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FORWARD AND INVERSE ANALYSIS OF TENSILE PROPETIES OF DUAL-PHASE STEELS

Takayuki Shiraiwa[1]*, Fabien Briffod[1], and Manabu Enoki[1]

[1]The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
** Presenting Author email: shiraiwa@rme.mm.t.u-tokyo.ac.jp*

Abstract

This study proposed a forward analysis method to predict tensile strength and total elongation by considering the three-dimensional microstructure of dual-phase steels. By repeating the forward analysis, an inverse analysis was performed to search for a microstructure with higher tensile properties. The optimal microstructures found by the inverse analysis were consistent with conventional materials engineering findings, demonstrating that the proposed inverse analysis method is effective in solving the structure-properties linkages in the inverse direction.

1. Introduction

This study targeted the structur-properties (SP) linkage of dual-phase (DP) steels. The DP steels consist of a soft ferrite phase and a hard martensite phase, and are classified as advanced high-strength steels (AHSS). A typical indicator to quantify the performances is the product of tensile strength (TS) and total elongation (EL), TS×EL. The TS can be predicted by calculating the average stress response of the microstructure in a finite element method (FEM) based simulation. However, the EL is the sum of uniform elongation and local elongation, and predicting local elongation remains a complex problem. The local deformation process from necking to fracture involves void formation, growth and coalescence and is sensitive to local microstructure. In our previous works, we proposed a method for predicting the total elongation of DP steels considering local damage evolution by crystal plasticity finite element (CPFE) method with a ductile damage model[1-2]. The purpose of this study is to develop a method of deriving the optimal 3D microstructures that exhibit higher TS×EL value under a given loading condition using forward/inverse analyses.

2. Method

The experiments and forward/inverse analyses performed in this study are summarized in Fig. 1. In the experiments, tensile tests were conducted on DP steel specimens with different microstructures to obtain experimental values of tensile properties for calibration of the forward model. The forward model was then created to calculate tensile properties from the 3D microstructure based on CPFE method. The three-dimensional representative volume elements (RVEs) were created using a Gaussian random field (GRF) method. To simulate the plastic deformation behavior of the polycrystalline aggregates, the crystal plasticity constitutive model was used in the finite element analysis. To reproduce ductile fracture behavior, stress triaxiality-dependent fracture strains were introduced into the CPFE framework. In the inverse analysis method, a large number of synthetic dual-phase microstructure models with different morphologies were randomly generated, and 24 microstructural descriptors were extracted by two-point spatial correlation[3] functions and persistent homology[4]. Feature importance analysis using random forest regression was used to further select the important descriptors for predicting tensile properties. Using the selected descriptors as explanatory variables and the forward model as the objective function, microstructures that maximize the product of tensile strength and total elongation (TS×EL) were explored.

3. Results

In the forward analysis, stress-strain curves were calculated for microstructures with different volume fractions of the martensite. Comparison of experimental results showed that the forward analysis predicted the TS and EL of DP steels accurately. In the CPFE analysis, damage initiation was located in the vicinity of ferrite/martensite interfaces. These damage evolution behaviors were consistent with previous experimental reports. Based on the results of the forward analysis, the relationship between TS, EL and volume fraction of martensite (VF_M) was discussed. There was an almost one-to-one relationship between TS and VF_M, while the EL varied considerably even for the same volume fraction.

In the inverse analysis, a database containing 100000 synthetic dual-phase microstructures was created. As features of the microstructures, VF_M and principal components of two-point spatial correlation and persistent diagrams were calculated in 3D. To identify important descriptors to improve TS×EL, the forward analysis was performed on 100 randomly selected microstructural models. Importance analysis using random forest regression revealed that TS could be predicted almost exclusively by VF_M, while the other microstructural descriptors are required to predict EL and TS×EL. Among the selected descriptors, the second principal component of the spatial correlation function was correlated to the third principal axis of the martensite grain, and the second principal component of the zeroth persistent homology was correlated to the solidity of the martensite grain. Both geometric features affect the stress concentration and stress triaxiality at the ferrite/martensite interface.

Based on the selected descriptors, several types of exploration methods were used to search for the optimal microstructures under uniaxial tensile deformation. As a results, all methods discovered microstructures with TS×EL > 40 GPa･% within 100 iterations. These TS×EL values were considerably higher than that found in the random search, indicating that the exploration methods improve the efficiency of the exploration. After the exploration, lamellar and rod-like microstructures with the ferrite/martensite interface parallel to the loading direction were selected as optimal microstructures under uniaxial tensile conditions. These results were consistent with mechanical considerations. It suggests that the proposed framework is effective in solving the inverse problem of structure-properties relationships of DP steels without expert knowledge.

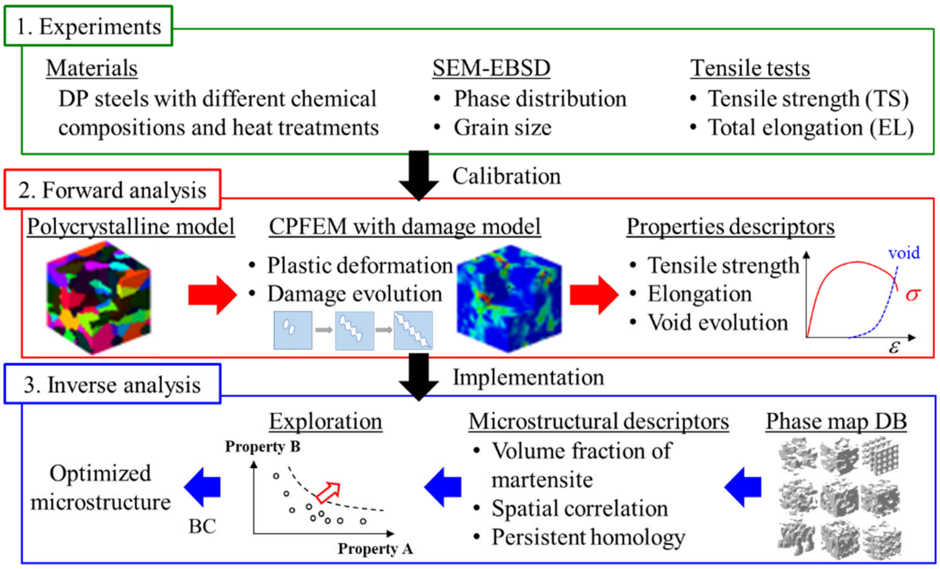

Fig.1 – Forward and inverse problem analysis to improve tensile properties of DP steels

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