg.de (J.-H. You).

[1] Current address: 2G Italia Srl, Italy.

0927-0256/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2013.11.067

ultimate elongation which reaches the maximum at 300 °C and decreases at higher temperatures.

The aim of this study is to understand the failure behavior of the present composite based on the microstructure. Focus is placed on ductile damage and fracture feature in the targeted operation temperature range between 300 °C and 550 °C. To this end, we applied so called microstructure-based finite element analysis (Mb-FEA) using a dedicated mapping tool OOF2 (Object-Oriented FEA) developed at NIST, USA. Direct mapping of a micrograph into a finite element model allows one to simulate the macroscopic behavior of a composite material based on the real microstructure. In Mb-FEA the field quantities are computed both on macro- and microscopic length scales simultaneously. In this study, the emphasis is placed on local processes of damage accumulation and crack initiation. The impact of microstructure on the failure mechanism is also elucidated.

2. Materials

Fig. 1 shows a scanning electron microscopy (SEM) image of the typical microstructure of the reference material (W volume fraction: 30%) in which a skeleton-like network of W particles is filled with the Cu1CrZr alloy matrix. In the following this reference material is referred to as W30–CuCrZr. The micrograph exhibits that the reinforcing W particles are distributed uniformly in the matrix on a macroscopic length scale, but it also reveals local agglomeration or depletion of the particles on a microscopic scale. The average spacing between the particles is comparable to the mean diameter of the particles (~4 μm). The micrograph indicates that the interfacial wetting is complete. Thus, the interfaces are assumed to be perfect in the present modeling. The composite was heat-treated after the infiltration process for precipitation hardening of the Cu1CrZr alloy. The ageing temperature was 480 °C.

The tensile stress–strain curves of the W30–CuCrZr composite, measured at 300 °C and 550 °C respectively, are plotted in Fig. 2(a and b) [6]. For each test temperature two tensile curves were measured. For comparison, the tensile curves of the Cu1CrZr alloy are also plotted. The tensile curve at 300 °C clearly exhibits a strengthening effect by the W particle reinforcement. However, the hardening effect almost diminishes at 550 °C. At 300 °C the hardening effect is accompanied by strong reduction in ultimate elongation. At 550 °C the composite shows the minimum elongation which is comparable to the unreinforced alloy. Since the uniform tensile elongation is a key parameter in the strain-based failure criteria of a structural design code, the reduction in ductility is a critical issue for structural application of the composite material.

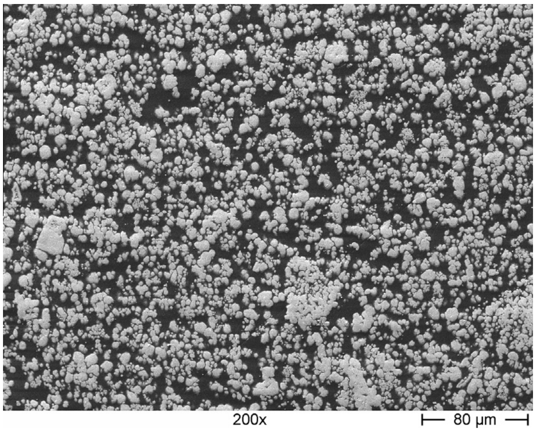

Fig. 1. SEM micrograph of the reference W30–CuCrZr composite material. A skeleton-like network of sintered tungsten particles is filled with the Cu1CrZr alloy matrix.

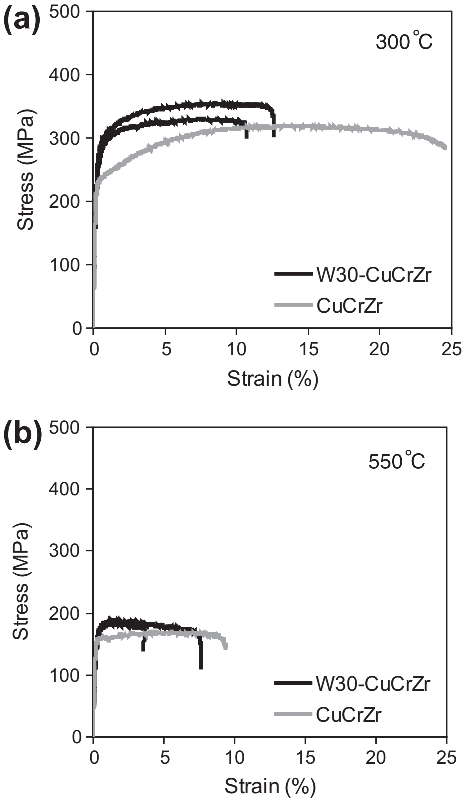

Fig. 2. Tensile stress–strain curves of the W30–CuCrZr composite measured at 300 °C (a) and 550 °C (b).

Some selected material properties used for the simulation are listed in Table 1 [8]. The yield stress of the Cu alloy is two orders of magnitude higher than pure copper. One encounters a difficulty in determining the material data for the W particle, since there is no experimental data available. The plastic properties of the W particle are subject to significant changes in the course of thermo-mechanical history during fabrication [7]. One may try to assess the plastic properties of the W particle based on the known data of other W materials.

The fully annealed (fully recrystallized) bulk W shows ductility with lower yield stress (~150 MPa) and some work hardening above its ductile-to-brittle transition temperature (DBTT: 300–400 °C). The cold worked bulk W shows brittleness with higher yield stress (~1000 MPa) and small elongation (no work hardening) below the corresponding DBTT (600–700 °C). Since our W particles have experienced both work hardening (ball milling) and partly annealing (melt infiltration), we assumed that they would have intermediate properties at the test temperatures. The input data used for the W particles are listed in Table 1.

Upon cooling from the ageing temperature to room temperature (RT), each phase undergoes differential thermal straining producing thermal stresses owing to the mismatch of thermal expansion coefficient (CTE) between tungsten and the copper alloy.

3. Direct mapping and finite element model

The direct mapping tool OOF2 used here has been already applied for various simulations in materials science [9,10]. This software can create the finite element mesh of a microstructure-based model by mapping and phase-segmenting the gray scale pixel image of a digitized micrograph taken at a specific magnification. The detailed description on the OOF2 code and the direct mapping procedure is found elsewhere [11]. Here we used the