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(54) Title: METHOD FOR GENERATING CELLS WITH DESIRED STATISTICAL PROPERTIES

(57) Abstract

The invention provides a method of generating cell with given statistical properties. The method to obtain the desired structure involves following steps: laying an array of seeds on a plane dividing the plane into a plurality of cells to obtain a cell network; optimizing the cell network by optimizing the cell network by displacing polygon vertices, checking if the minimization condition has been fulfilled by minimizing a suitable mathematical function which describes the difference of the obtain cell network and the desired changing the vertices of the cells until a predetermined statistical distribution of a cell–property is achieved, finishing the program in case the suitable mathematical function has reached a predetermined value. Applying the method of the present invention it is possible to predict the time–to–failure of known but also of unknown structures.

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Method for Generating Cells with Desired Statistical Properties

Field of the Invention

The invention relates to the field of generating polygon structures and especially to the application of polygon structures to simulate grain structures of materials.

Background of the Invention

The polygon networks are used to perform mathematical calculations and to investigate phenomena in many fields, for example, in hydrodynamics, geology, astronomy, biology, chemistry etc.

Numerical methods used to generate cell structures suffer, however, from a drawback that polygons have only fixed size distribution, so that no variation of statistical distribution is possible to obtain.

There are some methods in literature described which can generate a grain structure by simulating the physical process leading to a structure with variable statistical properties (e.g., M.J.FROST et al., J. Appl. Phys., 1994 V. 76, p 73390-7346). In this case however the variation is achieved by changing the parameters which govern the physical process. Therefore the variation of the end cell structure can only be achieved in the case that the parameters are known. There is however no method that would be general enough to generate any structure independent from the physical process. The method needed is a numerical method, which is flexible enough to be able to generate any structure needed, and also one that fulfills other requirements, such as reproducibility and reliability.

A need for such a method exists in the field of simulating grain structures of materials, as grain structure influences many physical properties of materials such as deformation, strength etc. It is very common that deposited metal films do not have lognormally distributed grain sizes. Besides, different bimodal distribution can arise, due to annealing of metal films. In order to investigate those structures it was necessary to find a method which would allow generation of any possible structure.

It is therefore the object of this invention to provide a method to generate cell structures with any predetermined statistical distribution, which could then be applied to simulate any desired grain structures of materials.

Brief Description of the Drawings

FIG. 1 shows a flow chart diagram of a method according to the present invention;

FIG. 2 shows a random seed distribution formed by common methods to choose a defined number of random points on the plane and the formation of the first Voronoi polygon;

FIG. 3 shows Voronoi polygon network of polygons obtained in a usual way starting from the random seed distribution shown in FIG. 2;

FIG. 4 shows the structure of FIG. 3 after the optimization has been carried out according to this invention; and

FIG. 5 shows statistical distribution of the size of the polygons shown in FIG. 4 (size being defined as $\sqrt{A}$; A representing polygon area).

Detailed Description of the preferred embodiment

FIG. 1 shows a flow chart diagram of method 100 according to the present invention.

In the following the structure is explained in terms of vertices, joined by edges, which surround faces and in the tree dimensional structures, the faces surround cells. In this invention the word "cell" is used both for two and tree dimensional structures, so that for two dimensional structures the word "cell" has the same meaning as the word "face".

The method used in the further example is used to generate cells in order to simulate grain structure. Persons skilled in the art will know that it is possible to use the following method for different purposes, which might need small suitable variations, which are however not important for the invention.

The first step 110 is to generate an array of input points. These points could serve as a seed around which a polygon is formed.

This array of input points may be random or have a specific pattern, depending on the purposes for which the cell structure is generated and on the structure which is being simulated. In principal it could be sometimes desirable to divide the plane into a number of triangles or squares having a regular pattern in which case the array of points would also have a regular pattern. In some other cases it could be of advantage to have data points which are completely random. In some other cases it could be important to have areas of regular patterns and areas of random pattern. Persons skilled in art will know how to generate an array of data points, depending on simulations they want to undertake and on the results they want to obtain.

