THREE DIMENSIONAL COMPLEX SHAPES ANALYSIS FROM 3D LOCAL CURVATURE MEASUREMENTS. APPLICATION TO INTERMETALLIC PARTICLES IN ALUMINIUM ALLOY 5XXX

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ABSTRACT

The studied material is a 5xxx aluminium alloys containing 2 types of intermetallic particles : $Al_x(Fe,Mn)$ and Mg_2Si. It is usually used in car industry as reinforcement pieces or in packaging industry, such as bottle liquid box lid. Scanning electronic microscope coupled with EDX analysis shows complex shapes of intermetallic particles. The particle shape is obtained during the solidification of alloys. Particles fill vacant spaces between aluminium grains. Therefore final sheet properties depend on intermetallic particles shapes and notably on the matrix-particle interface properties. The goal of the present study is to classify intermetallic particles versus their shapes using local curvature information. The aluminium alloys sample is observed by X ray micro tomography performed at the ESRF. Three dimensional images are segmented, and intermetallic particles are identified in a data base. Each particle is stored as a set of voxels. The surface of each particle is meshed by a marching cubes triangular meshing with the software Amira©. A simplification of the surface is performed by an algorithm contracting the edges. Finally, principal curvatures: k_{min} and k_{max} are estimated by Amira© on each facet centre of the mesh. From the full intermetallic population, the bivariate distribution of k_{min} and k_{max} is estimated. The obtained graph $k_{min} - k_{max}$ shows geometrical properties of interface portions of the surface of particles. A factorial correspondence analysis is performed to summarize the information on all intermetallic particles. In the obtained subspace, particles are classified into five shape families, in relation with their interface geometrical properties.

Keywords: 3D, classification, complex shape, local curvature, statistical analysis.

INTRODUCTION

The study of the microstructure of materials allows to predict its mechanical properties, and to develop a product with desired properties.

X ray micro tomography performed at the ESRF (European Synchrotron Radiation Facility) provides the acquisition of three dimensional images of materials in a non destructive way with a high resolution (up to 0.7 μm in the present case). Image analysis is then fundamental to extract information within scanned images, and to quantitatively characterize the micro structure of materials from three dimensional measurements.

In the case of metallic materials, as aluminium alloys 5xxx, the microstructure contains intermetallic particles showing 3D complex shapes. Their analysis requires characterization method suited to the complex nature of information. Many 3D shape analysis methods exist in the literature. Nevertheless, in most cases they are used for simple 3D shape analysis, such as for instance star shapes are described with the help of Fourier descriptors (Gardner *et al.*, 2003; Hobolth, 2003). For more complex shapes, parametric studies

have been efficiently applied (Parra-Denis *et al.*, 2007; Parra-Denis, 2007).

In this paper, we propose an alternate methodology to the parametric one for the three dimensional complex shapes analysis. This analysis is based on the study of the principal local curvature k_{min} and k_{max} at the surface of objects. This methodology follows the ideas of Alkemper and Voorhees (2001); Voorhees *et al.* (2002) to study the growth of aluminium grain dendrites. In the present study, we use the bivariate distribution of k_{min} and k_{max} to analyse the three dimensional complex shapes of intermetallic particles.

The paper is organized as follows: in the first part, we provide the method used to obtain the local curvature's information. Firstly, the definition of principal curvatures on an object surface is given. Secondly, the object's meshing method used in the present study is detailed. Lastly, we give parameters of the meshing for intermetallic particles contained in aluminium alloy 5xxx. In the second part, we present the bivariate distribution of k_{min} and k_{max}. Firstly, we give interpretation of the graph. Then, an example on a typical intermetallic particle illustrates the information of the graph. In the third part, the

statistical analysis of the results on an intermetallic particles population is presented. Its implementation is first given. Then the results obtained are presented. Finally, a classification depending on intermetallic particle shapes is performed. In the last part, we conclude with presenting the advantages and the limits of the proposed method, and present some possible projects for future works.
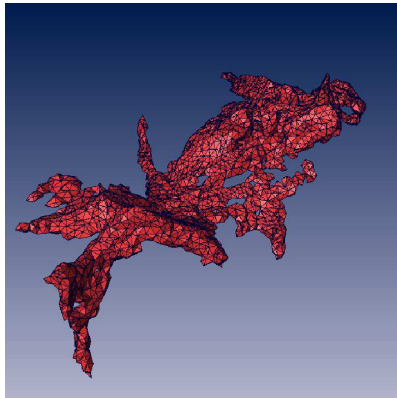

