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HEAT TREATMENT AND SURFACE ENGINEERING OF LIGHT ALLOYS

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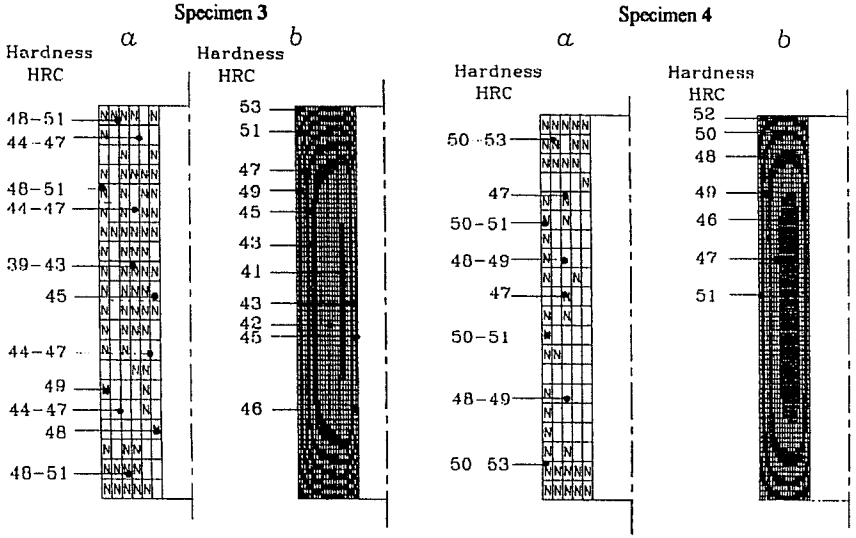

Fig. 4, Hardness distribution of quenched specimen 3 and specimen 4: (a) computer simulation, (b) experiment

4. Conclusions

The finite volume method of 2-D dimensional transient temperature field can be used for computer simulation of quenching of axially symmetrical steel workpieces of complex shape.

Based on experimental results it can be concluded that hardness distribution in quenched cylindrical specimens, with and without an axial hole can be successfully estimated on the basis of time of cooling from 800°C to 500°C and on Jominy hardenability curve.

Hardness distribution in as-quenched steel specimens can be successfully calculated by using values of heat transfer coefficients evaluated by the LISCIC/NANMAC probe. Further investigations have to be done with specimens of different shapes and by using different quenchants.

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TOPOLOGICAL ASPECTS OF ORDERING

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Keywords: random pattern, cellular structure, topological correlation

Abstract

Intensive development has recently taken place in two- and three-dimensional (2D and 3D) cellular pattern studies. These random pattern-formations are interdisciplinary, appearing in metallurgy (grain growth, metallic glass structures), biology, geology and they have numerous technological aspects as well. Despite the basic differences between the actual appearance of these processes and their ruling dynamic conditions, the resulting patterns have a common behaviour: their topology, a set of polygons in 2D, which cover the sheet without gaps and overlaps, and the space-filling polyhedral structure in 3D. The main aims of this paper are to answer the following questions: How could a global topological order be developed from a random pattern generated by only local interactions? How do the actual local interactions affect the global topological order? How does the system develop from a non-equilibrium state to an equilibrium one (energy minimum)?

Topological correlations

Well-known topological conditions in 3D structures are described as follows: (three edges bisect in a vertex)

