

# **SIMULATION OF COARSENING DURING LASER ENGINEERED NET\_SHAPING**

by

Veena Tikare, Michelle Griffith  
Eric Schlienger, John Smugeresky\*  
Sandia National Laboratories  
Albuquerque, NM  
\*Livermore, CA

## **Abstract**

Laser Engineered Net\_Shaping, otherwise known as LENS™, is an advanced manufacturing technique used to fabricate complex near net shaped components directly from engineering solid models without the use of dies or machining. The ultimate objective of this project is to develop predictive simulation capability which will allow the LENS™ processors to determine fabrication conditions given the material, shape, and application of the final part. In this paper, we will present an incremental achievement to meeting the ultimate goal, a model capable of simulating the coarsening of microstructural features under the unique thermal history to which a LENS™ part is subjected during processing. The simulation results show how grains of very different shapes and sizes form within the same deposition line. They also show that relatively minor changes in the dynamic temperature profile results in microstructures with vastly different characteristics. The implications of this work for LENS™ fabrication is that controlling the temperature profile is essential to tailoring the microstructure of a component to its application.

## **Introduction**

In the past, the development cost of a product was amortized over a large number of manufactured units. Current markets often demand small quantities of many different components with highly specialized performance requirements. Thus, development cost of each component cannot be amortized over large numbers and becomes prohibitively expensive. To reduce development cost, a number of solid free-form fabrication techniques are being developed. One such free-form technique, Laser Engineered Net\_Shaping, LENS™, is being developed at Sandia for rapid forming of complex shaped engineering components made from a variety of metals<sup>1</sup>. LENS™ parts are made by depositing metal particles directly into a weld pool formed by an Nd:YAG laser; the particles are melted and the weld pool is rastered under the laser beam to build each cross section or layer of a component. Subsequent layers are additively fabricated to form the part.

This fabrication process results in microstructures which are unique. Each deposited line has features which are inherent to it. Some features extend into the neighboring lines and into the adjoining layers as shown in figure 1, an SEM micrograph of a tool steel component fabricated by the LENS™ process. These features such as grain size and shape have a large effect on materials

properties and performance. Therefore, it is essential that microstructural evolution during LENS™ fabrication be controlled. To this end, we are developing a model which will predict microstructural evolution during fabrication. In this paper, we will present a model which is capable of simulating coarsening in a single-phase system under an assumed temperature profile of a LENS™ fabrication technique.

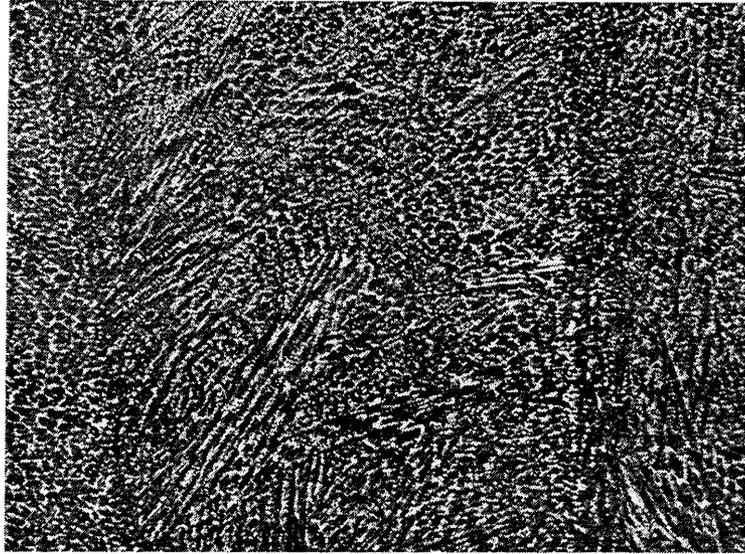


Figure 1. Optical micrograph of a LENS™ component showing microstructure within a deposition line. The direction of raster is to the top. (250 x)