Fig. 1. *Example of intermetallic particles contained in AA 5xxx meshed by Amira. The facets number of the meshing is equal to 8044.*

MEASUREMENTS OF LOCAL 3D CURVATURE

In image analysis, the study of the curvature is used to measure the total curvature integral which presents topological features, and the mean curvature integral which presents metrical features. They are estimated by stereological methods (Ohser and Mücklich, 2000). The study of the curvature is also currently used in computer generated images. In these studies, the discrete surface of objects is characterized by the local curvature measurement (Besl and Jain, 1986; Stokely and Wu, 1992). These methods are based on a triangular meshing of the surface (Polthier and Rossman, 2002).

In metalworking industry, the studies performed by Mendoza, Alkemper and Voorhees (Alkemper and Voorhees, 2001; Voorhees *et al.*, 2002) on the local curvature histograms ensure to follow the evolution of aluminium dendrites during the solidification process. An application of these studies to intermetallic particle shapes contained in aluminium alloys seems to be appropriate.

In this section, we present the measurement of local curvature to characterize three dimensional complex shapes. The definition of surface curvature in the three dimensional space is first defined. Then,

its implementation is presented. Lastly, parameters of the meshing for intermetallic particles contained in aluminium alloy are given.

THE CURVATURE OF A SURFACE

Let S be a smooth surface in the Euclidean space $\mathbb{R}^3$, and x be a point of S. The normal vector n is defined at x on the surface S. Every plane P containing n intersects S with a curve C. For each plane P_i, the radius of curvature r_i of C_i at x is given. The minimum curvature radius R_{min} and the maximum one R_{max} are obtained for a set of two orthogonal planes. They define the maximum curvature k_{max} (reciprocal of the radius) and the minimum curvature k_{min} , called principal curvatures.

IMPLEMENTATION

The surface meshing of an object is usually used in materials field, to carry out a mechanical analysis of an object by finite elements calculation, directly from three dimensional images. The choice of the technique to mesh the surface is a difficult problem (Frey and George, 1999).

In the present study, the local curvature measurement is performed with Amira© software. The principal curvatures of intermetallic particles are measured on the mesh produced by Amira©.

The geometry of aluminium alloys containing particles is complex (Fig. 1). It is far from simple geometries and the use of regular meshing of points is not possible; then the method used to mesh particles is a frontal non structuring method.

Frontal methods mesh the field by successive iterations, propagating a front inside the surface (starting on the surrounding area of the field), until its complete covering.

The non structuring meshing method used is based on the Marching Cube algorithm (Lorensen and Cline, 1987). From the 3D image, the surface of the object is digitized into triangles to mesh. Then from the discrete surface, the volume is meshed into linear tetrahedrons by using a frontal method implemented into Amira© software. This method allows us to vary the length of elements of the model without creating discontinuities. The number of triangular elements needed to cover the surface depends on its complexity. It is optimized to obtain a good definition of the surface with a low number of degrees of freedom.

After meshing, a simplification algorithm of the surface by collapsing edges is applied (Hoppe *et al.*, 1993). This algorithm consists in merging the two

extremities of edges into an apex, with a collapsing criterion based on the minimization of an energy function (Tables 1 and 2).

MEASURES PARAMETERS USED

The measure of the curvature in Amira© software is based on the meshing obtained by the Marching Cubes algorithm. Thus the principal curvatures are estimated either for each triangle of the surface, or for each point of the meshing. The algorithm works by a local fit of the surface according to a quadratic form. The eigenvalues and eigenvectors of the quadratic form correspond to the principal curvature values and to the directions of principal curvature.

Then a smoothing is made, depending on two parameters:

– The number of neighbours: it determines which triangles and which points are considered to be neighbours of a given triangle and of a given point. If the value of this input is one, then only triangles sharing an edge with a given triangle, and only points directly connected to a given point are considered.

