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Unified framework for microstructure evolution and property quantification

Chen, Hailong, endylon@gmail.com; Jiao, Yang; Liu, Yongming, Arizona State University, United States

ABSTRACT

In this study, a novel unified framework for the study of both microstructural evolution and the mechanical property quantification is proposed. The multistate Potts model is used to simulate the microstructural evolution, whereas a volume-compensated particle method (VCPM) is used for the mechanical property quantification of the steady state microstructure. The VCPM proposed by Chen and colleagues was originally developed for the investigation of the fracture phenomenon of solid materials. The model was also successfully extended to study the elastoplastic properties of solids by introducing a volume conservation scheme. In the VCPM framework, the domain of interest is discretized into regular unit cells according to the triangle and square packing for 2D and simple cubic, body centered cubic and face-centered cubic packing for 3D. Both local pair-wise and nonlocal multibody potential are proposed to account for the interactions between particles. The multistate Potts models have been used extensively to model a variety of microstructural phenomena, such as the grain growth in a single or multiple-phase system, recrystallization, solidification, and many others. The space-filling array of regular cells is used to represent the Potts domain which is the same as the one used in VCPM. The microstructure evolves such that the system Hamiltonian is minimized. To consider different external effects on the states of the microstructure, different energy terms can be introduced into the system Hamiltonian, such as surface energy to account for the interface effect and strain energy for the grain orientation. Once the final steady state is obtained using the multistate Potts model, usually some other techniques, such as FEM, are used to calculate the effective properties of the microstructural system. It requires the mapping between the FEM meshes and the microstructure. The mapping is very difficult, especially for the interface mapping when the microstructure is very complex. In this study, the VCPM is coupled with the multistate Potts model to simulate the microstructural evolution and quantify the effective mechanical properties of the system within one framework. No mapping between these two models is required since they share the same underlying domain structures. The nonlocal potential proposed in VCPM is introduced into the multistate Potts model as an alternative of the original strain energy term. By doing this, effective simulation of the microstructure evolution for multiple-phase materials can be achieved. Given the final microstructure, the VCPM simulation is carried out to calculate the effective properties of the obtained system.