### **LENS™ Process Description**

In the LENS™ process, a metal part is formed by depositing lines with widths and heights of approximately 300  $\mu\text{m}$  to form a layer with the topographical features of the part at the height of that layer. Once that layer is deposited, the next layer is deposited above it, again in a line by line sequence. The actual deposition process is accomplished by melting a pool at the part surface using a laser beam. Next, material in the form of particles is fed into the molten pool. The laser beam and feed material are rastered across the part surface to form deposition lines. As the laser beam moves away, the material cools and solidifies incorporating the added material. The previously formed layer will be heated as the laser beam rasters across. At higher temperatures, microstructural evolution will occur in this layer. The process which will be simulated in this work is the coarsening of grains driven by capillarity in the layer under the current deposition layer.

### **Model Description**

The Potts model, a statistical-mechanical model<sup>2</sup>, was used to simulate microstructural evolution during the LENS™ process. It has been used to simulate a number of microstructural evolution processes, including grain growth, recrystallization, Ostwald ripening, and phase-

transformations. In this study, we have modified the Potts model to simulate two-dimensional coarsening in the dynamic temperature profile of the rastering laser used by the LENS™ process.

Microstructural representation in the Potts model is done by populating a lattice with a canonical ensemble. We use a square lattice and each lattice site is assigned a “spin”\*. Contiguous sites of the same spin form a grain with a sharp grain boundary between adjacent grains. The number of different, degenerate spins that the lattice sites can assume is  $Q$ . The individual state is designated by the symbol  $q$  and the total number of states in the system is  $Q$ ,  $q_{grain} = [1, 2, \dots, Q]$ . All the simulations in this work used  $Q = 100$ . The equation of state for these simulation is the sum of all the neighbor interaction energies in the system given by

$$E = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^8 (1 - \delta(q_i, q_j)) \quad eq. 1$$

where  $N$  is the total number of sites,  $\delta$  is the Kronecker delta with  $\delta(q_i = q_j) = 1$  and  $\delta(q_i \neq q_j) = 0$ ,  $q_i$  is the state of the grain at site  $i$  and  $q_j$  is the state of the nearest neighbor at site  $j$ . Thus, the only energy considered in the simulation is the interfacial energy and all unlike neighbors contribute one arbitrary unit of energy to the system. This yields a single-component, single-phase system with uniform, isotropic<sup>3</sup> interfacial energies between grains.

Now that the microstructural representation and system energies are defined in the simulation, we turn to the grain growth mechanism and kinetics. Grain growth is simulated using the method developed in previous works<sup>4,5</sup>. First, a grain site is chosen at random from the simulation space. Then a new state  $q$  is chosen at random from the  $Q$  possible states in the system. The grain site is temporarily assigned the new state and the change in energy is evaluated using eq. 1. Next the standard Metropolis algorithm is used to perform the grain growth step based on Boltzmann statistics. A random number,  $R$ , between 0 and 1 is generated. Next, the transition probability,  $P$ , is calculated using

$$P = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T}\right) & \text{for } \Delta E > 0 \\ 1 & \text{for } \Delta E \leq 0 \end{cases} \quad eq. 2$$

where  $k_B$  is the Boltzmann constant and  $T$  is absolute temperature. If the  $R \leq P$ , then the grain growth step is accepted, if not, the original state is restored. The simulation temperature used for grain growth was  $k_B T = 0$  which has been shown to simulate grain growth well. Time in the Potts

---

\*The term spin originates from the original application of the Potts model which was used to study domain growth in magnetic materials.

model is measured in units of Monte Carlo step; IMCS corresponds to  $N$  attempted changes where  $N$  is the total number of sites in the system.

