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Numerical exploration into the potential of tungsten reinforced CuCrZr matrix composites

Jörg Hohe [a,*], Sascha Fliegener [a], Claudio Findeisen [a], Jens Reiser [b], Verena Widak [b], Michael Rieth [b]

[a] Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg, Germany
[b] Karlsruher Institut für Technologie, Institut für Angewandte Materialien (IAM), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

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ABSTRACT

The present study provides a numerical investigation into the potential of tungsten reinforced CuCrZr materials in order to overcome their limited performance at higher temperatures. Metal matrix composites including (i) particle reinforced microstructures, (ii) short fiber reinforced microstructures with both randomly orientated and (iii) aligned fibers as well as (iv) laminates consisting of stacked tungsten and CuCrZr layers are considered. The numerical analysis is performed by means of an energy based homogenization procedure in conjunction with a finite element analysis of representative volume elements for the respective microstructures. The results of the screening analysis reveal a distinct improvement of the mechanical properties of CuCrZr materials by the tungsten reinforcements even for moderate tungsten volume fractions. In a comparison of the different microstructures, the ordered microstructures, i.e. laminates and the aligned short fiber reinforced composites in most cases outperform their disordered counterparts.

1. Introduction

Nuclear fusion environments provide ambitious requirements for the choice of materials. Materials have to withstand rather high temperatures, possess a reasonable toughness even at lower temperatures and provide a considerable stress-carrying capacity throughout the entire thermal operation window. In order to enable cooling for keeping the temperature within acceptable limits and – depending on the task of the considered plant component – ensure a rapid transport of the generated heat, an excellent thermal conductivity in many cases is mandatory. Furthermore, aspects of radiation embrittlement and nuclear waste management have to be considered, which shrink the range of possible materials significantly. Finally, limits due to the availability of several candidate materials have to be considered (Tavassoli [1], Zinkle and Ghoniem [2]).

For the heat sink components in nuclear fusion, copper and copper alloys have promising properties in many aspects (Fenici et al. [3], Li et al. [4], [5]). Nevertheless, in high temperature application, they suffer from the low upper end of their thermal operation window. For the high temperature range, tungsten as the element featuring the second-highest melting temperature (and the highest one among all metals, although several kinds of ceramics have higher melting temperatures) might be a natural choice. On the other hand, tungsten suffers from its high ductile-to-brittle transitions temperature (DBTT) and its rather low fracture toughness in the brittle regime.

A possibility to circumvent the problem of the limited thermal application range for either of the materials and thus to enhance the thermal design window (Zinkle and Ghoniem [1]) is the design of composite materials where one of the constituents provides a reasonable toughness at low temperature and the other one ensures a sufficient strength and creep resistance towards the upper limit. Possible applications for tungsten composite materials can be found in the divertor technology. In particular water cooled divertor concepts provide a demand for advanced structural materials such as reinforced CuCrZr. Furthermore tungsten composite materials may be used as a functional material positioned between materials with different coefficients of thermal expansion. The design of such high

* Corresponding author.
E-mail address: joerg.hohe@iwm.fraunhofer.de (J. Hohe).

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temperature materials has first been studied by Vill et al. [6] in a study on tungsten-molybdenum microlaminates where molybdenum layers were attached in between thin tungsten layers in order to provide an enhanced toughness of the material. Hohe and Gumbsch [7] studied the design of tungsten-vanadium composites, considering a variety of possible types of microstructure. In a recent approach, Reiser et al. [8] demonstrated the possibility to improve the ductility of tungsten by rolling the material to thin foils and to assemble a three-dimensional material thereof by re-combining the individual foils to a tungsten laminate.

Regarding the design of tungsten-copper composites, a significant amount of work has been performed during the past two decades. In an early contribution, Itoh et al. [9] studied a tungsten-copper composite with interpenetrating microstructure. A functionally graded composite material was designed by means of a theoretical model based on Timoshenko beam theory and processed by infiltration of a graded porous tungsten precursor with a copper melt. A similar type of tungsten-copper composite was produced by Jedamzik et al. [10] where the graded tungsten precursor was processed by electrochemical gradation. An alternative route for processing of tungsten-copper composites resulting in a particle based microstructure has been proposed by Shen et al. [11] as well as by Zhou et al. [12] who studied the properties of functionally graded tungsten-copper composites manufactured by resistance sintering under ultrahigh pressure. Pintsuk et al. [13] compared the properties of tungsten-copper composites with different graded microstructures processed by powder metallurgical routes using laser sintering and plasma spraying to the properties of composites with interpenetrating microstructure obtained by infiltration technique mentioned before.