– The number of iterations: it determines how many times the initial curvature values computed for a triangle or for a point are being averaged with the curvature values of direct neighbour triangles or points. This parameter only applies to the scalar curvature values, not to the directional curvature.

A code written in Amira© software automatically generates the measurement of the curvature on an images set of raw type. For a sample of aluminium alloys with dimensions $(1 \times 1 \times 4)$ mm^3, each intermetallic particle corresponds to a single binary image. Typically there are among 4.000 particles in a sample. Each particle is then meshed. Amira© gives, for each facet of the meshed object, the coordinates of the three points which compose the triangle, and the values of the principal curvatures. A file containing each facet of the meshing its surface and its principal curvatures values is created. A preliminary study on different usual shapes with varying length was being performed, in order to validate the method of estimation. We have tested different shapes: cylinder (with different orientations), sphere, torus, and ellipsoid. For each tested shape, we introduce variations of all the parameters: simplification of the meshing varying between $0; 1, 4; 2, 8$, number of neighbours varying between $1; 6; 16$. Finally the retained parameters for further measurements are a simplification of the meshing equal to 1.4, a number of layers equal to 6, and a number of average equal to zero (Fig. 1 and Table 1).

The time needed to numerically compute the different curvatures on a data base of 4921 images of particles is 2hrs 21min (on a AMD Athlon 2600+ with 2 GB of RAM).

THE $k_{min} - k_{max}$ GRAPH

It is possible to quantify the shape of the object-matrix interface by looking at the distribution of the principal curvatures ($k_{min} - k_{max}$). The papers written by Alkemper, Voorhes and Mendoza present the use of the obtained graph to characterize the growth of dendrites during the solidification process of copper aluminium alloys (Alkemper and Voorhees, 2001; Voorhees *et al.*, 2002).
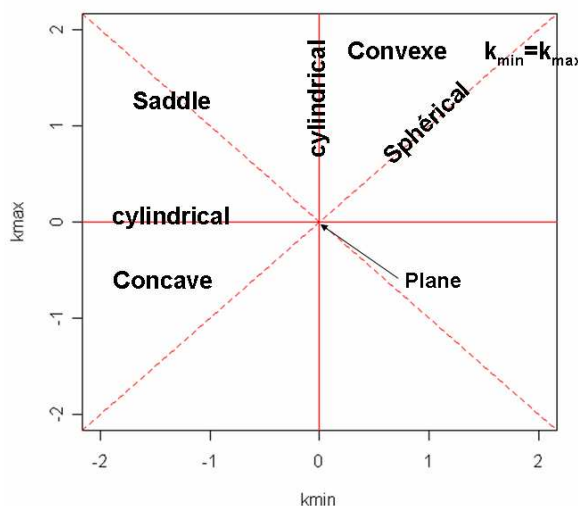

Fig. 2. $k_{min} - k_{max}$ *graph with the different types of portion intrefaces corresponding region.*

GEOMETRICAL PROPERTIES

The ($k_{min} - k_{max}$) graph presented in the reference article of Besl and Jain (1986) presents the geometrical properties of interface portions (Fig. 2). The shape of the interface can be determined from the values of k_{min} and k_{max}. Examples of different geometrical interface portion types are illustrated in Fig. 3. We present the striking properties of this graph (see Fig. 2):

– All the points of the surface are located on the left of the line corresponding to $k_{min} = k_{max}$. All the interface portions belonging to this line have a spherical shape.

– The planar interface portions are located at the origin of the graph, where $k_{min} = k_{max} = 0$.