In order to simulate the LENS™ process, the Potts model was modified to include a dynamic temperature profile. This was done by considering the grain boundaries to have a velocity,  $V_{gb}$ , which is proportional to grain boundary mobility,  $M_{gb}$ , and to the driving force,  $\mu$ , as

$$V_{gb} = M_{gb}\mu \quad \text{eq. 3}$$

Assuming that the mobility of the grain boundaries is a function of temperature, one can simulate coarsening in a dynamic temperature environment by using a temperature dependent mobility term,  $M_{gb}(T)$ . At high temperatures, the mobility term is large and at lower temperatures it is small. Since we are simulating a laser beam rastering across a part, the mobility term becomes a function of position,  $x$ , and of time,  $t$ ,  $M_{gb}(x,t)$ . The transition probability given in eq. 2 is modified to include temperature dependence by multiplying by the mobility term as

$$P = M_{gb}(x,t) \begin{cases} \exp\left(\frac{-\Delta E}{k_B T}\right) & \text{for } \Delta E > 0 \\ 1 & \text{for } \Delta E \leq 0 \end{cases} \quad \text{eq. 4}$$

The temperature profile assumed for the LENS™ process is a laser beam with a Gaussian temperature distribution. Preliminary characterization of the laser beam indicated that the beam was elliptically shaped; thus, a Gaussian distribution as shown in figure 2 was used for the simulation. Grain growth in a single line width and of an arbitrary length was simulated in this work with a temperature profile, as shown in figure 2, rastered across the length of the line.

## Simulation Results

Simulation of normal grain growth of an isotropic, single phase system under isothermal conditions has been studied and reported in previous works<sup>3,6</sup>. The microstructures from the isothermal grain growth simulations are shown in figure 3. The resulting microstructures are characterized by grain growth exponent,  $n=2$ , as predicted by theory<sup>7</sup>. After an initial transition period, the microstructures exhibit self-scaling behavior, so that the grain size distributions normalized by the average grain size and topology are independent of grain size. Thus, it has been shown that the Potts model can accurately simulate isothermal normal grain growth when grain boundary mobility is constant with temperature.

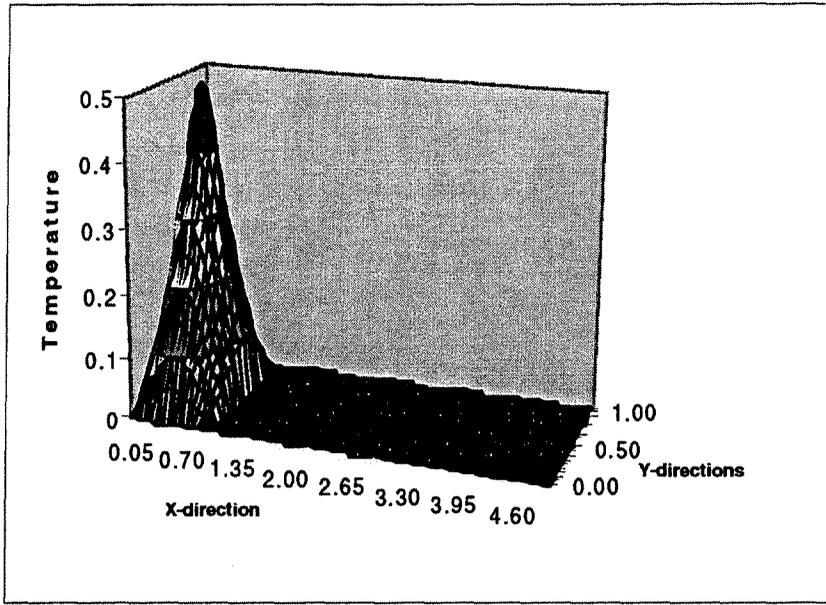


Figure 2. The temperature profile with Gaussian distribution in the X- and Y- directions was used to simulate coarsening.

