Comparison of phase-field and cellular automata models to simulate microstructure evolution during recrystallization of additively manufactured 316L austenitic stainless steel

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Motivation

316L SS is one of the most common materials used in additive manufacturing (AM) due to its excellent corrosion resistance and mechanical properties at elevated temperatures. Due to these properties, 316L is widely used in biomedical, aerospace, and nuclear plant applications, making it necessary to understand microstructure development during recrystallization at the mesoscale. Mesoscale modeling of microstructure evolution in AM materials enhances the process-structure-property relationship and enables the development of next-generation materials.

Background

This work aims to study the formation and growth of annealing twins in 316L during recrystallization using phase-field and cellular automaton models. Austenitic stainless steels with face-centered cubic (FCC) crystallographic structure consisting of low-to-medium stacking fault energy promote annealing twin formation. Annealing twin formation has been found to depend on material properties such as stack fault energy (SFE), grain size, texture, and thermomechanical processing parameters like pre-strain and annealing temperature. FCC structures consist of both coherent (parallel to {111} plane) and incoherent {112} Σ3 coincidence site lattice boundaries. Σ3 boundaries appear 60° about a rotation axis in <111> direction. Three points must be met in order to model the density and distribution of twin formation correctly:

i. rate of formation
ii. formed twin morphologies
iii. subsequent grain growth.

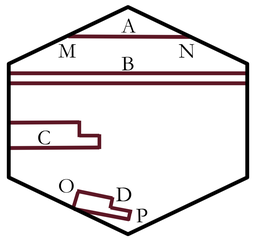


Fig. 1. Two-dimensional twin boundary appearances.

Future direction

Future work includes studying the mechanisms of annealing twins in relation to the thermomechanical history of selective laser melting (SLM) and wire-arc additive manufacturing (WAAM) processes. Annealing twins are generated during recrystallization, while twin density is primarily affected by high temperatures and prior strain levels. Results will be replicated (Fig. 2.), and information regarding crystal orientation, misorientation distribution, grain boundary characterization, and textures will be gathered with EBSD.

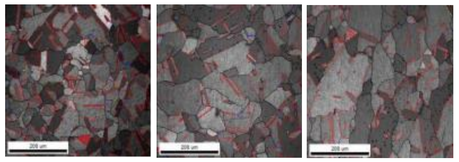


Fig. 2. Twin boundaries of samples heat treated at 1250°C for a duration of 12 minutes at varying heating rates: 10°C/s, 100°C/s, 200°C/s (from left to right). [1]

Phase-field

A grain encounter model, SFE model, and grain boundary dissociation model are considered to meet the previously listed points, but in this work, a growth accident (GA) model is chosen. The GA model presents twins forming on migrating grain boundaries (GB) and triple junctions (TJ) following recrystallization due to the occurrence of stacking fault accidents.

i. GB and TJ migration velocities have a great influence on the formation of twins.
ii. GA produces three types of twins. Type-A twins form behind moving triple junctions; type-b twins form parallel twins by two Type-A twins forming one after another. Type-C twins form behind migrating GB, leading to plate-like twins terminating inside the grain.
iii. During grain growth, the annealing twin boundaries (ATB) may extend in length or get annihilated, affecting the density. This creates an essential interaction between the various types of twins and grain growth [2].

GB migration rate is directly influenced by grain storage energy. Storage energy is incorporated in the phase-field model by varying the free energy parameter and GB mobility as a function of their character through the mobility parameter. A description of GB migration velocity and misorientation is also included in the model. The construction of the local free energy density is given by the Fan-Chen [3] model,

$$F(\eta_i) = \int_V \left(f_0 + \sum_{i=1}^{p} \frac{k_i}{2} |\nabla \eta_i| \right) dV ,$$

where $\eta_i (i = 1, \dots, p)$ are the orientation field variables for distinguishing different grain orientations, p is the number of possible orientations, $|\nabla \eta_i|$ is the grain boundary energy term, and k_i is the gradient coefficient. The bulk energy term, f_0, is a function of field variables and gradient coefficients written as,

$$f_0(\eta_i) = \sum_{i=1}^{p} \left[\alpha_i \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) \right] + \beta \sum_{j=1}^{p} \sum_{\substack{j=1 \\ j \neq i}}^{p} \eta_i^2 \eta_j^2 ,$$

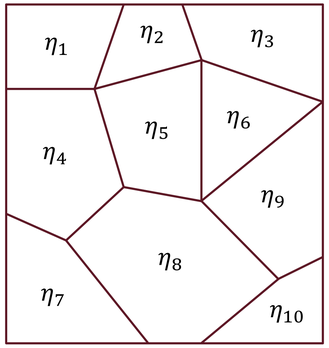


Fig. 3. Two-dimensional microstructure described using orientation field variables.

