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A novel artificial dual-phase microstructure generator based on topology optimization

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ABSTRACT

The mechanical properties of dual-phase (DP) steel are mostly derived from its microstructure, e.g., volume fraction, size, distribution and morphology of each constituent phase. An artificial microstructure generator with an enhanced *novel* phase assignment algorithm based on material topology optimization is proposed to investigate the mechanical properties of DP steel. With this algorithm, phase assignment process is performed on a *modified Voronoï tessellation* to achieve the targeted representative volume element (RVE) with a good convergence. This method also includes a proper orthogonal decomposition (POD) reduction of flow curves (snapshots) to identify the optimal controlling parameters for DP steel. This numerical method significantly improves the representation of the generated RVE with low computational cost. The proposed method is verified using a DP590 steel which indicates a good agreement with experimental material behavior and RVE predictions based on real microstructures. Predictions of plastic strain patterns including shear bands using the artificial microstructure closely resemble the actual material behavior under similar loading conditions. Robustness of this approach provides a new dimension for RVE development based on artificial microstructure which can effectively be implemented in material characterization.

1. Introduction

Dual-phase (DP) steel has been developed by automotive industry for the purpose of weight reduction, improvement in passive safety performance and fuel efficiency. Usually, DP steel contains hard martensite islands embedded in a soft ferrite matrix [1]. Synergy between these two phases with the inhomogeneous microstructure exhibits excellent mechanical properties [2–6], such as relatively high ultimate tensile strength (UTS), low yield to tensile strength ratio, absence of yield point elongation and a good balance of strength and formability.

Recently, several researchers [7–16] used computational models of representative volume element (RVE), which are constructed based on metallographic images, to predict the flow behavior and failure of DP steels. Sun et al. [7] investigated driving mechanisms of material failure for different grades of DP steel using microstructure based modeling approach and found that the failure is affected by material softening and plastic strain localization. Hosseini-Toudeshky et al. [8] studied the deformation pattern and mechanical behavior using large and small deformation theories in a series of RVE models obtained from scanning electron microscopy (SEM) images. Ramazani et al. [10,12] applied the Gurson-Tvergaard-Needleman (GTN) fracture model and extended finite element method (XFEM) to predict the ductile failure and micro-cracks propagation in real microstructure based RVEs.

Real microstructure based models are constructed using experimental data to investigate the influence of grain morphology or size changes on effective properties of DP steel. However, highly heterogeneous materials are produced during industrial welding, forging or heat treatment processes. They have special localized microstructures: microstructure at one material point could be different from another. For example, the welding zone formed during arc welding process can be divided into 3 regions: base material, heat affected zone (HAZ) and nugget [9]. In the HAZ, the microstructure is also dissimilar point-by-point, which is difficult to obtain experimentally. It is comparatively easier to use a computed artificial microstructure based on local phase proportions and chemical compositions to predict the flow behavior of each material point. Accordingly, the local phase proportions and chemical compositions can be obtained from the phase transformation model incorporating concerned diffuse mechanisms [17–21]. Therefore, this method particularly requires the development of

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an artificial microstructure with similar statistical properties to replace the real one.

Based on statistical descriptions of DP steel, artificial microstructures are often generated using geometry primitives (e.g., spheres, polygons or polyhedra). Al-Abbasi and Nemes [22] developed a micromechanical model for DP steel, which is dispersed of spherical martensitic particles with two different sizes in a ferrite matrix. However, this model has disadvantages such as inexact geometric representation and no reliable data close to the interface between different phases. Alternatively, Voronoï tessellation [23] is considered as an efficient tool for approximating the microstructure in DP steel. Nygårds et al. [24,25] modeled dual-phase microstructures using 2D and 3D periodic Voronoï tessellations with limited grain number to predict the effective mechanical properties. Due to the lack of an automate phase assignment algorithm, the second phase was just determined in a random grain growth way. Abid et al. [26] developed a random 2D RVE using Voronoï tessellation followed by an optimization and filtering algorithm to obtain tailored microstructures. However, the used Voronoï seeds were sowed in a pseudo-random way, which underestimates the variability of the grain size, while overestimates the number of nearest neighboring cells. Moreover, their model is not suitable for RVEs with less than 100 μm side length, since no periodicity exists in it. Fillafer et al. [6] simulated 3D microstructures using periodic Voronoï tessellation and subsequent phase coloring to investigate the macroscopic stress-strain behavior of DP steel with different martensite fractions. In their work, the martensite contiguity was well considered and "soft" optimization criteria were used to reach the microstructure with predefined controlling parameters. However, the randomness of the generating seeds was neglected and no more details of the "soft" criteria were given.

