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Geometrical and Component Modelling Approaches for Recrystallization and Grain Growth Simulation

K. Sreelatha*[1], C. S. Ananda Kumar[2], K. Sreelekha[1], N. Madhuri Rose[1], A. Himasri Bindu[1], S. V. G. V. A. Prasad[3]

[1] Department of Physics & Electronics, Ch. S. D. St. Theresa's College for Women (Autonomous), Eluru – 534003, Andhra Pradesh, India

[2] Department of Physics, SVKP & KS Raju Arts & Science College (Autonomous), Penugonda – 534320, Andhra Pradesh, India

[3] Department of Physics, P. R. Government College (Autonomous), Kakinada – 521001, Andhra Pradesh, India

* Corresponding Author: srilatha.prathap@gmail.com

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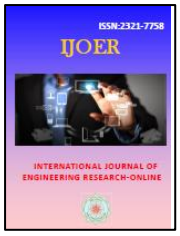

Abstract

Recrystallization and grain growth are fundamental microstructural processes that govern the mechanical and physical properties of polycrystalline materials. Accurate prediction of grain topology, size distribution, and texture evolution remains a central challenge in materials science. Among the various modelling strategies developed to address this problem, geometrical and component-based models have emerged as powerful mesoscale simulation tools. These approaches rely on geometrical principles of nucleation, isotropic growth, and impingement to describe microstructural evolution in a computationally efficient manner. This article presents a comprehensive review of geometrical and component models used for simulating recrystallization and grain growth phenomena. Mahin, Hanson, and Morris Jr. first proposed the geometrical model, which Frost and associates later refined is based on elementary spatial constructions that describe grain boundary formation under site-saturated and continuous nucleation conditions. The model successfully reproduces characteristic microstructural features such as Voronoi, Wigner–Seitz, Johnson–Mehl, and Dirichlet tessellations, making it particularly suitable for thin films and idealized grain structures.

To overcome the limitations of purely geometrical approaches, the component model introduced by Juul Jensen extends the framework by incorporating spatially resolved nucleation, growth kinetics, texture components, and anisotropic growth behaviour. Implemented on a three-dimensional computational grid, this model enables realistic simulation of recrystallization textures and grain topologies under experimentally relevant conditions. The article further discusses key applications of these models in materials science, including texture prediction, microstructure optimization,

and interpretation of experimental observations. Representative simulation examples are reviewed to illustrate the influence of nucleation timing, growth rates, and exclusion zones on grain morphology. The study concludes that geometrical and component models remain indispensable tools for fast and reliable microstructure prediction, especially when combined with experimental input and advanced computational techniques.
Keywords: Geometrical models; Component model; Recrystallization; Grain growth; Microstructure simulation.

1. Introduction

The evolution of microstructure during recrystallization and grain growth plays a decisive role in determining the mechanical, thermal, and functional characteristics of crystalline materials. Properties such as strength enhancement, ductility control, electrical conductivity optimization, and texture development are strongly influenced by grain size, shape, and orientation distribution. Consequently, understanding and predicting microstructural evolution has long been a central objective in materials science and engineering.

Recrystallization and grain growth are inherently mesoscale phenomena, bridging atomic-scale mechanisms and macroscopic material behaviour. While atomistic simulations provide fundamental insights, they are computationally prohibitive for practical microstructural length and time scales. Analytical models, on the other hand, often lack spatial resolution and are unable to capture realistic grain topology. This gap has motivated the development of mesoscale models that incorporate physical realism while remaining computationally efficient.

Among these approaches, geometrical and component-based models have proven particularly effective. These models describe microstructural evolution using simplified but physically meaningful representations of nucleation, growth, and impingement. Rather than resolving atomic details, they focus on spatial relationships between growing grains, enabling large-scale simulations with relatively modest computational effort.

The geometrical model represents one of the earliest systematic attempts to simulate recrystallization microstructures using purely geometrical rules. In this framework, nuclei are introduced either instantaneously (site-saturated nucleation) or continuously over time, and all nuclei are assumed to grow isotropically at a constant rate. Grain boundaries emerge naturally as a consequence of impingement between growing grains. Despite its simplicity, the model successfully reproduces characteristic grain topologies observed experimentally, including straight interfaces, triple junctions, and polygonal grain shapes.