Even though not important for the success of this invention, the number of points generated can be determined by the number of cells that are to be obtained. It is, however, possible to have number of points not being equal to the number of cells, especially in cases where data points represent vertices of the polygon to be obtained. This all depends on the purposes of the simulation and the results desired.

Even though any method for generating a polygon network could be used for the purpose of this invention the method described below is a well known method for generating polygons, to obtain a polygon network known as Voronoi diagram. A Voronoi diagram of a point set is a subdivision of the plane into polygonal regions, where each region is the set of points in the plane that are closer to some input point than to any other input point. Therefore from a geometrically defined point set only one polygon network will be formed. The construction of Voronoi diagram is well known to persons skilled in the art (e.g. Franco Preparata, Computational Geometry, Springer-Verlag 1985, New York, p.217-248).

The number of input points for grain structure simulation is usually the same as the number of cells that have to be obtained, if Voronoi polygons are generated. This has also an advantage that it is possible to compare properties of grain structures of a defined number of grains having different statistical properties such as area, size etc. In the case Voronoi triangulation of the plane is used as a method to generate polygons the first step is to lay down a random array of predetermined number of seeds in a sufficiently large region.

Voronoi triangulation is used in the further example as it is preferable to use a method which generates a set of cells with statistical properties close to the desired ones. Persons skilled in the art know, that this is done only because of practical reason, as it is much easier to optimize a set which is close to the desired one, than the which deviates very much from the desired one. The reason why Voronoi polygons are constructed in the further example, is that they have lognormal distribution. Even though the distribution is not the desired one, it is much easier to optimize this polygon network, than the one where the polygon network consists, for example, of triangles having the same area.

In order to preserve transparency it will be shown, how a 2-D Voronoi network with the lognormal grain size distribution of predetermined spreading can be constructed. It is however possible to vary the distribution function at will, as well as to construct Voronoi network in a 3-D region.

The second step 120 is to divide the plane into the number of cells which are generated around the data points.

Persons skilled in the art will know that there is a number of methods apart from constructing a pure Voronoi diagram describing executing the steps 110 and 120, such as Delaunay triangulation or generation of Voronoi polygons under certain conditions such as presence of barriers (AK CLINE, R.J. RENKE, SIAM, J. Num. Anal. 1990, V.27, N5, p 1305-1321).

The first two steps are known to the persons skilled in the art can be done with any common methods as this original network does not have to have any special properties.

The result obtained after performing the step 110 and constructing the first polygon is shown FIG. 2. Even though construction of Voronoi network was applied to generate a predetermined number of cells, people skilled in the art know that it is not decisive for the invention how the plane is divided into cells. The most important thing is the result of the division, i.e. to have a plane divided into a defined number of cells. In principle, it is possible to start with cells constructed in any way, for example with squares, triangles or of polyhedra of any desirable shape. In any case it is possible to apply the method described of this invention to a set of cells with versatile shape, whereas the cells can be of any desired shape or shape combinations. The same applies to the statistical distributions of the properties that have to be normalized. In the case of Voronoi network the distribution of polyhedra is normally lognormal. As mentioned above the choice of a starting structure and distribution should consider the final structure and distribution in order to save the optimization time. Typically, closer the final distribution to the desired one, less time is needed to normalize the original structure in order to obtain the desired one.

The step 130 consists of displacing of polygon vertices in order to obtain the desired structure. The minimization is done in such a way that a suitable mathematical function is found that describes the difference between the desired and the obtained structure as described later. when the desired structure is obtained the mathematical function must be 0. As it is however very difficult to obtain a structure which would match the desired one 100%, the structure obtained is only very close to the desired one so that the mathematical function is not 0 but very close to it. A value is chosen, hereafter called optimization condition, which should be reached during the minimization, which might be 0, but also a number close to it, depending to what extent the structure obtained should be close to the desired one.

