

Potts model for grain growth during welding using SPPARKS¹

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Introduction

1 Model grain nucleation and growth in fusion zone and HAZ

Heat source interacting with metal

Melting, solidification and microstructural evolution² in the fusion zone largely depend upon size and shape of pool

2 Model overview

- Initial microstructure
- Grain growth model
- Geometry/motion of weld pool & heat affected zone

Kinetic Monte Carlo Potts³ model implemented in SPPARKS

Elements of model^{4,5}

3 Potts model context

- Digitize space (lattice)
- Lattice sites represent discrete bits of material
- Each color represents membership in phase/grain
- KMC algorithm seeks to minimize grain boundary energy

$$E = \frac{J}{2} \sum_i^N \sum_j^n (1 - \delta_{ij})$$

4 Spatial and temporal temperature profile

- Simulates melting: $T > T_m$
- Simulates solidification: $T < T_m$
- Implicitly defines liquid/solid interface: $T = T_m$
- Mobility function of temperature

Energy: E_1

Grain boundary mobility: $M(T)$

Energy: E_2

Event rate: P

$$P = \begin{cases} M(T) & \Delta E \leq 0 \\ M(T)e^{-\frac{\Delta E}{kT}} & \Delta E > 0 \end{cases}$$

5 Pool motion and algorithm concepts

- Incoming sites may be associated with grains
- However, by the time they exit, grains are melted.

- Interface roughly @ T_{melt}
- No grains
- Move pool
- Randomly assign site spins within pool
- Sites at trailing edge exit
- Trailing edge sites are generally not associated with a grain
- Sites exit as singletons

Demonstration calculations

6 Types of grain growth

Normal growth

Epitaxial

FZ nucleation and normal growth

7 On weld speed and pool shape effects

Top view **weld speed (pool shape fixed)**

Longitudinal centerline cut view

Transverse cut view

Top view **weld pool shape (weld speed fixed)** ★

Longitudinal centerline cut view

Transverse cut view

compare pool size and shape
★ Same weld speed

Weld pool speed and shape are important factors in welded microstructure

8 Simulating pulsed arc power

Top view

Arc power

Time

Peak

Background

Temporal period fixed; different weld speeds

References

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