In order to further enhance the properties of the aforementioned tungsten-copper composites, You et al. [14] proposed the use of melt-infiltrated microstructures using precipitation hardened CuCrZr alloy instead of pure copper. Characterization of the material with three different tungsten volume fractions showed distinct advantages compared to composites with pure copper as a constituent material as well as compared to non-reinforced CuCrZr alloy. In a metallographic analysis, a rather good bonding of the two constituents has been observed. In order to further investigate the properties of tungsten-copper composites and the underlying mechanisms, Zivelonghi and You [15] provided a computational study on deformation and fracture of tungsten-particle reinforced copper matrix composites. Nevertheless, a two-dimensional model has been used in their analysis so that the microstructure considered in fact consists of prismatic inclusions with infinite extent normal to the meshed plane and thus defines an infinite fiber reinforced microstructure loaded perpendicular to the fiber direction rather than a particle reinforced composite.

The present study is concerned with an extensive numerical survey into the potential of CuCrZr-tungsten composite materials for nuclear fusion applications using full three-dimensional models. In a similar manner as in a previous study on the effective properties of tungsten-vanadium composites (Hohe and Gumbsch [7]), a numerical screening analysis is performed, considering the thermal and mechanical response of different microstructural design options, all at a variety of tungsten volume fractions, covering the entire possible range. The range of microstructural design options considered includes (i) particle reinforced composites, (ii) short fiber reinforced composites with aligned and (iii) randomly orientated fibers as well as (iv) CuCrZr-tungsten laminates. Their effective thermal, thermo-mechanical and mechanical response is predicted by means of a numerical homogenization analysis of the response of representative volume elements for the respective microstructures using the finite element method. The results are evaluated in terms of the thermal conductivity, coefficient of thermal expansion, elastic constants, yield curves and creep rates.

2. Homogenization analysis

2.1. General outline

The present contribution is concerned with a numerical screening analysis into the macroscopic material properties of tungsten reinforced CuCrZr matrix composite materials. For the determination of the effective thermal and mechanical properties, an energy based numerical homogenization scheme proposed in previous studies is adopted (Beckmann and Hohe [16], Hohe and Gumbsch [7]). For a concise presentation, the scheme is briefly outlined: Consider a body Ω according to Fig. 1, consisting of a material with a distinct microstructure. For an efficient numerical analysis of the thermo-mechanical response, the body Ω is to be substituted by a similar body Ω^* consisting of a quasi-homogeneous “effective” material with yet unknown properties. The effective properties have to be determined such that the thermo-mechanical response of Ω and Ω^* is equivalent. Provided that the microstructure of Ω does not depend on the position within the body, the effective properties can be determined from the condition that the response of a representative volume element Ω^{RVE} for the microstructure and a similar volume element $\Omega^{\mathrm{RVE}*}$ consisting of the effective medium has to be equivalent (Fig. 1). The mechanical response of both volume elements is defined to be equivalent, if the volume average

$$\overline{w} = \frac{1}{V^{\mathrm{RVE}}} \int_{\Omega^{\mathrm{RVE}}} w \, \mathrm{d}V = \frac{1}{V^{\mathrm{RVE}*}} \int_{\Omega^{\mathrm{RVE}*}} w^* \, \mathrm{d}V \tag{1}$$

of the strain energy density in both volume elements is equal, provided that the volume average

$$\bar{\varepsilon}_{ij} = \frac{1}{V^{\mathrm{RVE}}} \int_{\Omega^{\mathrm{RVE}}} \varepsilon_{ij} \, \mathrm{d}V = \frac{1}{V^{\mathrm{RVE}*}} \int_{\Omega^{\mathrm{RVE}*}} \varepsilon_{ij}^* \, \mathrm{d}V \tag{2}$$

of the infinitesimal strain tensor $\varepsilon_{ij} = 1/2\ (u_{i,j} + u_{j,i})$ with the gradient $u_{i,j} = \mathrm{d}u_i/\mathrm{d}x_j$ of the displacement vector u_i is equal for both, Ω^{RVE} and $\Omega^{\mathrm{RVE}*}$. Similar equivalence conditions

$$\bar{\dot{q}}_i = \frac{1}{V^{\mathrm{RVE}}} \int_{\Omega^{\mathrm{RVE}}} \dot{q}_i \, \mathrm{d}V = \frac{1}{V^{\mathrm{RVE}*}} \int_{\Omega^{\mathrm{RVE}*}} \dot{q}_i^* \, \mathrm{d}V \tag{3}$$

and

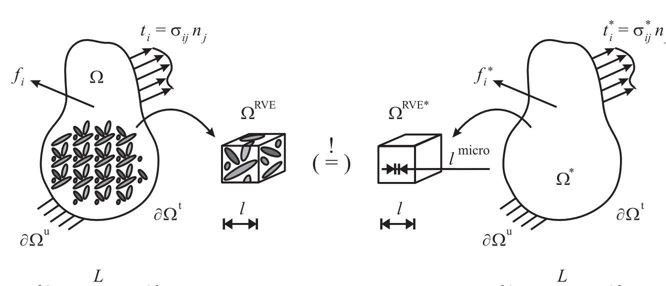

Fig. 1. Representative volume element.