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Application of Centroidal Voronoi Diagram in Numerical Model of Microforming process

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Keywords: Microfingming, Size effects, Centroidal voronoi diagram, Simplex integration

Abstract. Grain size, shape and orientation play an important role on the deformability of micro workpiece as the geometrical dimensions approach to a characteristic scale in micro-forming process. This paper addresses the three-dimensional (3D) finite element (FE) model with weighed centroidal voronoi diagram (WCVD). Steady-state grains are generated when the voronoi generating points approach the grain centroid utilising a simplex integration algorithm. As a result of the centroidal process, the topological features of grains advance the uniform and steady state gradually, which may cause a decrease of interfacial energy. The grain size distribution is compared between the 3D domain and random cross-sectional plan. The effects of centroidal process on the distributions of grain size and number of grain corners, facet and edge are analysed.

Introduction

In recent years, driven by the increasing demand for these products due to the trend towards micro system technology (MST) and one of its increasingly important outcomes, micro electro-mechanical systems (MEMS), microforming has been developed successfully as an appropriate technology to manufacture metallic micro components with at least two dimensions in the sub-millimeter range [1, 2]. Components of this size are commonly used in electronics production and other fields including the medical sector.

Material size effects arise as the geometry of the part approaches a characteristic length scale i.e. at least two of workpiece size under the sub-millimeter range [2]. The deformation behaviour of single grain is anisotropic. The mechanical properties of polycrystalline material is considered as isotropic since the dimension of workpiece is much larger than that of grain inside and the unique properties of individual grain such as grain size, shape and orientation are neglected within the macro scale. In microforming process, as the specimen size approaches the dimension of grain size, there are a small number of grains locating in the specimen as shown in Fig. 1 [3]. Therefore, the size effects become significant, and the grains with different sizes, shapes and orientations result in the scatter of the measured mechanical properties. This size effects are captured in the numerical model utilising voronoi diagram.

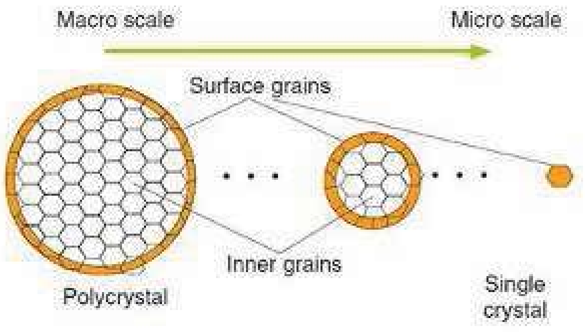

Figure 1. The ratio of surface grains to volume grains Increases with miniaturization [3]

Voronoi Tessellations

Voronoi diagram has been utilised to conduct significant research by generating polycrystalline material structure [4]. The voronoi diagram subdivides an area space into convex polygons or cells that fills the space without overlap. In the application, each voronoi cell is regarded as a grain. Voronoi tessellations can be conducted in both two- and three- dimensions. The grain radius R is defined as the cubic root of the grain volume and the average grain radius $\langle R \rangle$ is defined as the cubic root of average grain volume within in the 3D grain. The radius R of a grain in a cross section is defined as the square root of the polygonal area of Voronoi diagram and the average grain radius $\langle R \rangle$ is defined as the square root of average polygonal area. The grain size distributions obtained from the entire 3 dimensional (3D) domain and from the random cross section of that 3D domain are shown in Fig. 2a and b respectively. It can be seen that the distribution of Fig. 2b is significantly broader than that of 3D domain. This result suggests that the grain distribution obtained from the cross section is not appropriate to represent the grain size distribution for the entire 3D domain. For the FE application, 3D Voronoi tessellations will be focused in this paper.

