From Simple Shapes to Microstructural Grain Structure: An Inquiry

E. Begum Gulsoy

egulsoy@andrew.cmu.edu

CMU, Department of Materials Science and Engineering

17.12.2007

***Abstract*—Based on serial sectioning data, materials microstructure can be reconstructed to digitally represent each grain in three dimensions. This paper attempts to calculate the average shape of the grains through Principal Component Analysis(PCA) , with a theoretical introduction to how this method can be generalized into calculating an average shape of the microstructure. Also investigated is the relation between the commonly assumed average shapes, sphere and ellipsoid, and the average shapes calculated, which for the current case proves to be very similar. Finally, the knowledge acquired from the first two steps is applied to creating new grain shapes which possess the characteristic of the microstructure.**

***Index Terms*—Three-dimensional Morphing, PCA, Three-dimensional Reconstruction, Microstructure**

I. Introduction

THREE-DIMENSIONAL reconstruction of microstructures from two-dimensional serial sectioning data, acquired through different techniques have been around for some time now. Following the development of new technical opportunities, one of the latest ideas is to acquire the serial sectioning data with a focused ion beam microscope, combine it with information detected from orientation imaging microscopy and to apply both pieces of information as an attempt to build more accurate representation of microstructures. Starting with a 3D reconstructed Ni-based superalloy microstructure, this project aims to investigate the shape characteristics of the microstructure acquired through a principal component analysis (PCA) approach. The major curiosity is to be able to calculate an average shape of the grains and see if this average shape deviates from the commonly assumed sphere or ellipsoid, and if yes, how. Also, investigated is a beginners approach to 3D morphing and see if this can be applied to microstructural grains.

II. Parameterization

Two entities can only be compared using a common basis. In this case this basis will be constructed through defining a set of corresponding points in 3D, for both shapes. Assuming the shapes are different, as would be the case with microstructural grains, correspondence is to be defined by directions. This process involves several steps.

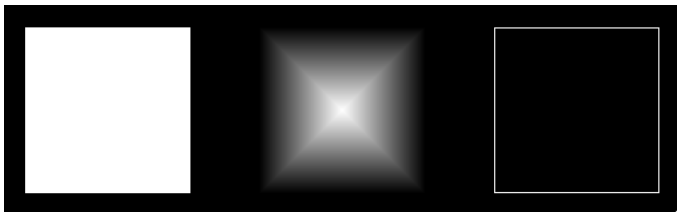

Fig. 1. The distance mapping procedure; Left: A layer from a solid cube, Middle: Distance map of the cube, shown is a cut through the structure, Right: The thresholded image showing the surface voxels

First, the chosen grains are thresholded and separated from the microsturcture. Then, the orientation information is extracted from the experimental data in terms of euler angles and the grains are aligned with respect to the 'laboratory reference frame'. This involves defining three rotation matrices corresponding to these euler angles and multiplying each voxel with the inverse of these matrices. Once done, the xyz corrdinates of each voxel in the structure is used to calculate a center of mass, such that

$$\mathbf{c_m} = [(\sum \mathrm{X_{coord}})/\mathrm{n}, (\sum \mathrm{Y_{coord}})/\mathrm{n}, (\sum \mathrm{Z_{coord}})/\mathrm{n}] \quad (1)$$

where $\mathbf{n}$ is the number of points used and $\mathbf{c_m}$ corresponds to the xyz coordinates of the center of mass of the grain. The center of mass is calculated for all grains of interest, separately. Then, a global center is defined, which most of the time corresponds to the center of the array the grains are extracted from. Each grain is then shifted such that their center of mass corresponds to this global center.

As the grains are aligned in the right manner, next step is to define the voxels that contribute to the outermost surface of the structure and eliminate the enclosed ones. This arises the need for a distance map. The aim is to construct a grain map such that the farthest voxels from the center of the structure will be assumed as the surface. For this project a three-dimensional distance map is constructed using Interactive Data Language(IDL)'s the built-in MORPH_DISTANCE function.