After checking the minimization conditions in step 140, the execution is either stopped (step 150) if the optimization conditions are met, or steps 130 and 140 are repeated until the conditions are fulfilled.

FIG. 2 shows one possible random seed distribution and the formation of the first Voronoi polygon. The plane is then being subdivided into polygonal regions, where each region is the set of points in the plane that are closer to some input point than to any other input point.

The result obtain after generating Voronoi network from the seed distribution shown in FIG. 2 in a usual manner, is shown in FIG. 3. This network does not have properties that are desired, so that it has to be optimized. This structure is the result of executing steps 110 and 120 of the flowchart diagram shown in FIG. 1. The step 130 of the flowchart diagram in FIG. 1 still has to be applied in order to obtain the desired structure.

The optimization step 130 of FIG 1. is done in such a way that vertices of the polygons shown in FIG. 3 are displaced. In step 140 checking if the minimization condition has been satisfied takes place. In case the minimization has been successful the optimization is stopped. Otherwise the optimization will be continued until some criteria are satisfies.

Optimization of the original obtained polygon network is done in such a way that in order to obtain the desired statistical distribution, as mentioned before, a suitable mathematical function describing the difference between a desired and the starting structure has to be found and subsequently minimized. Minimization of this function is achieved by displacing the polygon vertices in such a way as to obtain areas which have been determined before (see below) or at least to get close to those areas as much as possible. The areas which are to be obtained can be calculated because knowing a given distribution it is possible to calculate how many polygons would have an area which is for example 2/3 of the mean value and how polygons would have an area which is 1/2 of the mean value and so on. This can be done for any statistical distribution. By the way of example if a Gaussian curve of a specific property, for example area of a polygon, is to be obtained, one knows that 68% of all the polygons would have a value between $\bar{A} \pm \sigma$, whereas A represents the mean value of the areas of the polygons and σ the standard deviation of the Gaussian distribution curve. By the way of example, if 99 polygons having areas distribution according to the Gaussian distribution curve are present, each polygon being designated as A(i), whereas (i) can take any value from 1 to 99, whereas A(1) is the polygon with the smallest area and A(99) a polygon with the largest area, polygons A(17) until A(83) would have area which would be within the limits of σ.

The other possibility is to have calculated values from the digitized picture of the surface under investigation and find the mathematical expression for the statistical distribution. In both case all values are already known. What has to be done is to correlate original polygon network with the desired one.

In order to establish which polygon from the generated set {V(i)} has to be fitted to the desire grain having area A(i) one does not change the numbering of {V(i)} but instead of that the numbering of the set {A(i)} is changed. The polygons which has the maximal area is brought in correspondence with the grain having the maximal area in the set {A(i)}. The maximal area in the set {A(i)} is called then A(j). Then the next polygon V(k) has been chosen having the area which is nearest to V(j) and is brought in correspondence with polygon having the area nearest to A(j). This polygon is then named A(k) etc.

After sorting is completed it is possible to minimize the function using one of the standard procedure e.g. (Hook and Jeev's algorithm can be used, described in ACM 1961, V8, p 212-229). In the preferred embodiment of the invention, because of physical reasons an additional condition to the Hook and Jeev's algorithm has been imposed that each polygon has to be convex. This condition has been imposed on vertex displacements and was performed for every step of the procedure. People skilled in the art will know that this specified imposed condition is only optional and that any other condition(s) can be imposed or omitted if necessary.

For persons skilled in the art it is also known that there are different mathematical functions which can be used in order to obtain the desire distribution. By the way of example, a function **(1)** can be a function which can be used for optimization. The only condition that the function has to fulfill is to be normalized i.e., to predetermined value, preferably 0 when an ideal solution is found (as in case of function **(1)**)and that every member of the sequence has to have the same sign and preferably to be positive. In our case this has been achieved by raising each member of the sequence to an even power of preferably 2 i.e. $\left\{1-\frac{A(i)}{V(i))}\right\}^2$ in order to obtain only positive values, which are then added together. Another possibility such as $\left\{1-\frac{A(i)}{V(i))}\right\}^4$ is possible also, but it was found that better results are obtained with power of 2 than with the power of 4.