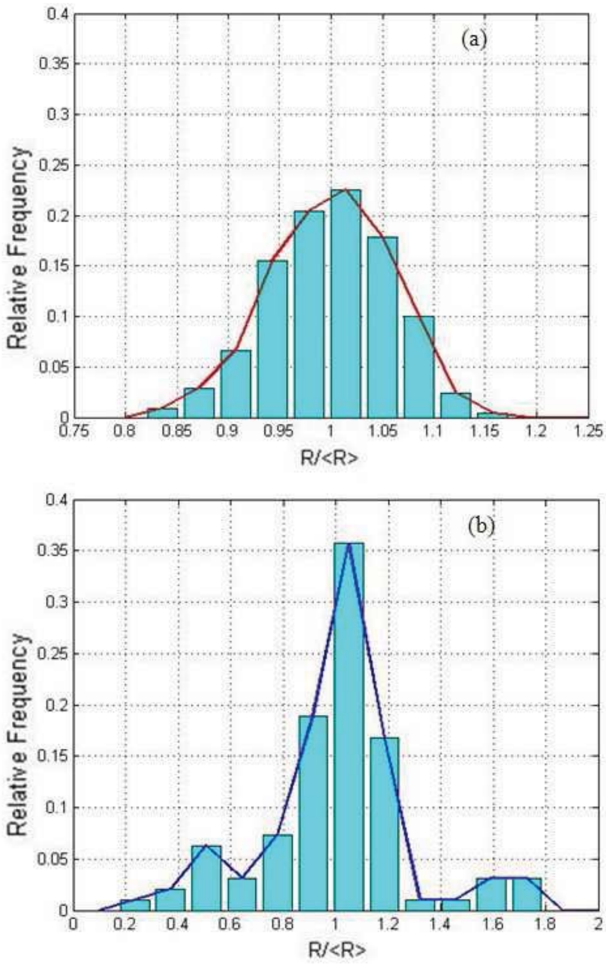

Figure 2. Normalized grain distributions (a) for the entire 3D domain and (b) for the random cross-sectional plan

Stable Grain Structure and 3D Centoidal Voronoi Diagram.

The geometric form of the grain structure is defined by the system of grain boundary, which constitutes a topological network. In metals, it is characterised by a progressive magnification of grain size without seeming to change their geometric form, which follows after a growth period when the grained topological state towards a constant average ratio of corners to faces to edges 6:7:12 and on a cell this ratio is 24:14:36 as shown in Fig. 3 [5, 6].

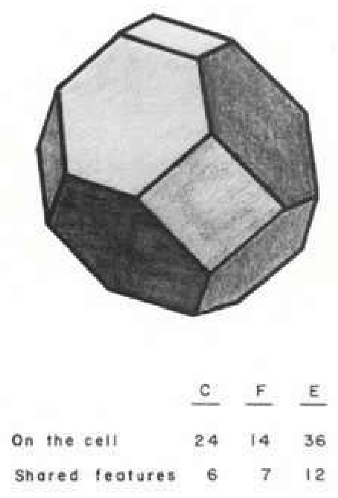

Figure 3. A 14-sided figure representing the average topological form of grains in the polycrystalline metal

According to the characteristics of the stable magnification process of grain in metals, centroidal Voronoi diagram is proposed to generate the topological structure of stable polycrystalline metals. A centroidal Voronoi diagram has the odd property that each generating point lies exactly on the centroid of their Voronoi region. The centroid of a region is defined as

$$c = \frac{\int_A x\rho(x)dA}{\int_A \rho(x)dA} \tag{1}$$

where A is the region, x is the position and $\rho(x)$ is the density function [7]. In this study, the grain density is regarded as homogeneous, so 1. 3D simplex integration method is used to calculate the weight centroids of the 3D Voronoi cells.

Procedure to Generate Stable Polycrystalline Structure

In this study, a 3D domain including 1000 grains is set up. The space is divided into $10\times10\times10$ cubes with volumes $a\times a\times a$ mm^3. Then, the seeds are spread into these cubes. Assuming the centre of a cube is (x, y, z), the seed will lie $\lambda\delta a/2$ away from the central point. Exactly, the coordinate of the seed position should be $(x+\lambda\delta a/2, y+\lambda\delta a/2, z+\lambda\delta a/2)$. δ is the maximum distance between the seed and the cubic centre, and λ is a random number between -1 and 1. Both of δ and λ is so called shape factors which will determine the shapes of Voronoi cells. A critical distance d between different seeds is defined to prevent seeds from being excessively close to one the other. After that, the 3D Voronoi diagram is generated taking the seeds as the generating points. Calculations of the topological features per grain are conducted. If the distributions of grain corner, facet and edges satisfy the value of stable grain, continue the procedure. Otherwise, identify the centroids of Voronoi cells applying the 3D simplex integration algorithm. Then based on these centroids, a new set of voronoi tessellations is generated. The procedure is shown in Fig. 4.