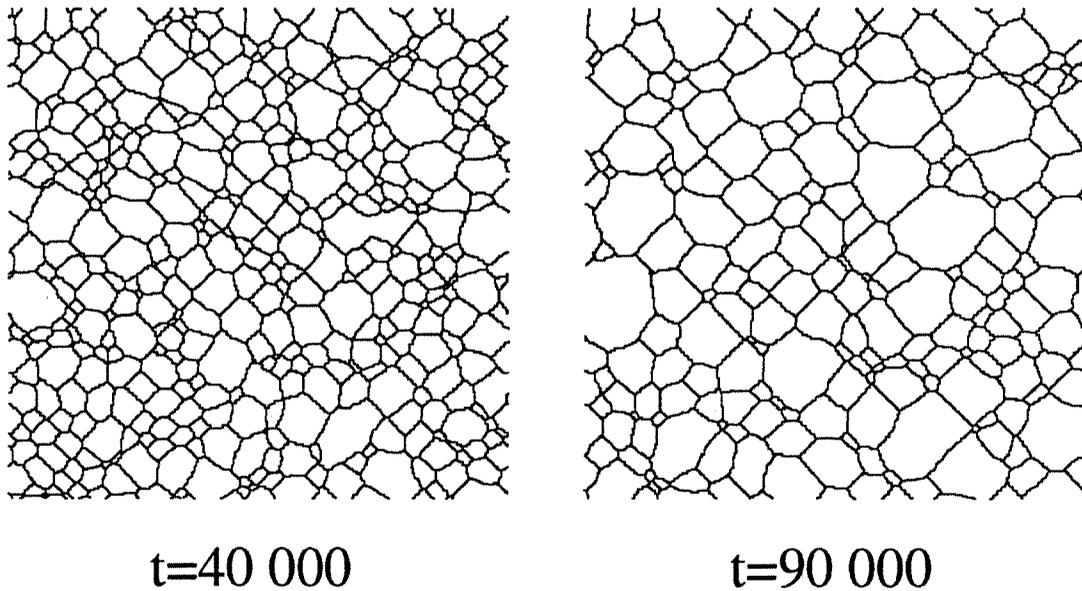


Figure 3. Simulation of isothermal grain growth using the Potts model at 40,000 and 90,000 MCS.

Next, we turn our attention to the simulation of grain growth under a rastering temperature profile of a laser beam. As shown in figure 2, a Gaussian temperature profile with a hot center and progressively cooler edges was rastered with a speed of  $V_{lb} = 0.05$  sites/MCS. The resulting microstructures at mid- and full-raster are shown in figure 4. At the higher temperatures in the center of the line, grains have grown larger. They are also slightly elongated in the center. Another simulation under the same conditions was run with the same temperature profile, but

with a laser raster speed of half the previous simulation speed,  $V_{lb} = 0.001$  sites/MCS. The resulting microstructures is shown in figure 5. This microstructure is dramatically different from the one at the faster raster rate, shown in figure 4. At the slower raster speed, the grain in the higher temperature region are highly elongated in the direction of laser raster. The grains in the cooler region are progressively less elongated and become equiaxed at the coolest region.