Under site-saturated conditions, the geometrical model leads to Voronoi or Wigner–Seitz tessellations, where each grain occupies the region closest to its nucleation site. When nucleation occurs continuously, Johnson–Mehl-type structures emerge, capturing more realistic recrystallization scenarios. These topologies provide valuable insight into how nucleation density, timing, and growth rates influence final grain size distributions.

However, purely geometrical models are limited in their ability to incorporate crystallographic texture, anisotropic growth, and experimentally measured nucleation behaviour. To address these limitations, Juul Jensen introduced the component model, representing a significant advancement in recrystallization modelling. This approach combines analytical growth expressions with a computer sample, implemented as a three-dimensional spatial grid, allowing explicit representation of grain positions, orientations, and growth histories.

In the component model, each nucleus is assigned a spatial position, nucleation time, texture component, and growth rate. The simulation proceeds by determining, for every point in the grid, which nucleus arrives first, thereby defining grain boundaries through a non-overlapping growth rule. This method preserves the physical constraint of impingement while allowing grains to continue growing in unimpeded directions. As a result, realistic grain topologies and texture distributions can be generated.

The strength of the component model lies in its flexibility. It can incorporate experimentally measured nucleation rates, orientation-dependent growth, and initial textures, making it highly suitable for practical materials science applications. Moreover, the model can simulate both partial and complete recrystallization, providing insight into transient microstructural states that are difficult to observe experimentally.

Together, geometrical and component models form a complementary modelling framework. While geometrical models offer conceptual clarity and computational efficiency, component models provide enhanced realism and predictive capability. Their continued development and application have significantly advanced the understanding of recrystallization and grain growth phenomena.

2. Geometrical Modelling of Recrystallization

Like all models of grain development and mesoscale recrystallization, geometrical models are continuum-based techniques. Their three main stages comprise nucleation, crystal growth until impingement, and, in certain cases, subsequent grain coarsening. The final phase is discussed in Chapter 14. Nuclei are either continuously supplied to the non-recrystallized volume fraction as a linear or decreasing function of time, or they are initially distributed in a site-saturated manner, as in most comparable models. All nuclei are assumed to grow isotropically in space at a fixed growth rate after nucleation. This implies that each nucleus expands uniformly as a sphere until impingement occurs.

Simple geometrical considerations can be used to construct the final grain topology under site-saturated nucleation conditions [2]. If two nuclei nucleate simultaneously and grow at the same constant rate, the interface between the two adjacent grains will be a straight line. This interface corresponds to the perpendicular bisector of the line connecting the two nucleation sites. This geometrical result forms the basis of the Wigner–Seitz cell construction [3].

When three neighbouring crystals grow under identical conditions, the resulting topology includes a triple point located at the intersection of the three perpendicular bisectors of the edges of the triangle formed by the nucleation sites [4] (Fig. 1). If the three nuclei are created at different times but expand at the same rate, they collide along hyperbolic interface lines [4] (Fig. 2). The final position of the triple point is given by

$$r_1 + Gt_1 = r_2 + Gt_2 = r_3 + Gt_3$$

where G is the isotropic growth rate, t_i is the nucleation time of grain i, and r_i is the distance between the nucleation site of grain i and the triple point [4].

Applying this algorithm under site-saturated nucleation conditions produces the well-known Voronoi structure, equivalent to a Wigner–Seitz construction based on randomly distributed lattice points in space [3], [5] (Fig. 3). Voronoi topologies are also referred to as Dirichlet or Theissen structures. Geometrical models with a constant nucleation rate generate similar structures, commonly known as Johnson–Mehl topologies [4], [5] (Fig. 4).

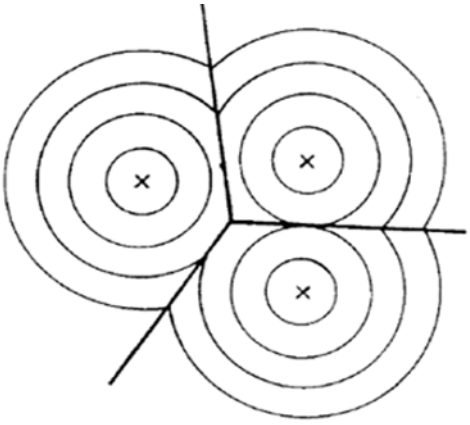

Fig:1 Development of straight interfaces between three crystals formed at the same time, under isotropic and constant growth rate conditions.