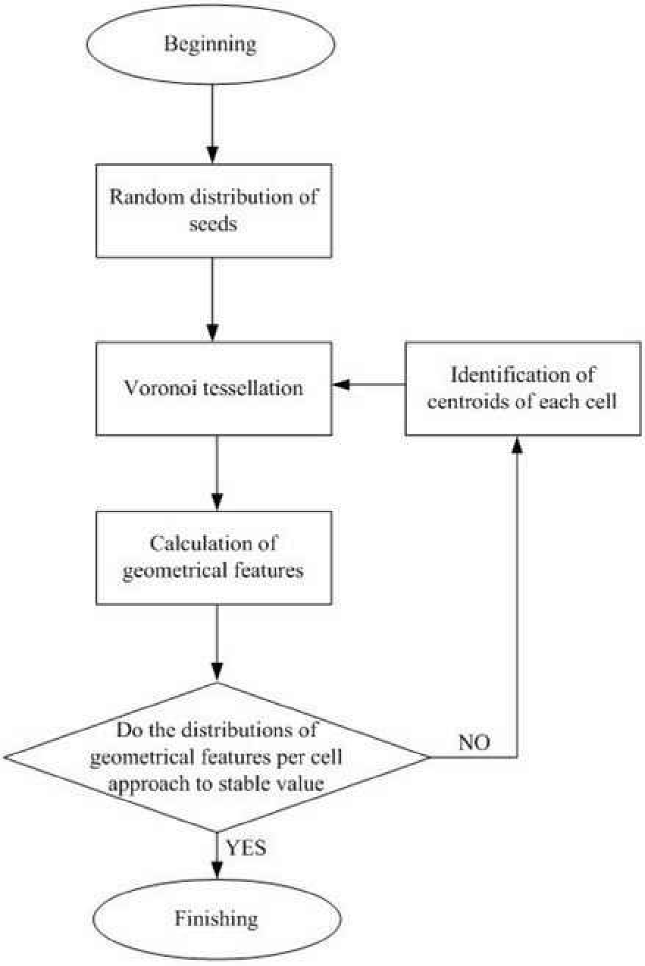

Figure 4. Procedure of generating stable polycrystalline structure

Analysis. Fig. 5a shows the normalised grain size distributions obtained become narrower as the centroidal process evolves. The number of grain with the average volume increase significantly as shown in Fig. 5b, which indicates the centroidal process make the grain size more even.

As the influence of CS on the geometrical features, Fig. 6 shows the distributions of the number of corners, facets and edges per grain N_c, N_f and N_e. All of these three distributions appear to become narrower with an increase of CS. Moreover, as the centroidal process evolves, there is an increase of grains whose ratio of corners to faces to edges approaches to 24:14:36, which is geometrical features of steady-state grains.

Application of Voronoi diagram in FE modeling. After generating the appropriate topological structure of grains within the specimen, this geometrical feature should be imported to FEM software and randomly meshed. However, free meshing may generate abnormal elements and increase computational error. In order to eliminate the effects of meshing, the specimen is meshed with regular cubic elements at first. According to the properties of Voronoi cell, the distance between any point inside a Voronoi cell to its own generating point is shorter than the distance between this point and any other generating point, the elements can be identified to belong the grain by measuring the distance between the element and all of generating point of Voronoi tessellation. As shown in Fig. 7, the application of Voronoi tessellation in FE modeling is accomplished by modifying the keyword file of ANSYS/LS-DYNA.

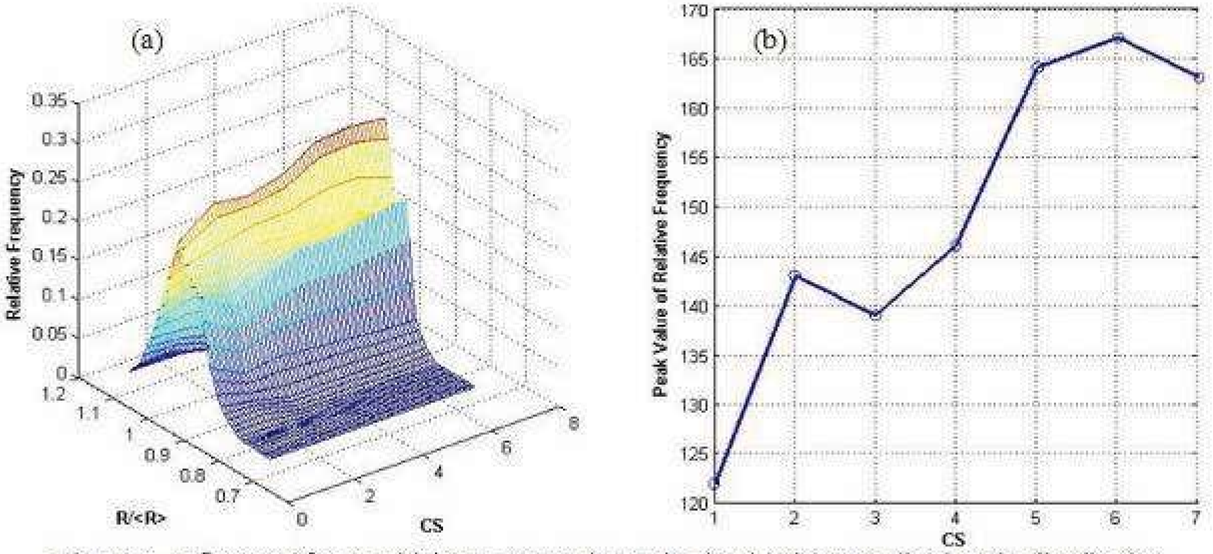

Figure 5. Influence of centroidal process on the grain size (a) the nomalized grain distribution (b) the peak vaule of the relative frequency of volume