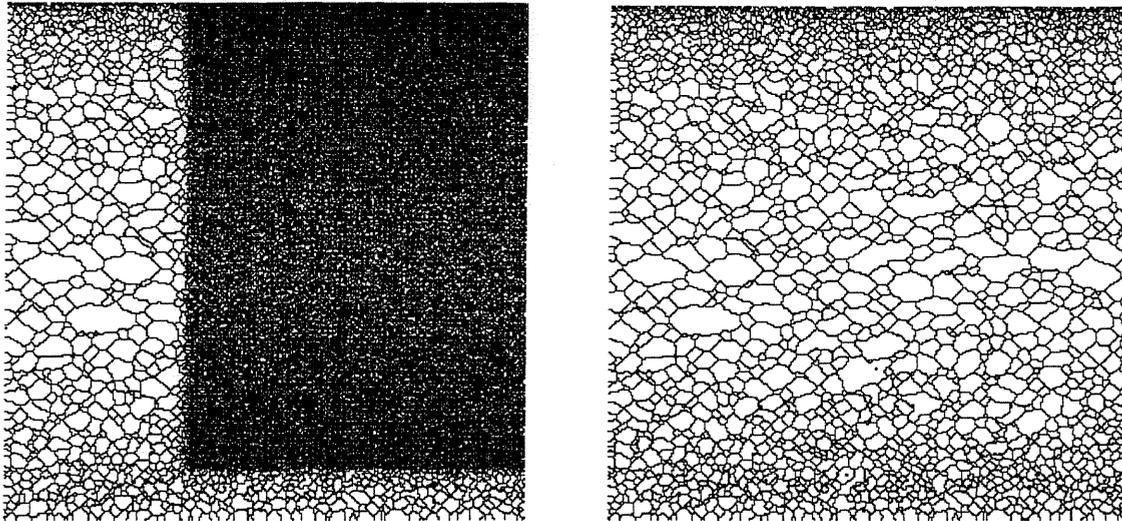


Figure 4. Coarsening in a deposition layer at mid- and full-raster of a laser beam. The raster velocity,  $V_{lb} = 0.05$  sites/MCS. The laser raster direction is to the right. The strip at the bottom of the figure is the previously deposited line.

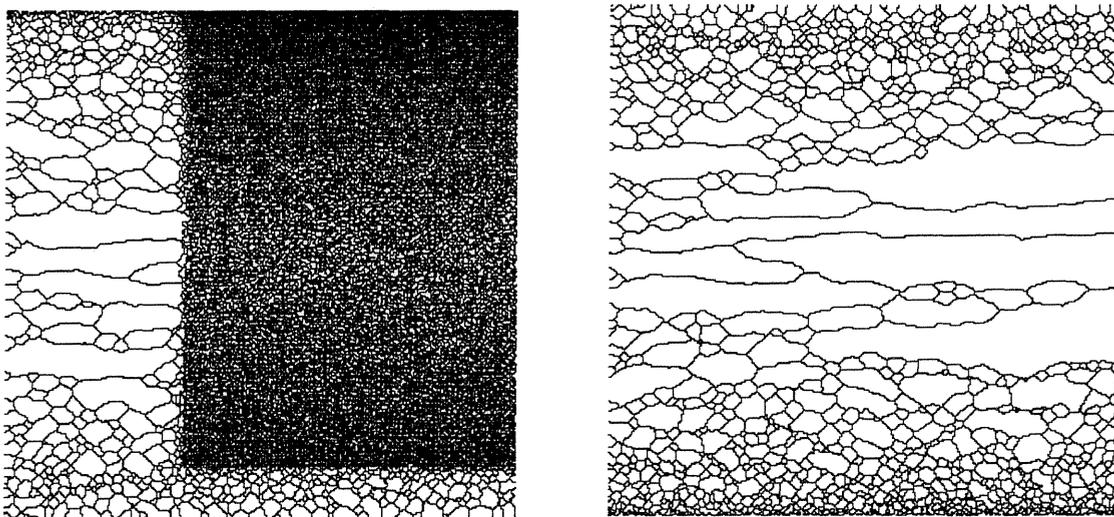


Figure 5. Coarsening in a deposition layer at raster velocity,  $V_{lb} = 0.001$  sites/MCS. The raster direction is to the right and strip is previously deposited line.

Preliminary characterization of the laser beam revealed that the elliptical Gaussian shape of the laser beam was not perpendicular to the laser raster direction, but tilted as shown in figure 6. To understand the effect of such a laser beam, we ran simulations with a tilted beam. The simulation parameters were the same as the previous simulation whose results are shown in figure 5, except

that a tilted temperature profile is used. As shown in figure 7 the grains are highly elongated which was expected as the slower raster speed of  $V_{lb} = 1 \times 10^{-3}$  sites/MCS was used. However, unlike the previous simulation, the elongation is tilted like the laser beam. The abrupt change in microstructure at the left end is due to the use of periodic boundary conditions. At the beginning of the simulation, the bottom of the laser beam is at bottom, left corner of the simulation space and the top is wrapped around to the right of the line at the left end of the simulation space. At the end of the raster, the laser beam is positioned at the line. This leads to the abrupt discontinuity in the microstructure seen in figure 7.