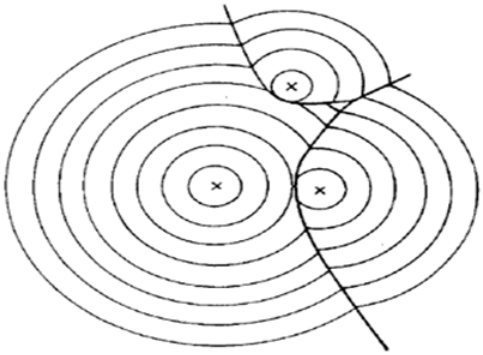

Fig: 2 Development of hyperbolic interfaces between three crystals, formed at different times, under isotropic and constant growth rate conditions.

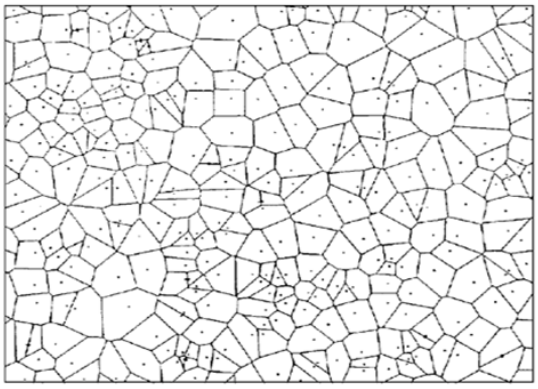

Fig. 3: 2D Voronoi (Dirichlet) topology from Wigner–Seitz construction under site-saturated, isotropic growth with straight interfaces (Frost *et al.*, 1986).

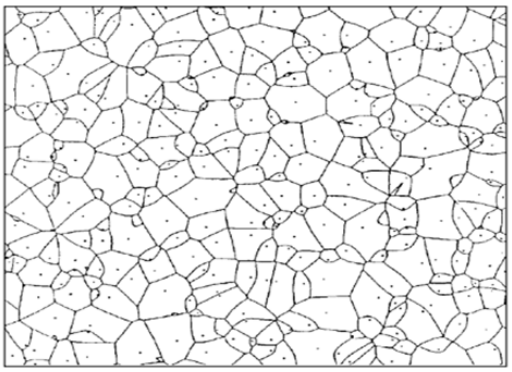

Fig: 4 2D Johnson–Mehl crystal topology from constant nucleation and isotropic growth, producing straight and hyperbolic interfaces (Frost *et al.*, 1986).

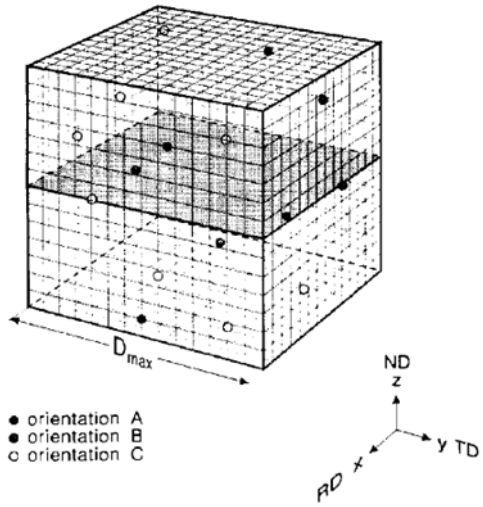

Fig: 5 3D calculation grid for the Juul Jensen (1992) component model showing nuclei with three initial crystal orientations and a shaded plane indicating a 2D slice.

3. Component Model for Microstructure Simulation

The component model extends geometrical principles by introducing spatial grids, multiple texture components, and orientation-dependent growth kinetics [6]. By tracking the arrival times of nuclei at each grid point, the model generates realistic recrystallized microstructures while preventing grain overlap.

Each nucleus is characterized by its position, nucleation time, crystallographic orientation, and growth rate, enabling spatially resolved simulations [6], [7]. The use of a three-dimensional computational lattice allows representation of realistic grain morphologies.

Growth continues in non-impinged directions, preserving physical realism while maintaining computational efficiency [6].

Texture evolution can be explicitly modelled through orientation-dependent growth behaviour, making the component model particularly suitable for predicting recrystallization textures in deformed metals [7]. This approach effectively bridges analytical growth theories and numerical microstructure simulations.