The whole function **(1)**, which is suitable to be an optimization function could look like this:

$$F(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, x_1^{(2)}, x_2^{(2)}, x_3^{(2)} \ldots\ldots x_1^{(M)}, x_2^{(M)}, x_3^{(M)}) = \sum_{i=1}^{N} \left\{ 1 - \frac{A(i)}{V(i))} \right\}^2 \quad (1)$$

where $x_i(j)$, are the vertex coordinates of the polygon structure; M is the number of vertices of N polygons; V(i) is the area of the i-th polygon in the course of the optimization; A(i) is the desired area of i-th polygon in accordance with the required grain size statistics.

Other terms can be added to the right side of the function (1) if there are special conditions to be met, such as the condition of convexity of the polygons, introduced due to physical reasons, as well as any other desired conditions.

FIG. 4 shows the same structure as in FIG. 3 after the optimization step 130 described above has been carried out according to this invention.

From the FIG. 5 which shows statistical distribution of area of the polygons obtained in FIG. 5. It can been seen that the distribution of the cell structure obtained matches very well the desired one. A big advantage of the present invention is that it is not necessary to know the physical process to obtain the desired structure, so that also structures not yet known, can be investigated.

It is known, for example, that metallization time-to-failure due to electromigration is strongly influences by distribution of poly- (Lp) and single grain (Ls) segments in length along a metal line. These distributions can be used for predictions of metal line time-to-failure.

It is possible to utilize the method of the present invention to predict the time-to-failure of known but also of unknown structures on account of such statistical distributions.

The present invention can be therefore very useful in designing new materials as it can be helpful to evaluate which structures would have most promising properties.

While the invention has been described in terms of particular structures and methods, those skilled in the art will understand based on the description herein that it is not limited merely to such examples and that the full scope of invention is properly determined by the claims that follow.

Claims

1. A method of producing cell structures with predetermined statistical distribution properties comprising following steps:

a) laying an array of seeds on a plane;

b) dividing the plane into a plurality of cells to obtain a cell network;

c) optimizing the of cell network by displacing polygon vertices;

d) checking if the minimization condition has been fulfilled by minimizing a suitable mathematical function which describes the difference of the obtained cell network and the desired changing the vertices of the cells until a predetermined statistical distribution of a cell-property is achieved;

e) finishing the program in case the suitable mathematical function has reached a predetermined value.

2. The method according to claim 1, wherein the property of the cell is a cell-area.

3. The method according to claim 1, wherein the cell property is a cell-size.

4. The method according any of the preceding claims, wherein the dividing the plane into cells is done in such a way as to obtain a Voronoi polyhedra network.

5 The method according to any of the preceding claims, wherein the distribution of the seeds is random.

6. The method according to any of the preceding claims, wherein the optimization is done with the suitable mathematical function normed so that the predetermined value is 0 when a desired solution has been found.

7. The method according to any of the preceding claims, wherein the restriction is imposed on the displacement of polygon vertices so that resulting polygons are convex.

8. Application of the method according to any of the preceding claims in simulating grain structures.

9. Application of the method according to any of the preceding claims in simulating grain structures of 2-D surfaces.

10. Application of the method according to any of the preceding claims in simulating grain structures of 3-D materials.

11. The method according to claims 8 or 9 wherein a statistical distribution is used to predict time-to-failure of materials.