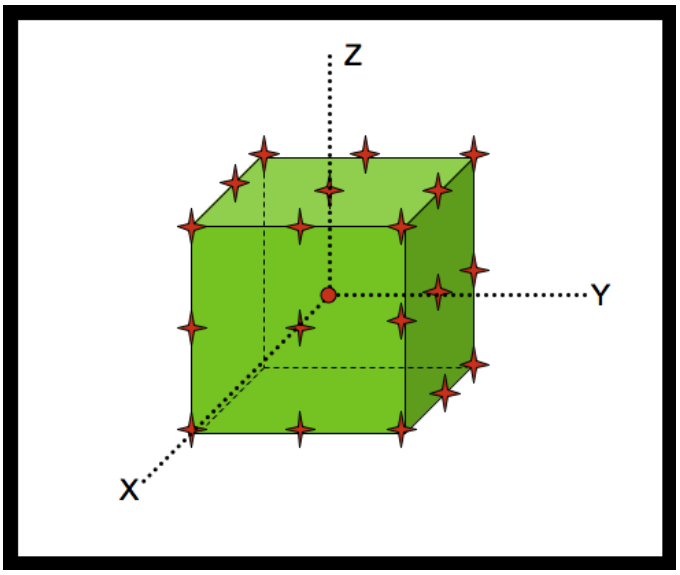

Fig. 2. The {100},{110},{111}directions, half shown

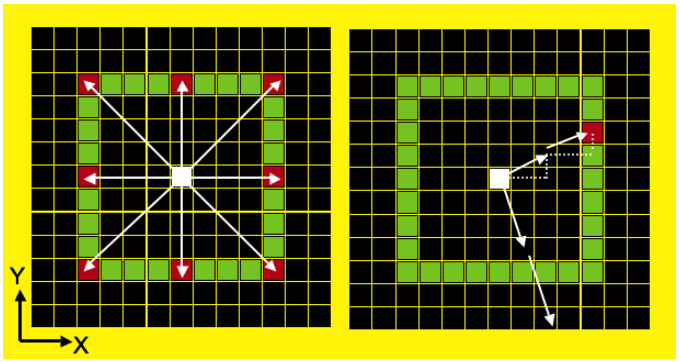

Fig. 3. Determination of directions; Left: March to find the surface voxels in the corresponding pre-determined directions, Right: March in random directions, which may or may not end up at a surface voxel

This function assigns the maximum value to the structure center and decreases this value by one calculating the next-nearest neighbors until the surrounding is reached, which is defined by 0's. Thresholding the map by 1, as seen in figure 1, it is possible to extract the surface voxels.

Next step is to define a set of directions. In this case, dimensions fall into two categories: the pre-defined ones and the randomly generated ones. The pre-defined directions are the {100},{110} and {111}. These directions are shown, using a cube, in figure 2 where the center of the cube is assumed to be origin, at [0,0,0], and the cube has dimensions 2unitsx2unitsx2units.

Next step is to define a set of directions. In this case, dimensions fall into two categories: the pre-defined ones and the randomly generated ones. The pre-defined directions are the 100, 110 and 111. These directions are shown, using a cube, in figure where the center of the cube is assumed to be origin, at [0,0,0], and the cube has dimensions 2unitsx2unitsx2units. The random direction generation is a little more tricky. The idea is that, in order to move in 3D one has to take steps in x, y, and z directions. The algorithm developed, generates three random numbers, where these numbers have the freedom of being positive or negative, and assumes these to be the step sizes taken in corresponding directions. Theoretically, since the outcome of the random number generator can be negative or positive, the system is allowed to march in all possible directions. An example, simplified to 2D for visualization purposes can be observed in figure 3.

When dealing with voxelized structures, the surface voxels determined do not span a continuous surface. Therefore, depending on the shape of the structure, it is possible not to land on a surface voxel or in other words to 'miss' the surface in any given direction. An example has been given on figure 3, right. These directions are eliminated and instead a new direction is randomly generated in order to account for the desired density of sampling. While dealing with multiple images, the aim is to sample the structures by finding their corresponding surface voxels along the same directions. Therefore, one has to account for the fact that if a surface is missed in one of the structures in a certain direction then the results of that direction should be eliminated from all the surfaces.

III. Approach

Given any two shapes, the corresponding points can be acquired, at a desired sampling density, using the approach which has been extensively explained in section two. The denser the sampling is, the closer the shapes can be approximated. The mean shape can be directly calculated by finding the average coordinates of each sampling point, such that

$$\mathbf{ave_c} = [(\mathrm{X_{i1}} + \mathrm{X_{i2}})/2, (\mathrm{Y_{i1}} + \mathrm{Y_{i2}})/2, (\mathrm{Z_{i1}} + \mathrm{Z_{i2}})/2] \quad (2)$$

where $\mathbf{ave_c}$ is the average coordinate array of the form 3 by n and $\mathbf{X_{i1}}$, $\mathbf{X_{i2}}$.... indicate the xyz coordinates of a point in two different images.

However, the mean shape is not the only shape of interest. The aim of this project is to be able to generate any shape that lie in between two shapes as well as, given several shapes, extract the characteristics that correspond to the bunch and be able to create shapes that possess the same characteristics. This is possible through a principal component analysis (PCA).