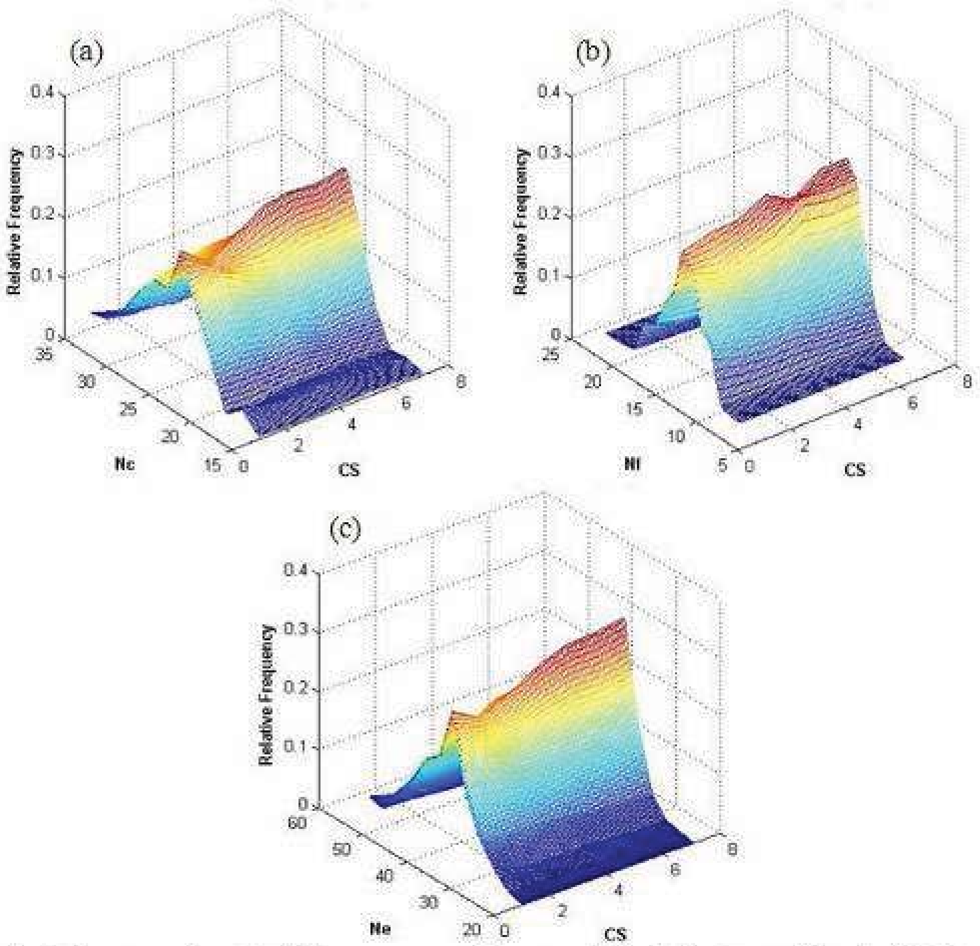

Figure 6. Influence of centroidal process on the geomitrical features of grain (a) Numbers of corners (b) Numbers of facets (c) Numbers of edges

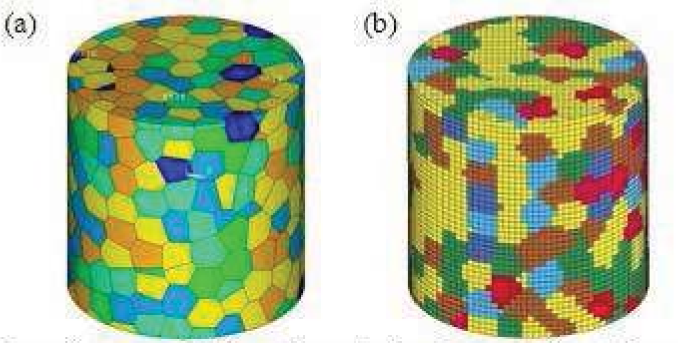

Figure 7.Application of voronoi tellessations in the FE modeling (a) voronoi cells (b) FE meshing

Conclusions

As the specimen dimension is scaled down to microscale, the traditional homogenous material model is no longer valid for the analysis of microforming process due to size effects. The influence of individual grain size, shape and orientation cannot be neglected when there are only a few grains locating in the deformation region. Voronoi diagram is used to generate the polycrystalline structure. Centroidal Voronoi tessellations are utilised to obtain the stable micro structure in terms of grain shape. The analysis indicates that the distributions of grain size and number of geometrical features per grain including grain corners, grain facets and edges appear towards a value of the steady-state polycrystalline structure. Finally, the application of Voronoi tessellation in FE modeling is realised with the numerical model composed by regular element.

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