Computational Materials Science 80 (2013) 96–103

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

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

A statistics based numerical investigation on the prediction of elasto-plastic behavior of WC–Co hard metal

G. Chen [a,*], U.A. Ozden [b], A. Bezold [b], C. Broeckmann [b]

[a] Institute for General Mechanics (IAM), RWTH Aachen, Templergraben 64, 52062 Aachen, Germany
[b] Institute for Materials Applications in Mechanical Engineering (IWM), RWTH Aachen, Nizzaallee 32, 52072 Aachen, Germany

ARTICLE INFO

Article history:
Received 14 December 2012
Received in revised form 7 April 2013
Accepted 8 April 2013
Available online 28 April 2013

Keywords:
WC–Co hard metal
Composite material
Automatic adaptive modeling
Elasto-plastic behavior
Statistics

ABSTRACT

This paper focuses on the evaluation of the nonlinear elasto-plastic behavior of a WC–Co composite by a computational micromechanics approach. Due to the non-periodic nature of the material, the difficulty underlies primarily in determining a representative volume element (RVE) which is efficient in embodying the microstructure of the material and the global material feature predicted from it would not been strongly distorted. For this purpose a statistics based methodology is proposed as well as a model generation technique which is capable to convert real images taken from scanning electron microscopy (SEM) automatically into a finite element model. Based on this technique, a series of SEM images were studied with the emphasis to investigate the impact of the RVE size on the prediction of the composite behavior in a statistical manner. Furthermore, the paper discusses the impact coming from additional factors, such as boundary conditions and element type. Simulation results based on various case studies are compared with experimental observations and a statistical perspective in RVE size determination is introduced.

1. Introduction

In recent decades hard metals based on WC–Co became powerful tool materials in many industrial applications. The composite consists of an interpenetrating network of brittle tungsten carbides (WC) and a ductile Cobalt (Co) binder. Volume fractions of WC range from 70% to 95%. By this composition major advantages of ceramics and metals are combined resulting in materials with high hardness, high wear resistance and sufficient toughness.

One of the long lasting research interests regarding composite materials lies in predicting their macroscopic effective behavior from the micro-constituents' configurations. The existing methodologies employed to serve this purpose include vast variances which belongs to analytical mathematical or numerical categories [1]. Among them the numerical homogenization based on the finite element method (FEM) is the most generic and flexible one, owing to the simplifications it makes in describing the material as well as the growing availability of computational power.

WC–Co is one of several major materials which are frequently taken as representative materials for aforementioned homogenization studies. Due to the genetic non-periodicity of its microstructural morphology, the prediction of material's linear behavior alone is a significant challenge. Jaensson and Sundström has initially investigated the effective elasticity of this composite by using a very coarse 2D representative surface element model (RSE) constructed from one micrograph of the alloy [2]. Laterally this approach is further developed and performed by Sundström to study the material behavior in the scope of small plastic deformation [3]. More recently, Poech has performed a comprehensive study regarding various methodological aspects of the problem including mesh density and model size [4]. Most recently Sadowski tested the response of a 2D RVE model to different element types (plane stress vs. plane strain) and suggested a transition algorithm that converts the volume fraction of a certain phase to corresponding area ratio in a 2D model [5].

Among various theoretical and technical issues related to the accurate prediction of effective material properties, the determination of minimum required model size and the proper embodiment of the microstructural geometry play the most critical roles. The former one arises from the need to capture the global response of the composite with an infinite domain from a sample of limited size. The latter one is induced by irregularity and complexity of the morphology of the material.

Having realized the difficulty for determining a proper RVE size which can objectively reflect the macroscopic feature of the composite, Hill provided an insight from energetic point of view and developed initially a pragmatic criterion [6]. Another impor-

* Corresponding author. Tel.: +49 017620468688.
E-mail addresses: geng@iam.rwth-aachen.de (G. Chen), u.oezden@iwm.rwth-aachen.de (U.A. Ozden), a.bezold@iwm.rwth-aachen.de (A. Bezold), c.broeckmann@iwm.rwth-aachen.de (C. Broeckmann).

0927-0256/$ - see front matter
http://dx.doi.org/10.1016/j.commatsci.2013.04.004

tant criterion for linear elastic composite is the one proposed by Drugan and Willis [7]. This criterion determines the minimum RVE size by comparing the ratio of the magnitude of nonlocal terms to the magnitude of local terms. Accordingly, the minimum RVE size is required to be at most twice the reinforcement diameter for any reinforcement concentration level. Drugan's criterion was later approved in several studies [8], but disproved among others which attribute the discrepancy not only to the plasticity of the matrix, but also to the underlying geometrical arrangement of the particles [9]. Furthermore, it has been proven by Ostoja-Starzewski that a minimum RVE can be determined only either when the composite can be embodied by unit cell with periodic microstructure or when the volume containing a very large (mathematically infinite) set of microscale elements [10]. Meanwhile, some researchers see the need to adopt governing parameters other than the elastic moduli. In this context, Stroeven proposed key figures such as peak load, dissipated energy and strain concentration factor [11], and among others also peak stress and experimental strain distribution [12,13]. In this sense, as concluded by Stroeven, the determination of the RVE size is by no means straightforward. It depends on the material under consideration, but also on the sensitivity of the physical quantity that is measured. This means a uniform criterion determining a minimum RVE size is not applicable; the size of RVE has to be specified by considering the morphology of microstructure as well as the material behavior and the purpose of application. This objective oriented mechanism is strongly approved by Kanit et al. based on their study on a random composite [14]. In several most extreme cases, the existence of a minimum representation of the composite is questioned [15]. Nevertheless, in general a minimum sized RVE can be found which is capable of objectively reflect the global composite behavior. Also such a size depends largely on both structural and material features of each phase [16].