Table 1. *Values of the surface and volume measure on different shapes with different values of simplification meshing.*

		Cylinder 3D	3D turned cylinder	Oblate spheroid	Torus
Contract edges 2,8	volume	328274	327698	989383	1168340
	surface	26928,6	26929,2	539323	77845
Contract edges 2,0	volume	328520	328024	990032	1169135
	surface	26960,9	27142,1	54099	78073
Contract edges 1,4	volume	328691	327890	990394	1169416
	surface	27572,4	27829,2	55620	79970
Contract edges 0,0	volume	328918	328000	990371	1169213
	surface	28227,7	29818,8	58448	83872

Table 2. *Meshing number elements in relation to the simplification of the meshing applied and to the shapes of the studied object.*

		Cylinder 3D	3D turned cylinder	Oblate spheroid	Torus
Contract edges 2.8	points	878	821	1766	2464
	faces	1752	1638	3528	4928
	edges	2628	2457	5292	7392
Contract edges 2.0	points	1734	1642	3476	4986
	faces	3462	3278	6948	9972
	edges	5193	4917	10422	14958
Contract edges 1.4	points	3994	3558	6805	9952
	faces	7984	7112	13602	19886
	edges	11976	10668	20403	29829
Contract edges 0,0	points	32678	39816	76534	110656
	faces	6552	79628	153064	221312
	edges	98028	119442	229596	331968

Table 3. *Clustering of intermetallic particles into 5 shape families according to their matrix-particle interface properties.*

Type 1	Saddle IP $+++$	Branched particles
Type 2	Flat IP $+++$ Ridge IP. Valley IP $+$	Flat Particles with an important aspect ratio
Type 3	Flat IP $+++$ Concave (120)	Flat particles with concavity
Type 4	Ridge IP $+++$ Flat IP	Sharped particles
Type 5	Spherical IP $+++$	Particles with a rounded interface

- The cylindrical interface portions have $k_{min} = 0$ or $k_{max} = 0$; if $k_{min} = 0$ the portion has a valley shape, if kmax = 0 it has a ridge shape.

- The hyperbolic interface portions or saddle shape have one positive and one negative curvature.

- If the two principal curvature values are positive, the interface portion is concave.

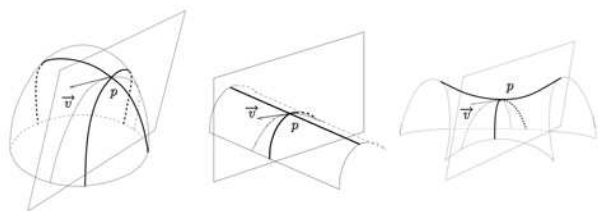- If the two principal curvature values are negative, the interface portion is convex.

Fig. 3. *Geometry of typical interface at the point p.*

Fig. 4. *($k_{min} - k_{max}$) graph of particle illustrated in Fig. 1.*

THE BIVARIATE DISTRIBUTION OF ($k_{min} - k_{max}$)

On the ($k_{min} - k_{max}$) graph each point represents a portion of the object interface. In the case of intermetallic particles the obtained meshing is defined by a large number of facets, from one thousand up to at least ten thousands (Table 2). A two-dimensional histogram can then be used to correctly exploit the available information.

From the curvature result files we have plotted the ($k_{min} - k_{max}$) graph (see Fig. 4) and the empirical bivariate distribution of ($k_{min} - k_{max}$) (see Fig. 5) for each intermetallic particles contained in the data base. The bivariate distributions of ($k_{min} - k_{max}$) are weighted, each facet being counted according to the amount of the object surface it represents (see Fig. 5).