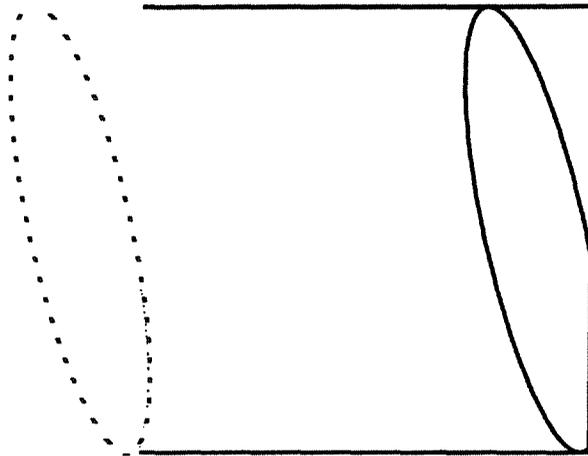


Figure 6. The temperature distribution across the simulation space with periodic boundary conditions at time  $t = 0$ . Light areas are at higher temperature than dark areas

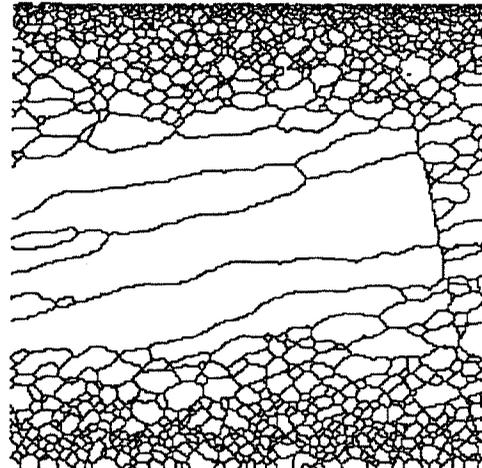


Figure 7. Grain growth with a tilted temperature distribution.

## Discussion

The Potts model has been used extensively to study many different coarsening phenomena, however incorporating a dynamic, non-linear temperature in the Potts model to simulate coarsening in a <sup>TM</sup> part during fabrication is a unique application of this model. In this work, simulation of coarsening in a dynamic temperature environment was achieved by varying the mobility of the grain boundaries with temperature. This is an accurate modeling method as long as the grain growth mechanism and driving force for grain growth are temperature independent and only grain boundary mobility changes with temperature. This is a valid assumption as the growth mechanism and driving force for a number of thermally activated processes is temperature independent over fairly large temperature ranges. Furthermore, in the current study, we were not interested in the effects of multiple grain growth mechanisms or temperature dependent driving force on coarsening. The objective here was to understand coarsening in single-phase, isotropic, material subject to an unusual thermal history.

The simulations presented in this paper show that the raster speed of the laser beam and the temperature distribution around it has a large effect on the grain size and shape. At the faster

laser beam raster speed of  $V_{lb} = 0.05$  sites/MCS, the grains were slightly elongated in the hot section. At this speed, the grain boundary velocity was too slow to grow with the laser beam. When the laser raster speed was slowed to 0.001 sites/MCS, the grain boundary velocity was able to move with the laser. In the cooler regions, on the top and bottom of the simulations, the grain boundary velocity was slower, thus, unable to move with the laser beam. This resulted in progressively smaller, more equi-axed grains away from the center line of the simulation.

The tilted grains seen in figure 7 were unexpected. While the laser beam is tilted, the hot-zone still rasters in the same position, the center of the deposition line. It is only the distribution around the hot-zone that changes slightly. This result demonstrates that grain growth is highly sensitive to any asymmetry in the temperature profile of the system.

The microstructure within a deposition line of the a LENS<sup>TM</sup> component is shown in figure 1. One can see the highly elongated features and as well as the equiaxed features in the microstructure. From our simulation results, we know that the elongated features are forming in the regions where the grain boundary velocity is sufficiently large to move with the moving high temperature of the laser. The equiaxed features are forming in the lower temperature region of the deposition line where the grain boundary velocity is slower and cannot keep pace with the rastering laser beam.