- Euler-law [1]: $F-E+V-P=1$ (1)
  where F is the number of faces of a cell, E is the number of edges, V is the number of vertexes, P is the number of cells in the system.
- Consequences of Euler-law [1]: $\langle F\rangle = \frac{12}{6-\langle n\rangle}$ (2)
  where $\langle F\rangle$ is the average polyhedra-face in cellular pattern, $\langle n\rangle$ is the average number of edges of the polyhedra faces in the system. Note the difference between the 3D and 2D patterns: the value of $\langle F\rangle$ is constantly 6 in 2D, but it varies system by system in 3D.
- Aboav-law [2]: $m(F) = \langle F\rangle - a + \frac{\langle F\rangle a + \mu_2}{F}$ (3)
  where m(F) is the average number of faces of next-neighbour cells of a given cell, $\mu_2 = \sum_{F\neq 4} B(F)(F-\langle F\rangle)^2$ is the second momentum of the face-distribution, B(F) is the ratio of F-faced cells in the system, a is a system-constant (like $\langle F\rangle$ and μ_2 as well).
- Peshkin-law [3]: $A(G,F) = F + G - \langle F\rangle - \frac{a}{\mu_2}(G-\langle F\rangle)(F-\langle F\rangle)$ (4)
  where A(G,F)=M(G,F) / B(F) is the topologic correlator, and M(G,F) is the average number of the G-faced next-neighbour cells of F-faced ones, and
- Some metric conditions [3]: $V(F) \approx V_o\left(1+\frac{F-\langle F\rangle}{K_V}\right)$

$$A(F) \approx A_o\left(1+\frac{F-\langle F\rangle}{K_A}\right) \quad (5)$$

$$L(F) \approx L_n\left(1+\frac{F-\langle F\rangle}{K_L}\right)$$

where V(F), A(F) and L(F) are the average volume, surface and edge-length of the F-face cells respectively. The constants V_0, A_0, L_0 are the average volume, surface and edge-length in the system respectively, and K_V, K_A és K_L are constant system-parameters.

- The radius-law establishes a linear dependence of the cube-root of volume of average F-sided polyhedra versus F, [4].

- Angle-law [4]:
$$\Theta(F)=120^0\left[1+\frac{f}{3}\left(1-\frac{\langle F\rangle}{F}\right)\right] \qquad (6)$$

where $\Theta(F)$ is the average face-angle of the F-faced cells, and 'f' is constant characteristic for the actual pattern. In BCC f=0, for a serie of Platonic bodies f=0.88, and $0.6 < f < 0.75$ for random Voronoi patterns.

These conditions are similar for 2D structures, moreover Dubertret and Peshkin have shown the long-distance correlation of the cells in 2D, [5].

Effects of cellular interactions

Two-dimensional patterns

Taking global effects of pair-interactions into consideration, it can be found that random structures can evolve to the energetically optimal equilibrium arrangement, which is the honeycomb pattern in 2D. During this process the changes of 2D topological parameters are definite, Fig.1.

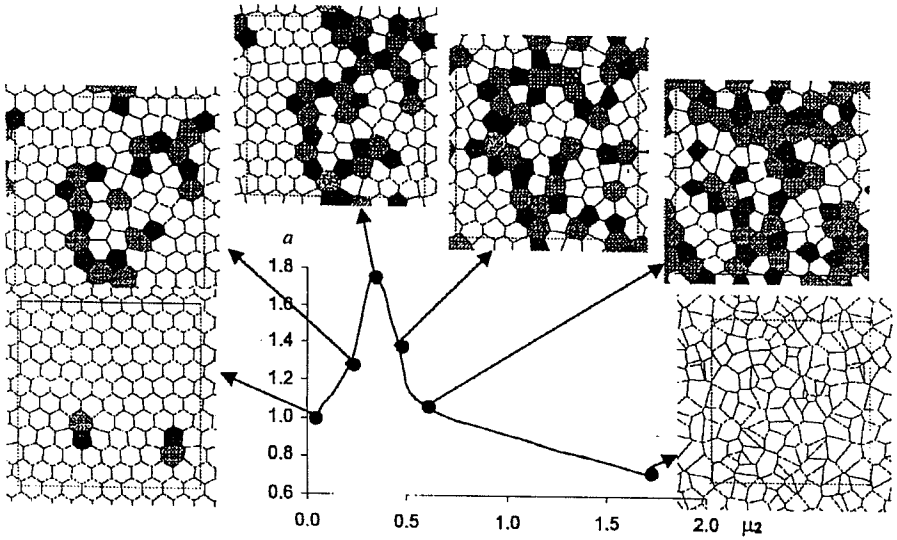

Figure 1. This computer simulation used energetic potential function (the Lennard-Jones potential) as pair-interaction. The patterns should be seen from right to left. It is visible, how honeycomb pattern develops from a random pattern. The detailed description of the computer simulation has already been published elsewhere [6]. a and μ_2 are topological parameters from the Aboav-law.