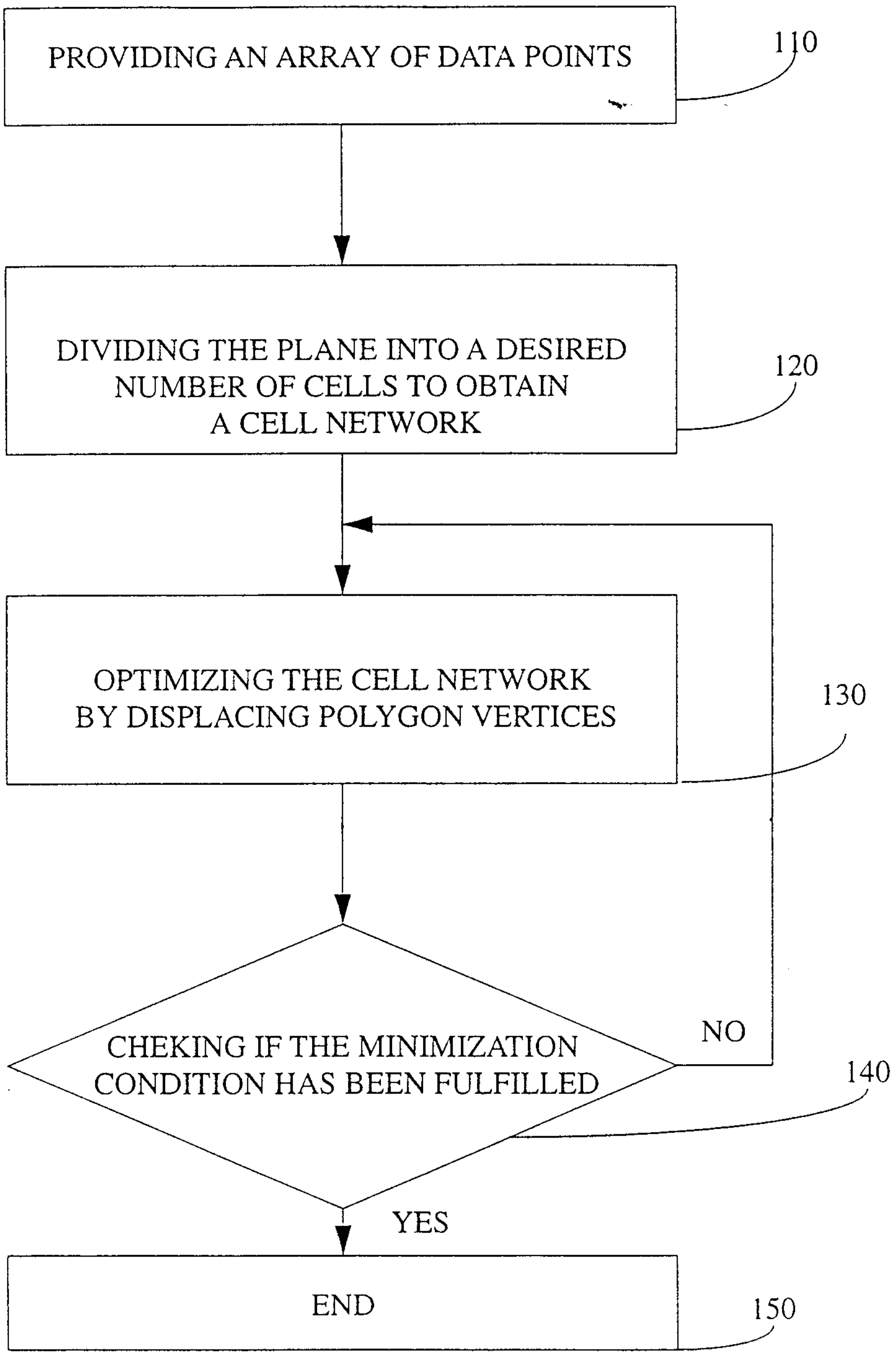
PROVIDING AN ARRAY OF DATA POINTS
110
DIVIDING THE PLANE INTO A DESIRED NUMBER OF CELLS TO OBTAIN A CELL NETWORK
120
OPTIMIZING THE CELL NETWORK BY DISPLACING POLYGON VERTICES
130
CHEKING IF THE MINIMIZATION CONDITION HAS BEEN FULFILLED
NO
140
YES
END
150