RESULTS

The bivariate distribution of ($k_{min} - k_{max}$) of the particle shown in Fig. 1 is given in Fig. 5. It presents a significant concentration of interface located: on the line $k_{max} = 0$, on the line $k_{min} = 0$, into the saddle shape interface portion area and in a peak area centred on zero. It suggests that the particle has an important number of cylindrical interface portions with ridge type, and also a large part of planar interface portions. The particle is then made of planar area and of branches with intersections.
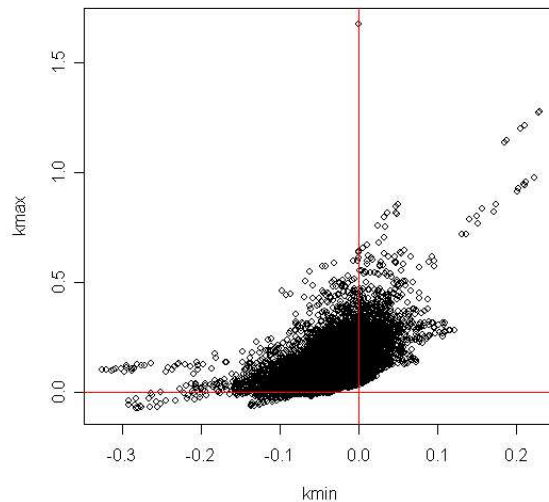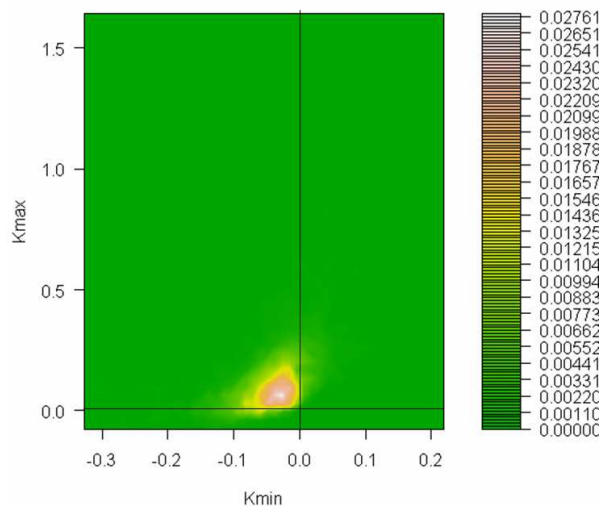

Fig. 5. *Bivariate distribution ($k_{min} - k_{max}$) of the particle illustrated in Fig. 1.*

STATISTICAL ANALYSIS OF THE BIVARIATE DISTRIBUTION ON A POPULATION OF INTERMETALLIC PARTICLES

PRINCIPLE

In the case of an important population of complex shape particles, we have to perform a statistical analysis. The goal of the study is to describe shapes of populations of objects by using an adapted representation space. For each intermetallic particle

extracted from the sample of aluminium alloy 5xxx, we estimate the bivariable distribution ($k_{min} - k_{max}$). The ranges of each graph are kept constant, in order to be able to compare the graphs of the particles.

A factor correspondence analysis of the bivariate distribution is performed, to compare the distributions in a space provided with the Khi 2 distance (Benzécri, 1980). In this space, it is possible to classify particles by using a Hierarchical Cluster Analysis (HCA). The Ward's algorithm is used (Ward, 1963). Initially, each particle is assigned to its own cluster. Then the algorithm proceeds iteratively. At each stage, it joins the two most similar clusters, by using as distance between two clusters, the loss of inertia generated by merging two classes. It is iterated until a single cluster is remaining.

The HCA leads to a hierarchical clustering into n clusters, represented by tree-like structures, called dendrograms (Fig. 6). A dendrogram shows the $n - 1$ steps of the clustering process leading to a single cluster. A truncation at a given level of the dendrogram, gives a partition of the population. The goal of the HCA is to globally indicate the presence of clusters. If at a level of the dendrogram the intra clusters inertia sharply increases, we consider that the classification of particles is pertinent.

RESULTS

Fig. 6 represents the dendrogram obtained by the Ward's method on the intermetallic particles population of the 5xxx aluminium alloy. The choice of the number of clusters by cutting the tree is obtained visually. The levels of aggregation are observed to vary between 0 and 160 in Fig. 6. The last knots, visualized by red dot lines in Fig. 6, represent the most significant aggregation jumps. We can expect a correct partition of the particles population by cutting the tree between the knots' values 35 and 45. Indeed, a cut at this level of the dendrogram represents an important aggregation jump, and gives five clusters. The five identified particle clusters have geometrical properties summarised in Table 3. Figs. 7 to 11 illustrate each particle family contained in the aluminium alloy.
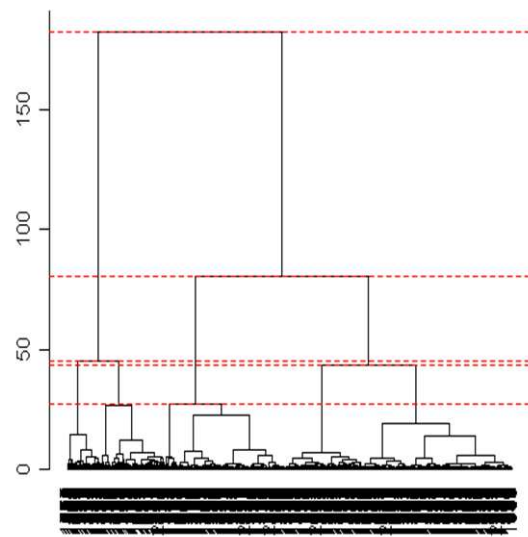