Three-dimensional structures

In atomic structures the energetic driving force means the dominance of the tetrahedral clustering where 20 tetrahedra forms an icosahedron shearing a common vertex, Fig.2. This arrangement of 12 atomic nearest-neighbours is the most stable available cluster proven by energy calculation, [1]. The periodic repetition of an icosahedron alone could not fill the space, the icosahedron can not be a unit cell of a crystalline structure. This contradiction causes the geometric frustration phenomena [7],[8]. 3D cellular structures are dual systems of atomic arrangements, therefore the geometric frustration is characteristic for the developing of cellular patterns as well.

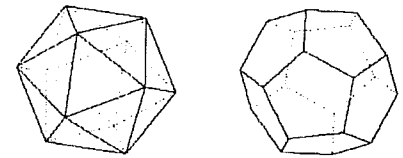

Figure 2. a: the icosahedron and its geometric dual: **b:** the dodecahedron

Taking global effects of pair-interactions into consideration, it can be found that random cellular structures can only approach the energetically optimal equilibrium because of the geometric frustration. Figs 3 and 4 show the results of a computer simulation, where the developing of Voronoi structures from random arrangements to the state of energy minimum was studied. The detailed description has been published elsewhere [4]. Fig.3. shows, that the equilibrium seeks to A15 crystalline structure, which is BCC in one of its substructure and icosahedron in the other one.

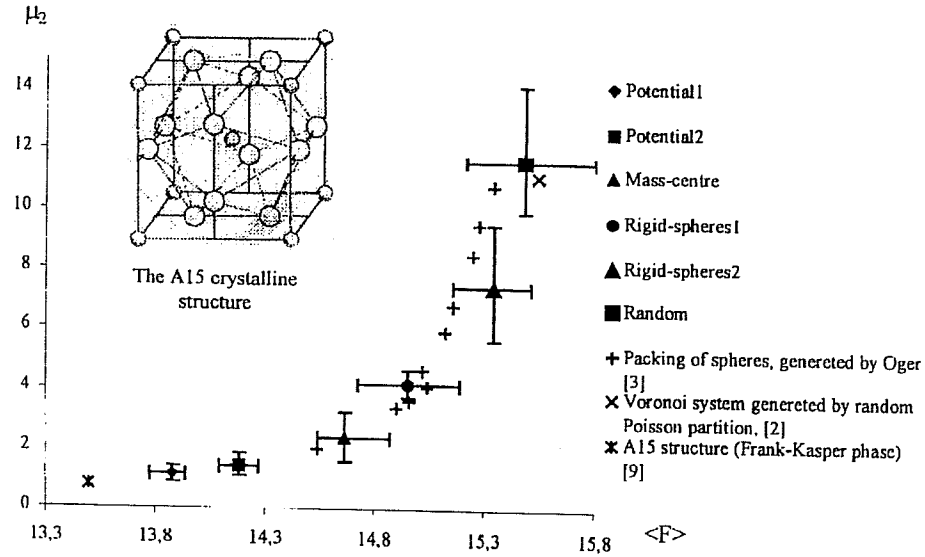

Figure 3. Topologic parameters μ_2 and $\langle F\rangle$ seem to approach parameters of the A15 crystalline structure, while systems develop from random patterns to the state of energy minimum. Results from the computer simulation [4] are denoted by filled symbols, while the data of other structures are illustrated with unfilled signs. The names Random, Rigid-spheres, Mass-centre and Potential denote various relaxation methods, taking various cell-interactions into consideration.

Fig.4. shows the characteristic cells in structures seeking the energy minimum. The numbers in the brackets: the polyhedral characterisation denotes the number of face-polygons in order of the polygonal edges. (The number has been underlined for clarity where it has two digits.) 'c' is the crystallization parameter, the ratio of the 3, 4, 6-fold (crystal conform) polygons to all the others. The five-fold symmetry dominates over the crystalline fore- and six-fold symmetry.