Figure 6 shows two two-dimensional crystal topologies with distinct exclusion zones calculated by Frost and Thompson under conditions of continuous nucleation [4].

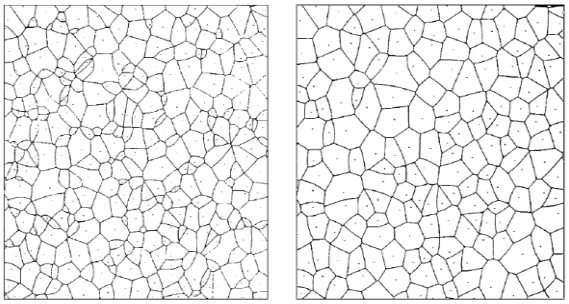

Fig: 6 shows two 2D crystal topologies with disti nct exclusion zones that were calculated by Fros t and Thompson under continuous nucleation [4].

4. Applications in Materials Science

Geometrical and component models are widely used for rapid microstructure prediction, texture evolution studies, and interpretation of recrystallization experiments [7], [8]. Advanced implementations allow the inclusion of initial textures, exclusion zones, and time-dependent nucleation behaviour, enabling improved agreement with experimental observations [6], [8].

These models are valuable tools for analysing the influence of processing parameters on final grain size and morphology. They assist in optimizing thermomechanical treatments in metals and alloys by providing predictive insight into grain refinement and texture control [8]. Simulated microstructures also offer access to transient recrystallization states that are difficult to capture experimentally, supporting model validation and experimental interpretation [7].

5. Summary

This article reviewed geometrical and component modelling approaches for simulating recrystallization and grain growth. The geometrical model provides fundamental insight into grain topology formation, while the component model enables realistic simulation of spatially resolved microstructures and textures.

Both models operate at the mesoscale, balancing computational efficiency with physical accuracy. They capture essential features of nucleation, growth, and impingement phenomena. The geometrical model excels in conceptual clarity, whereas the component model offers enhanced flexibility. Together, they form a complementary modelling framework that has significantly advanced microstructure prediction capabilities.

6. Conclusion and Future Scope

Geometrical and component models remain indispensable tools for mesoscale microstructure simulation due to their efficiency, clarity, and adaptability. Future developments are expected to integrate these models with phase-field methods, crystal plasticity simulations, and experimental data-driven approaches. The incorporation of anisotropic growth, solute effects, and coupling with deformation models will further enhance predictive power, supporting the design of next-generation structural and functional materials.

Advances in computational resources will enable larger and more detailed simulations, while hybrid modelling strategies combining statistical and physics-based approaches will improve robustness. Integration with in-situ experimental techniques will strengthen model validation, and machine learning methods may assist in parameter optimization and pattern recognition. Collectively, these developments will expand the applicability of recrystallization

modelling to complex, multi-phase material systems.

References

[1]. J. C. M. Li, "Recrystallization," *Metallurgical Transactions*, vol. 3, no. 6, pp. 1233–1242, 1972.

[2]. R. Mahin, B. Hanson, and J. W. Morris Jr., "A geometrical model for recrystallization," *Acta Metallurgica*, vol. 28, no. 4, pp. 443–453, 1980.

[3]. H. J. Frost, Y. Whang, and C. V. Thompson, "A two-dimensional computer simulation of recrystallization," *Acta Metallurgica*, vol. 34, no. 9, pp. 1733–1744, 1986.

[4]. H. J. Frost and C. V. Thompson, "The effect of nucleation conditions on grain structure," *Acta Metallurgica*, vol. 35, no. 3, pp. 529–540, 1987.

[5]. H. J. Frost, C. V. Thompson, and D. T. Walton, "Simulation of recrystallization and grain growth," *Acta Metallurgica et Materialia*, vol. 38, no. 8, pp. 1455–1462, 1990.

[6]. D. Juul Jensen, "A new model for the simulation of recrystallization textures," *Acta Metallurgica et Materialia*, vol. 40, no. 4, pp. 901–913, 1992.

[7]. D. Juul Jensen, "Simulation of recrystallization microstructures," *Scripta Materialia*, vol. 36, no. 4, pp. 405–410, 1997.

[8]. F. J. Humphreys and M. Hatherly, *Recrystallization and Related Annealing Phenomena*, 2nd ed. Oxford, U.K.: Elsevier, 2004.