A lot of effort has been spent in overcoming the difficulty of building finite element RVE models representing a certain microstructure. Neglecting some technical details the existing techniques for modeling the microstructure can coarsely be divided into two groups. The first group entails modeling techniques which aim to duplicate real microstructures of the composite. The second broad group of modeling techniques entails the development of idealized microstructures representing major features of the original one. Considering difficulties in particular applications, the methods in the first group are primarily adopted in the extent of 2D and rarely in the spectrum of 3D. These techniques include image processing from SEM [17], direct 3D modeling from holotomography and indirect 3D modeling from a series of 2D images by a sectioning process [18]. In contrast, the methods belonging to the second group are primarily applied to build up 3D RVE models and the most important representatives of them is the so called random sequential adsorption (RSA) algorithm [19]. Meanwhile, for most previous numerical homogenization studies of WC–Co hard metal, the development of a 2D RVE model from SEM images was taken as the primary strategy.

The microstructure of WC–Co is not only random and non-periodic but also geometrically complex. Therefore the challenge is that, on one hand, RVE model is required to be adequately large; and on the other hand the morphological details are required to be preserved. Because these two requirements must be satisfied simultaneously, they should not be treated individually. For this reason in this study a technique is proposed which is capable of building 2D finite element RVE models automatically from SEM images. This technique allows for the analysis of a large group of microstructures without excessive manual effort. Because of this advantage, the statistical analysis of material with random structure is possible. The determination of RVE size can be partially resolved by a statistical based procedure.

2. Statistical homogenization of the elasto-plastic material behavior

2.1. Micromechanical model

In the context of micromechanics, any field variable $*$ of the heterogeneous material is usually non-uniformly distributed in a material body. In this sense, its volumetric averaged counterpart (denoted in angle brackets) is frequently reckoned:

$$\langle * \rangle = \int_{\Omega} * dv \tag{1}$$

Ω denotes the domain of interest and dv represents a volume element. In 2D models an appropriate area average is defined. The effective feature of the material in this circumstance refers to the one linking two averaged physical variables. Taking exemplarily stress tensor $\boldsymbol{\sigma}$ and strain tensor $\boldsymbol{\varepsilon}$, in case that all components of the composite reside in the elastic regime, the relationship between $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ can be depicted via the effective elasticity in the manner:

$$\langle \boldsymbol{\sigma} \rangle = \overline{\boldsymbol{C}} : \langle \boldsymbol{\varepsilon} \rangle \tag{2}$$

$\overline{\boldsymbol{C}}$ stands for the effective elastic tensor. Depending on the characteristics of the microstructure, this tensor can be either isotropic or anisotropic.

In homogenization, the RVE size determination possesses an important significance; several conditions are raised to check if the size of a certain RVE is large enough to satisfy basic requirements. Among them one idea is the renowned Hill's criterion which states that two energy terms should be identical if RVE size is adequately large [1]. This condition is written as:

$$\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle \tag{3}$$

Hill's condition does not specify material behavior and in principle can be applied to any sort of materials. For a practical purpose, we adopt a parameter ψ to check a model's obedience with Hill's condition which is defined as:

$$\psi = \max\left(\frac{\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle}{\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle}, \frac{\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle}{\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle}\right) \tag{4}$$

According to its definition, it can be found that the more ψ approximates to the unit value; the better is the representativeness of the real microstructure by the RVE.

Another condition checking the representativeness of the RVE model which is suitable for a macroscopically isotropic material is the anisotropy coefficient. It is defined as the maximal ratio between three normal components of the elastic tensor:

$$\zeta \stackrel{!}{=} \max\left(\frac{\overline{C}_{iiii}}{\overline{C}_{jjjj}}\right) \quad (i, j = 1, 2, 3) \tag{5}$$

Unlike Hill's condition, parameter ζ is based upon the composite elasticity and it requires the macroscopic isotropy of the material. It should be pointed out that all these criteria are necessary but insufficient. The advantages of ψ and ζ are due to their convenience and efficiency: these values can be applied to make an initial check of the adequacy of the RVE size before start statistical analysis.

Since the ductile binder phase of the WC–Co composite exhibits plastic behavior, the effect of one plastically deforming component to the global composite behavior is also investigated. To analyze the macroscopic plasticity, we resort to the theory developed by Suquet [20]. According to it, the actual micro-stress can be divided into two parts: the first occurs if the material behaves perfectly elastic and the second belongs to a self-equilibrated residual stress field:

$$\boldsymbol{\sigma}(x) = \boldsymbol{L}(x) :< \boldsymbol{\sigma} > + \boldsymbol{\sigma}^r(x) \tag{6}$$

Here $\boldsymbol{L}$ represents the stress localization tensor which maps the averaged stress to a local stress of a purely elastic medium, and