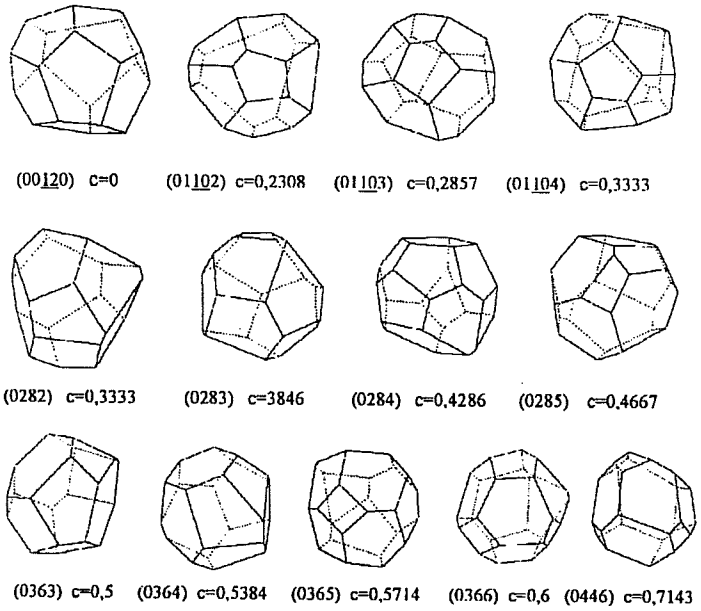

Figure 4. Most characteristic Voronoi polyhedra and their notations

Summary

Definite topologic correlations describe the global order of 2D and 3D random structures. Local pair-interactions have an effect on the global order. Random 2D structures can evolve to the energetically optimal equilibrium arrangement, the honeycomb pattern. Random 3D structures can only approach the state of energy minimum because of the geometric frustration, and the global topologic parameters seek the parameter-values of A15 crystalline structure.

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COMPUTER PROGRAM FOR CCT DIAGRAM ANALYSIS AND HEAT TREATMENT PROCESS PLANING

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Keywords: CCT diagram, computer aided process planning

The CCT diagrams are widely used for process planning of technologies working with heat cycles resulting austenit creation and transformation, as the welding or the heat treatment. In order to use the advantages of continuous development of personal computers, a system was developed for the analysis of continuous cooling diagrams [1] and its application for heat treatment technology [2,3].

The program module created for the analysis of CCT diagrams makes possible a more easy and adequate process planning work, as compared to the traditional methods, and its main properties can be summarised in the following points:

- The collection of CCT diagrams, based on [4] can be easily completed, the data input is facilitated by a CCT diagram-editor;
- The list of already implemented diagrams can be visualised on the screen, all features and numerical data of selected diagram can be printed;
- For the selected curves, different cooling rates can be choice and visualised in the diagram; the start and endpoints of given metallurgical transformations, the percentage of produced phases can be calculated.
- The cooling rate resulting a prescribed cooling time, phase quantity or hardness can be determined, and while the cooling curve can be visualised in the CCT diagram, the analysis presented above can be performed;
- Several CCT diagram can be superimposed making possible its comparisons.

On the Fig. 1 the analysis performed for given cooling rate are shown with the resulting microstructure.

As it was already mentioned, the CCT diagrams are widely used for the process planning of heat treatment. For the presented program, several independent modules were developed, to facilitate the industrial applications.

During hardening, the hardness distribution in the cross-section, so the so-called hardness-depth curve must be known. For hardening and tempering, the properties obtained after annealing depends on the microstructure developed during the hardening step, so it is important to know the cross-sectional distribution of the phases after hardening. For these purposes the cooling curves are calculated by a program module for axi-symmetrical workpieces in every 0.2 R distance from the centre to the surface, using several cooling media - oil, or moving water. The cooling curves are plotted into the selected CCT diagram, afterwards the ferrite, perlite and martensite contain can be calculated and stored. Finally, the hardness-depth curve is calculated from the stored points, as it shown in Fig. 2.