FIG. 1

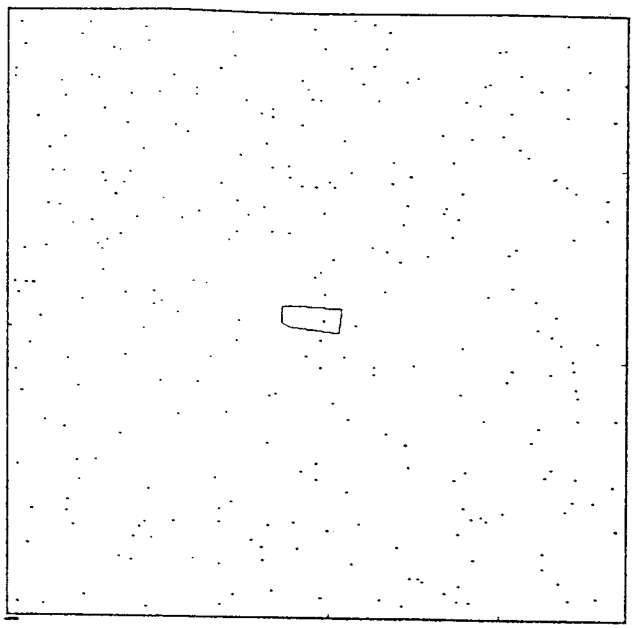

FIG. 2

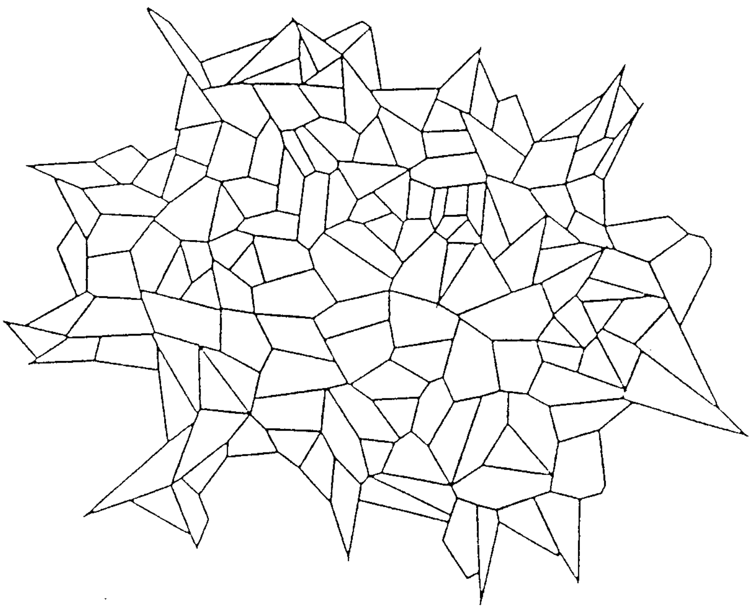

FIG. 3

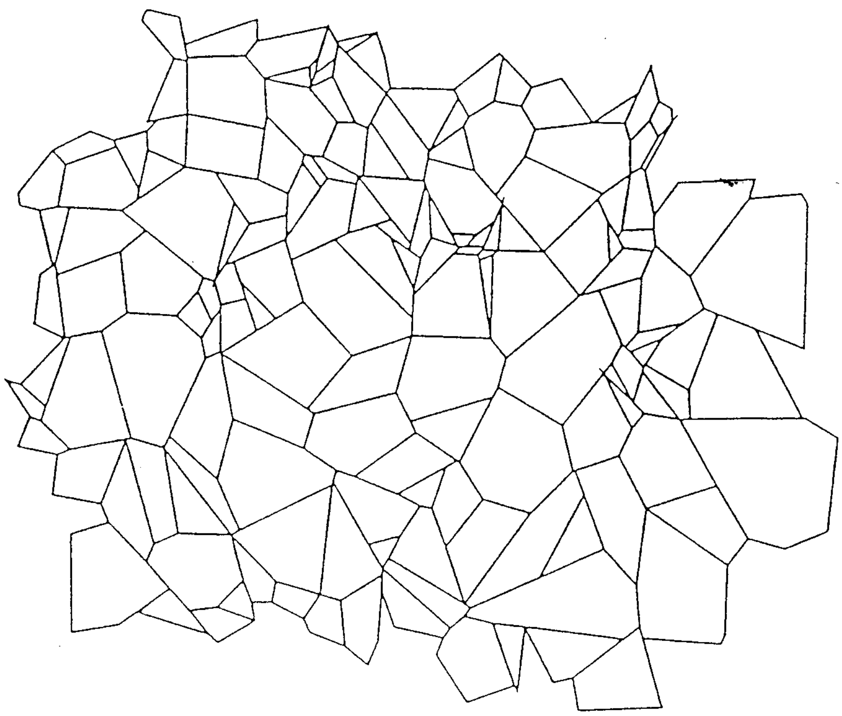

FIG. 4

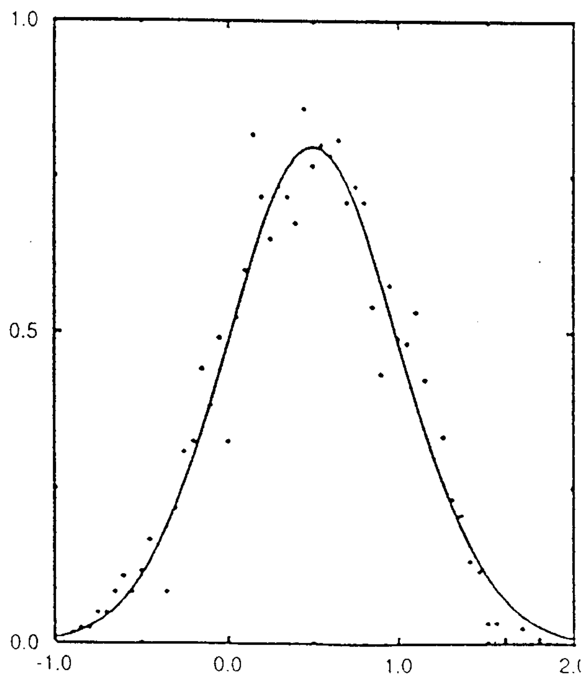

FIG. 5

INTERNATIONAL SEARCH REPORT

International Application No
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A. CLASSIFICATION OF SUBJECT MATTER
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According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
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Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	HUANG Y -P: "TRIANGULAR IRREGULAR NETWORK GENERATION AND TOPOGRAPHICAL MODELING" COMPUTERS IN INDUSTRY, vol. 12, no. 3, 1 July 1989, pages 203-213, XP000104026 see page 204, left-hand column, paragraph 2 - page 206; figure 1 ---	1
A	EP 0 801 364 A (INSTITUT FRAN AIS DU PÉTROLE) 15 October 1997 see page 3, line 10 - line 15 see page 5, line 30 - line 55; claim 7 ---	1
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[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	CIGNONI P ET AL: "MULTIRESOLUTION REPRESENTATION AND VISUALIZATION OF VOLUME DATA" IEEE TRANSACTIONS ON VISUALIZATION AND COMPUTER GRAPHICS, vol. 3, no. 4, 1 October 1997, pages 352-369, XP000730968 see page 354, right-hand column, paragraph 2.3 - page 356, right-hand column, paragraph 3 -----	1

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INTERNATIONAL SEARCH REPORT

Information on patent family members

Inter. ɔnal Application No
PCT/RU 98/00325

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
EP 801364 A	15-10-1997	FR 2747490 A	17-10-1997
		NO 971678 A	13-10-1997
		US 5844564 A	01-12-1998