Fig. 6. *Dendrogram of the intermetallic particles' contained into AA5xxx (HCA obtained by Ward's method).*
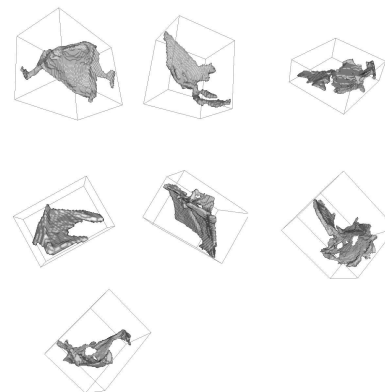

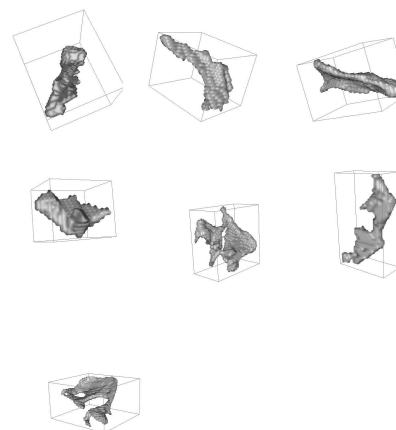Fig. 7. *Examples of intermetallic particles contained into type 1.*

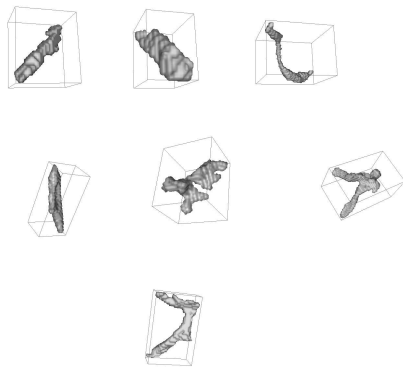Fig. 8. *Examples of intermetallic particles contained into type 2.*

Fig. 9. *Examples of intermetallic particles contained into type 3.*
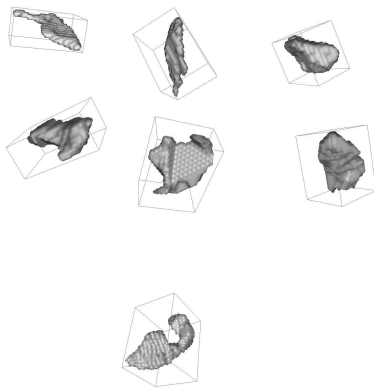

Fig. 10. *Examples of intermetallic particles contained into type 4.*
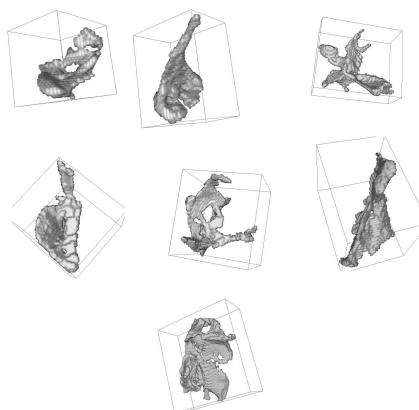

Fig. 11. *Examples of intermetallic particles contained into type 5.*

CONCLUSION

The characterization of the three-dimensional complex shape of objects by means of curvature information is efficient. This characterization method is original; it gives complex information about the nature of the interface between three dimensional objects and the material in their surrounding area. A relevant classification of objects with complex shape according to the statistics of their geometrical properties at the interface (namely the principal curvature) is possible. The curvature gives interesting information for mechanical studies on intermetallic particles; in particular for futures studies on the break up of intermetallic particles during industrial process according to their families.

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