PCA is a method that transforms the current coordinate system into another such that the largest variance will be visible and the eigenvectors acquired correspond to the dimensions with the strongest correlation.

$$\mathbf{A} = [\mathrm{U}][\mathrm{S}][\mathrm{V^T}] \quad (3)$$

where $\mathbf{U}, \mathbf{S}, \mathbf{V^T}$ are the orthogonal eigenspace vectors. Before PCA, the coordinates of the points has to be normalized such that the center of mass lies on [0,0,0]. The result gives a set of vector that define the characteristics of the major variances in the data set.

Once applied, out of the results, the first eigen vector turns out to be the step size that need to be taken while transforming

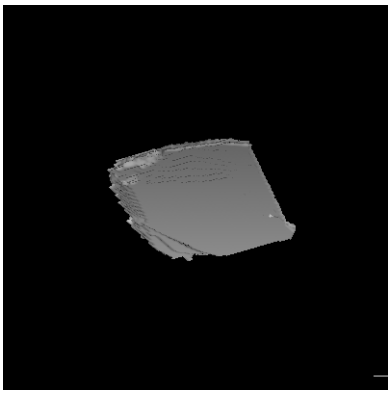

Fig. 4. The 3D reconstructed grains: Grain#1

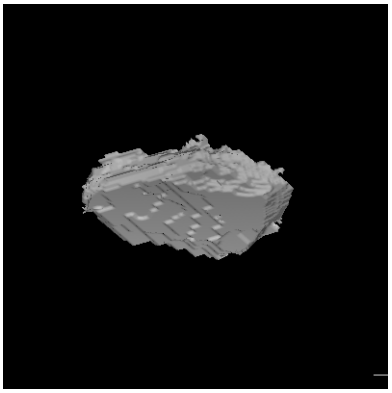

Fig. 5. The 3D reconstructed grains: Grain#2

one set of points to the next one, giving the average shape at 50-50. Therefore it is possible to morph one three-dimensional shape into another using a single eigen vector, assuming the sampling is dense enough to represent the shapes as close as possible. An example will be provided in the next section.

IV. Experimental Results

A. Application to Basic Shapes

The first shapes investigated include rectangular prisms and cubes since they are relatively easy to work with due to the almost perfect corresponding of their 8 corner points. Also important is the fact that rectangular prisms are easy to generate randomly. Using these shapes have provided insight to the project and have been very useful in improving the algorithm.

B. Application to Microstructural Grains

Grains possess far more complex shapes than the prisms. They are harder to deal with because, first of all, they are much bigger, which causes them to take up more memory as well as increasing the running time. They are also much more voxelized which makes finding random corresponding directions much harder, especially as the number of the grains taken into consideration increases. On the other hand, being able to extract the shape characteristics of a data set is very exciting from a materials science point of view. The information on whether these characteristics change from material to material may prove to be important in terms of investigating a link between microstructure and materials physical behavior. Although there is still a long way to the point where this link can be investigated, the explained method has been applied to two grains taken from a real Ni-based superalloy microstructure. The serial-sectioning data set is a courtesy of M. Uchic of Air Force Research Lab at Wright Patterson Air Force Base and has been digitally reconstructed at Carnegie Mellon University by E.B. Gulsoy and Prof. M. DeGraef where orientation work has been completed by Sukbin Lee.

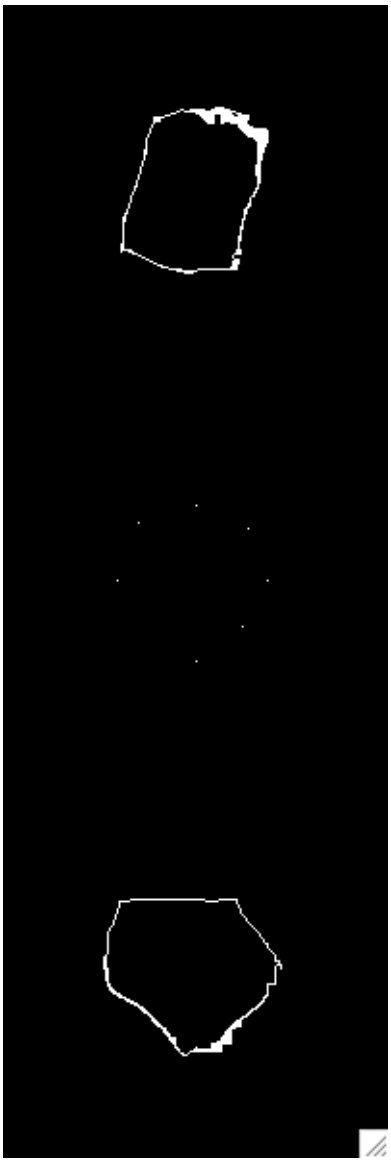

Fig. 6. The 3D reconstructed grains; Top: A cut through the surface of grain 1, Middle: The average shape calculated using equation (2), Bottom: A cut through the surface of grain 2