Although Voronoï tessellation is an adequate approximation for DP microstructure, the variability of grain size, shape and neighboring grains' correlation are affected by the design of generator seeds [27,28]. Moreover, typical existing phase assignment processes do not able to well capture the complete features of DP microstructure and obtain a convergent phase distribution. Therefore, in this work, a *modified Voronoï tessellation* is periodically generated from Halton (quasi-random) sequence [29], which statistically exhibits low discrepancy, to provide adequate grain morphology. A phase assignment algorithm based on material topology optimization is proposed to solve the phase distribution problem.

Over the past few decades, a dramatic development of topology optimization has been performed in both scientific research [30–39] and industrial applications [40]. Various approaches including density-based methods [41,42], evolutionary procedures [43,44] and level-set methods [45,46], have been proposed to enhance the topology optimization design of multiscale nonlinear heterogeneous structures, topological design of microstructures of multi-phase materials. Originally, the density-based topology optimization design technique can be regarded as a method that seeks the optimal structure to satisfy the given constraints, while minimizing the objective function, by defining a so-called "pseudo-density" within a fixed grid. This is quite similar to the phase assignment procedure in artificial DP microstructure generation. Therefore, an algorithm related to density-based methods in topology optimization is introduced in our generator.

The structure of the present paper is as follows: firstly, a *novel* artificial dual-phase microstructure generator based on topology optimization is developed to construct micromechanical model for DP steel. Secondly, the optimal controlling parameters for a DP steel are identified using a proper orthogonal decomposition (POD) reduction [47,48] on flow curves. Thirdly, an RVE model based on real microstructure of DP590 steel has also been simulated to predict the macroscopic flow behavior and the plastic strain distribution at the element level. Finally, micromechnical modeling of the generated microstructure using these optimal controlling parameters are performed and the results corroborate experimental material behavior and RVE predictions based on real microstructure. This study also confirms the robustness of our proposed generator.

2. Artificial microstructure generator

2.1. Modified Voronoï tessellation

Voronoï tessellation allows the generation of artificial microstructures with randomly distributed and orientated grains for metallic or ceramic materials. This kind of tessellation is a nearest neighbor diagram determined from a set of generating seeds. Since the resulting diagram is mainly affected by the choice of Voronoï generating seeds, a *modified point set* has been used to overcome the shortcomings (e.g., the inexact estimation of grain size and nearest neighboring grain number) found in the standard tessellation generated from a pseudo-random sequence [6,24,25,26]. The *modified point set* is generated using Halton (quasi-random) sequence [29], which statistically exhibits low discrepancy.

Halton sequence is constructed using a deterministic method that uses coprime numbers as its bases. An integer n in decimal notation can be written in base v as:

$$n = \sum_{i=1}^{m} w_i v^i \tag{1}$$

where w denotes the coordinate of each basis. Therefore, the n-th number in Halton sequence of base v can be given by:

$$h(n, \mathbf{v}) = \sum_{i=1}^{m} w_i v^{-(i+1)} \tag{2}$$

Throughout the construction of Halton sequence, the distribution of the sampling points that are considered as the Voronoï seeds, is more uniform than that of pseudo-random sequence.

Since periodic microstructures have favorable numerical properties in the context of computational homogenization [28], these seeds are repeated three times in each direction to ensure the periodicity of the *modified Voronoï tessellation*, as shown in Fig. 1. In order to demonstrate the advantages of the *modified Voronï tessellation*, an example has been compared with the standard one, as shown in Fig. 2. Two sets of seeds are generated from Halton (quasi-random) and pseudo-random sequences, respectively. The

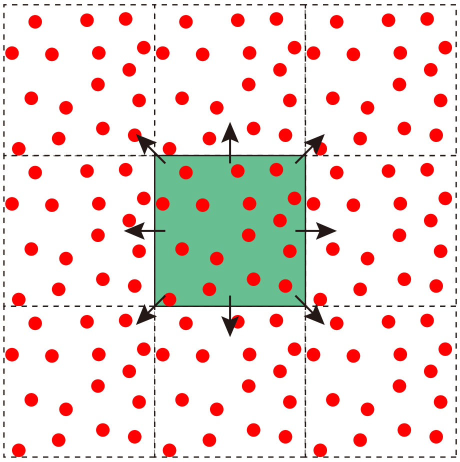

Fig. 1. Construction of a periodic set of Voronoï generating seeds.