

# DEVELOPMENT OF MATERIAL DESIGN SIMULATOR BY USING THE PHASE-FIELD METHOD AND THE HOMOGENIZATION METHOD

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**Key words:** Multi-Scale Analysis, Homogenization Method, Phase-Field Simulation, Spheroidizing, Carbon Steel, Image-Based Modeling

**Summary.** *The phase-field simulation and the multi-scale analysis are coupled in this paper to develop the material design simulator for carbon steel. We focus We employ the phase-field method to simulate the change caused by the thermal treatments and the multi-scale analysis based on the mathematical homogenization method to clarify the effects of it for macroscopic mechanical properties. Connecting by the concept of the digital image engineering, the whole simulations of the carbon steel are achieved on PC's as a material design simulator.*

## 1 INTRODUCTION

A steel is one of the most important materials used in all engineering fields, and especially has overwhelmingly a lot of the production compared with other metals. Reflected by its oldness of the history and technological importance, and a lot of profitable findings have been accumulated from various aspects like a mechanical engineering aspect and a metal studies standpoint. For example in carbon steels, it is experimentally well known fact that the mechanical properties, such as, the yielding stress and strength, are quite different depending upon their carbon contents. Even though for the steels with same carbon contents or same chemical compositions, the different thermal treatments also cause change in their mechanical properties. Addition to the macroscopic material properties, according to the SEM or TEM observation of the carbon steels, their micro

structures especially the shape of carbides are quite different depending on the thermal treatments which they are experienced. In order to produce materials of desired macroscopic mechanical properties, we often draw attention to their microstructures, by which their macro-scale material behavior is more or less affected.

On the other hand, recent years have seen a renewal of interest in the two-scale modeling of a heterogeneous elastic-plastic material based upon the mathematical homogenization method, and the efficient numerical algorithms have been implemented. This two-scale analysis method enables us to simulate the macroscopic inelastic behaviors which are affected by the microscopic structural responses.

In this paper, assuming that the carbon steel is two-phase material; that is, composed only of ferrite (Fe) and carbide ( $\text{Fe}_3\text{C}$ ), the authors develop a numerical simulation tool to obtain the desired macroscopic mechanical properties for the materials. First of all the numerical simulations, the microstructures are modeled by using SEM or TEM observation of the carbon steels and digital image processing. Then, the phase-field simulation is executed to simulate the spheroidization process for the carbon steel and we obtain a various kind of microstructures experienced the different thermal treatments. Finally, the global-local analysis based on the mathematical homogenization method for each microstructures gives its macroscopic material behavior, such as, the initial yielding stress and the uniaxial stress-strain curve. These simulations are combined by the concept of the digital image based engineering using the bitmap data in computers.

## REFERENCES

- [1] A. Benssousan, J.L. Lions and G. Papanicoulau *Asymptotic Analysis for Periodic Structures*, North-Holland, Amsterdam, 1978.
- [2] Babuska Homogenization and its application. Mathematical and computational problems, *Numerical solution of partial differential equations III*, Academic Press, New York, pp.89–115, 1976.
- [3] K. Terada and N. Kikuchi A class of general algorithms for multi-scale analyses of heterogeneous media *Comput. Meths. Appl. Mech. and Engrg.*, **190**, pp.5427–5464, 2001.