Figures 4 and 5 show the three dimensionally reconstructed grains. The two grains chosen appear to be thin and elongated. Following the procedure, figure 6 shows a cut through the 3D structures with the middle image representing the average shape calculated from equation 2. 27 attempts were made to determine

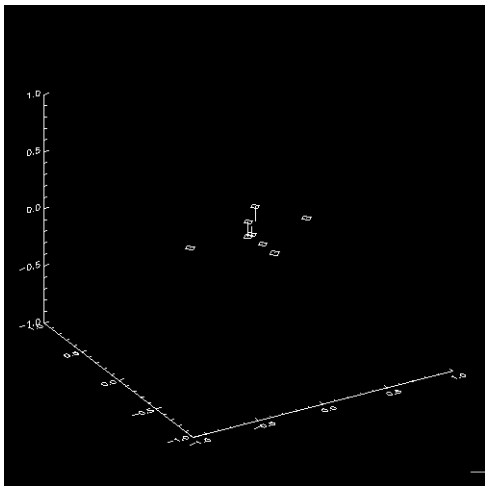

Fig. 7. The first eigen vector

Fig. 8. A new shape created by F=9 for e0 and F=30 for e1

corresponding directions between grains, 21 of which were succesful.The average shape, represented as a cut through the cloud of corresponding points, is a reasonable approximation between the top and bottom shapes in figure 6. This shows that the sampling was, even though not very dense, was enough.

Figure 7 represents the first eigen vector calculated through PCA of the two grains. Applying the first eigen vector to the sampling points from the first grain enables the generation of all the shapes that appear as one shape is morphed into another. A slice through the 3D shapes in showm on figure 9. The eigen vector has been applied as:

$$\mathbf{Newpts} = \mathrm{pt1arr} + \mathrm{e0} * \mathrm{F} \tag{4}$$

where $\mathbf{Newpts}$ represent the new coordinates of the sampling points, $\mathbf{pt1arr}$ holds the sampling points of the first grain, $\mathbf{e0}$ corresponds to the first eigen vector and $\mathbf{F}$ is a multiplication factor.

Using the same idea, and therefore the eigen vectors it is also possible to generate new grains, which have the same characteristics. An example has been given in 8

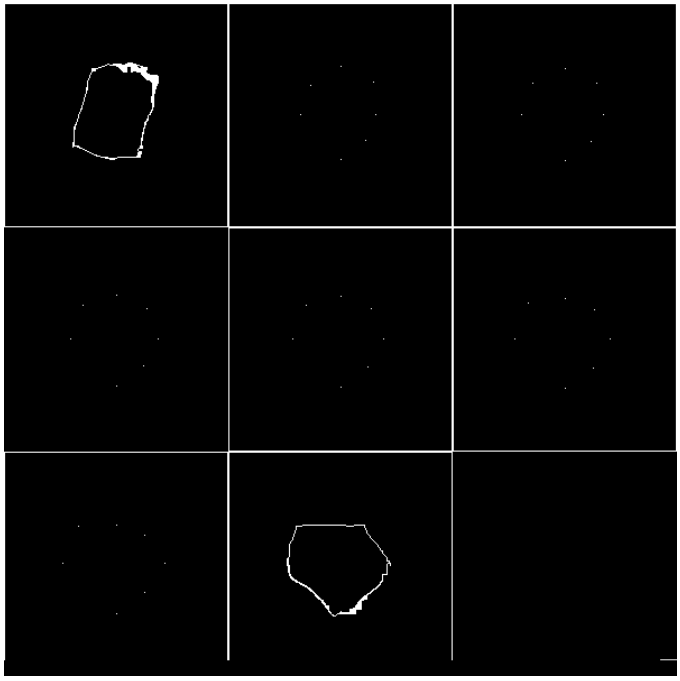

Fig. 9. Transforming from one shape into the next, using the first eigen vector

V. Conclusions

This project has attempted to investigate the shape characteristics of a microstructure. Although no large scale research could be done, it was shown that it is possible to transform shapes into each other in 3D through the usage of PCA analysis and eigen vectors. It was also shown that an average shape could be determined using the same approach. It would be interesting to see if this idea can be extended to compare different materials shape distribution and average shape with their physical behavior and investigate if a correlation exists.

Acknowledgements

The author would like to thank Professor A. Efros for his enthusiasm in making Computational Photography course available at CMU. It really has been a great experience. Also to mention, Jim McCann for his time, support and patience as the class TA.