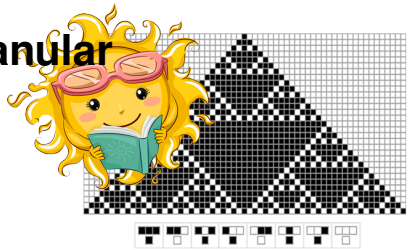
Hexagonal Cellular Automata Simulation of Intergranular Cracking in Polycrystalline Materials



Tarun Kumaar M K, Deeraj H, Suvetha M, PG Kubendran Amos
Mentor: Prince Gideon Kubendran Amos

August 24, 2022

In our everyday life, we can find a diverse range of materials that each have their own characteristic properties that decide which applications they can be employed in. Thus, we often group materials by their shared characteristics into groups such as metals, fabrics, glasses and so on. The properties of a material are closely correlated with its structure on the microscopic scale. Hence, it is very important to study and understand how the microstructure of a given material affects its response to certain conditions and thus, affects its characteristic properties.

Materials are composed of atoms or molecules and how these elements are arranged in three-dimensional space affects their interactions and their properties as well. When there is a regular ordered arrangement of atoms over a long distance, that material can be called crystalline and when the ordered arrangement of atoms is observed over a much shorter range, the material is deemed amorphous. Crystalline structures often arise when the material in consideration undergoes solidification from liquid to solid state. As the material is cooled, small nuclei that each have a particular orientation of crystalline structure expand to form large grains. The boundary separating two adjacent grains of different orientation is called the grain boundary.

Intergranular cracking occurs when a crack propagates along the grain boundaries of a boundary, usually when these boundaries are weakened. This can be compared to a wall of bricks where cracking takes place in the mortar that joins these bricks together. Intergranular cracking is likely to occur if there is a hostile environmental influence and is favoured by larger grain sizes and higher stresses. Though there are several mechanisms for intergranular fracture, all of them revolve around grain boundary orientation and the presence of solutes and impurities.

Our model takes an input of the desired number of nuclei, which are then distributed at random throughout the domain. For this system, we are considering 18 different grain orientations associated with their own unique colours. Conventionally, cellular automata are associated with square discretization but here we have implemented hexagonal discretization and attempt to undertake a qualitative comparison between them.

By applying a specific rule to evolve the automata synchronously, we can observe the nuclei that were introduced at the start of the evolution grow into large grains and develop grain boundaries. The rule implemented here is such that, the cell under consideration will also solidify or become alive if there is at least one live cell in the neighbourhood or radius 1. The use of hexagonal cells gives us a unique grain boundary shape compared to square cells that may appear more jagged upon close observation. By testing different neighbourhoods and rules, we were able to identify a few combinations that resulted in a satisfactory model for a polycrystalline system. One important thing to note is that once cells become “alive” or nucleated they should not be able to return to their *dead* state. After obtaining this polycrystalline structure, we are able to apply a rule to model the crack as it propagates along the grain boundary between two or more grains. This rule is capable of deciding between two paths where a junction between three or more grains is formed in the domain. Thus, the model is able to create a polycrystalline structure which can then be used as a sample to effectively model the growth of a crack across the domain as shown below.

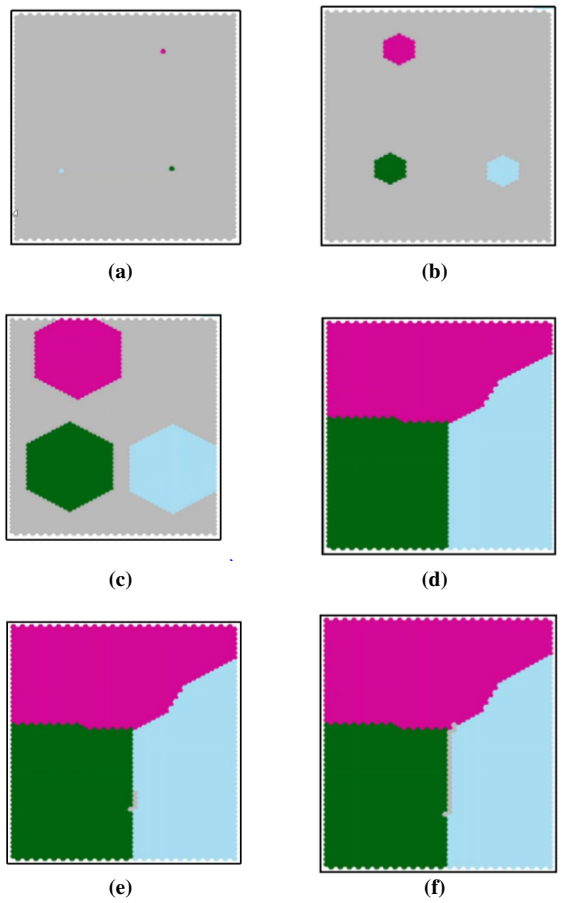


Figure 1: (a), (b), (c), (c) Three Nuclei developing into Polycrystalline System; (e), (f) Intergranular Crack Initiation and Propag ation along the green and blue boundarie;

It is also worthwhile to note that this model is not limited to materials science related applications. As the model is able to select a path at a junction of two or more possible options, it may be used as a path finding algorithm. If one were to consider the grains to be mountains with the centre of each grain being its peak, and the grain boundaries the narrow valleys at ground level; the model can be construed as a path finding algorithm that can be applied in mountainous terrain. We hope to expand this project to also model intergranular crack propagation within the grains and search for other potential applications outside the domain of materials science.