The elongated features are not in the direction of laser raster, rather they are at angle to the raster direction. The results of the simulation suggest that the temperature profile in the LENS<sup>TM</sup> part during fabrication is far more complex than was assumed for the purposes of this investigation. We assumed a Gaussian temperature distribution centered in the middle of the deposition line with symmetric distribution around it and moving at a constant rate in the direction of raster. Clearly, the LENS<sup>TM</sup> part experienced a temperature profile which is does not have these characteristics. The direction of elongation is not is the direction of laser raster. This suggests that the direction of temperature profile movement is not in the direction of laser raster. The part of the LENS<sup>TM</sup> component which has already been formed will act as a heat sink and draw heat away in the direction of previous deposition lines yielding asymmetry in the temperature profile of the part. Furthermore, the asymmetric cooling will move the high-temperature zone away from previously deposited lines. There are also abrupt changes in the microstructural features within a deposition line like the one seen in figure 7. This suggests that the temperature profile in a deposition line is not a continuous smooth raster, but has some discontinuities yielding the abrupt microstructural changes.

The simulations in this work demonstrate the importance of knowing and controlling the temperature distribution during fabrication of a LENS<sup>TM</sup> part. The temperature distribution influences microstructural evolution and therefore must be controlled to tailor the microstructure for optimal performance. Conversely, if certain microstructural features are desirable, this simulation capability can be used to determined the temperature profile necessary for their formation.

## Conclusions

The Potts Model can predict the coarsening of grains during LENS<sup>TM</sup> fabrication. It can simulate grain growth driven by capillarity in a non-linear, dynamic temperature profile of a rastering laser beam. The simulated microstructures had many of the features seen in the actual LENS<sup>TM</sup> parts, in particular they had elongated grains in the direction of a moving temperature profile, equiaxed grains at the cooler regions of the same moving temperature profile and abrupt change in size and shape of grains where there was a discontinuity in moving temperature profile. Thus, the grain size and shape were shown to vary within a deposition line depending on the thermal history of that particular region.

## References

- 
- <sup>1</sup>M. L. Griffith, D. M. Keicher, C. L. Atwood, J. A. Romero, J. E. Smugeresky, L. D. Harwell, D. L. Greene, *Free Form Fabrication of Metallic Components using Laser Engineered Net Shaping (LENS<sup>TM</sup>)*, proceedings of the Solid Freeform Fabrication Symposium, August 12-14, 1996, Austin, TX, p.125.
  - <sup>2</sup>F. Y. Wu "The Potts Model," *Rev. Modern Phys.*, 54 [1] 235-268 (1982).
  - <sup>3</sup>E.A. Holm, James A. Glazier, D.J. Srolovitz, G.S. Grest, "Effects of Lattice Anisotropy and Temperature on Domain Growth in the Two-Dimensional Potts Model," *Phys. Rev. A*, 43 [6] 2662-2668 (1991).
  - <sup>4</sup>D.J. Srolovitz, G.S. Grest, M.P. Anderson, and A.D. Rollett, "Computer Simulation of Recrystallization II. Heterogeneous Nucleation and Growth," *Acta Metall.*, 36 [8] 2115-2128 (1988).
  - <sup>5</sup>J. Wejchert, D. Weaire, J.P. Kermode, "Monte Carlo Simulation of the Evolution of a Two-Dimensional Soap Froth," *Phil. Mag.* B53 15-24 (1986).
  - <sup>6</sup>M.P. Anderson, D.J. Srolovitz, G.S. Grest, and P.S. Sahni, "Computer Simulation of Grain Growth I. Kinetics," *Acta Metall.* 32 [5] 783-791 (1984).
  - <sup>7</sup>M. Hillert, "On the Theory of Normal and Abnormal Grain Growth," *Acta Metall.*, 13 227-231 (1965).