where α_i and β are bulk energy parameters that relate to the thickness of the GB and energy of diffusion interface. The first term of the bulk energy equation describes energy at equal depths where one field variable is of a non-zero value while the others are set to zero, e.g., see Fig. 3.,

$$(\eta_1, \eta_2, \dots, \eta_p) = (\pm 1, 0, \dots, 0),$$
$$(0, \pm 1, 0, \dots 0), (0, 0, \pm 1, \dots 0), (0, 0, 0, \dots \pm 1).$$

The field variables are linearly proportional to the variational derivative of the total free energy with respect to the orientation field variable governed by the Ginzburg-Landau equations,

$$\frac{\partial \eta_i}{\partial t} = -L_i \frac{\partial F(\eta_i)}{\partial \eta_i},$$

which is then solved using a finite difference method and active parameter tracking algorithm.

Cellular Automata

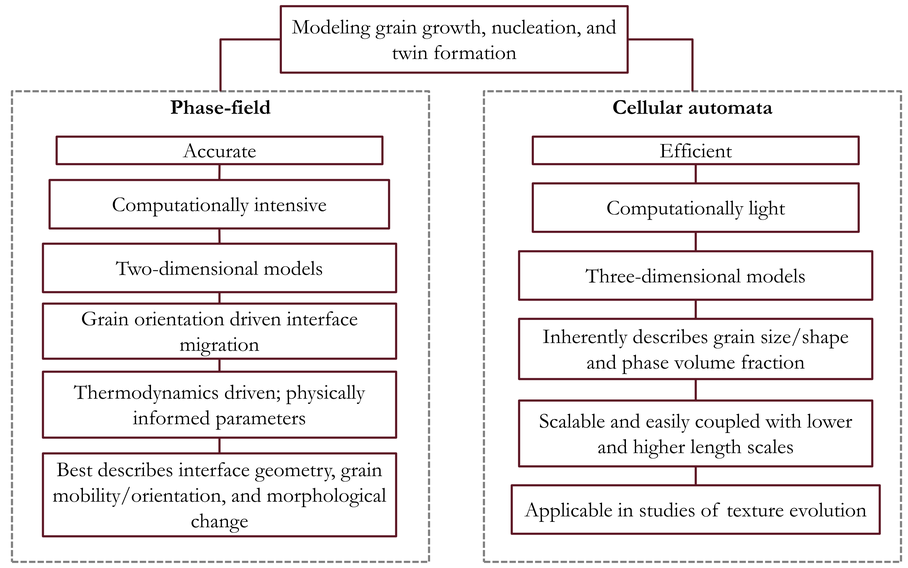
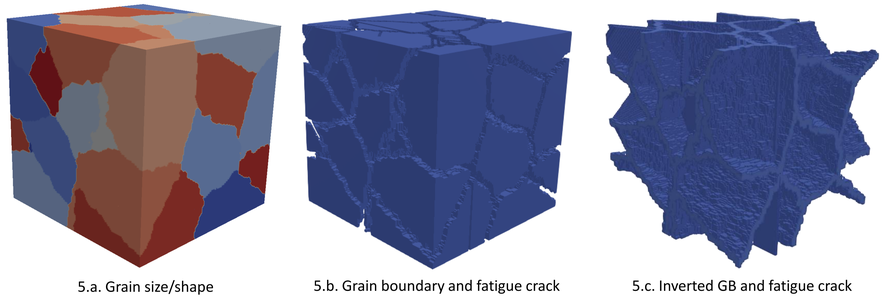


Fig. 5. Comparative diagram of phase-field and cellular automata for modeling 316L during recrystallization



5.a. Grain size/shape

5.b. Grain boundary and fatigue crack

5.c. Inverted GB and fatigue crack

Fig. 5. Simulation of formation and cleavage fracture of polycrystalline microstructure using CASUP.

References

1. Zhou, Y. (2020). *Effect of Heat Treatment on the Properties of Additively Manufactured Type 316L Stainless Steel* (thesis).
2. Jeyaraam, R., Subramanya Sarma, V., & Vedantam, S. (2020). Phase field modelling of annealing twin formation, evolution and interactions during grain growth. *Computational Materials Science*, *182*, 109787.
3. Fan, D., & Chen, L.-Q. (1997). Computer simulation of grain growth using a continuum field model. *Acta Materialia*, *45*(2), 611–622.