Bull. Nov. Comp. Center, Comp. Science, 25 (2006), 49–57

Cellular automata construction based on molecular dynamics simulation data analysis

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Abstract. The Delaunay Tessellation is used to construct a cellular automata resembling model based on data obtained from molecular dynamics experiment. Particle coordinates at each time step of required length are tessellated to compose a system of vertices and edges, which are classified to produce states and transitions. These states and transitions are used to describe a local order of structure and its evolution in cellular automata under consideration.

1. Introduction

Mechanical alloying often results in the formation of disordered non-equilibrium states of a material [1, 2]. There are numerous questions about this material inner structure, mechanisms of formation, etc. It can be stated that the problem of disordered solid state in general is one of the least investigated areas of solid state physics [3].

Physical methods often fail to give satisfactory results due to a specific structure of a material and undesirable transformations taking place in the course of analysis.

Computer-aided modeling is one of a few methods that can be used to study materials in question.

While attempting to model the structure and properties of the interfacial boundary between two solid metals, which constitute a sufficient part of the initial stage of forming a product (the so-called mechanocomposite) of intermetallic compounds, we performed the shape analysis of the structure alongside the interfacial boundary [4]. The Delaunay tessellation of particle coordinates obtained from Molecular Dynamics (MD) model was treated with S simplex coloring [5]. The analysis showed that most of "imperfect" simplexes are located near to the interfacial boundary on the side of a softer metal.

Further investigation showed that most versatile regions coincide with imperfect ones, whilst the rest structure remains nearly unchanged. In order to describe these specific regions and their evolution, the methods described further were proposed.

In this paper, 2D models are in the main investigated to improve efficiency and clearness of results. All the results obtained are also valid for 3D models.

2. Theory

2.1. Geometric properties of the Delaunay method. In mathematics and computational geometry, the Delaunay triangulation for a set P of points in the plane is the triangulation $T(P)$ such that no point in P is inside the circumcircle of any triangle in $T(P)$. The triangulation was invented by Boris Delaunay in 1934 [6].

In the general n-dimensional case, it is stated as follows: For a set P of points in the n-dimensional Euclidean space, the Delaunay tessellation is the tessellation $T(P)$ of P such that no point in P is inside the circumhypersphere of any simplex in $T(P)$.

The Delaunay simplexes constructed for the entire system form a mosaic covering the space without overlapping and gaps. Thus, the Delaunay simplexes can be regarded as the "bricks" composing the empty interatomic space in an atomic system.

An example of the Delaunay tessellation is shown in Figure 1.

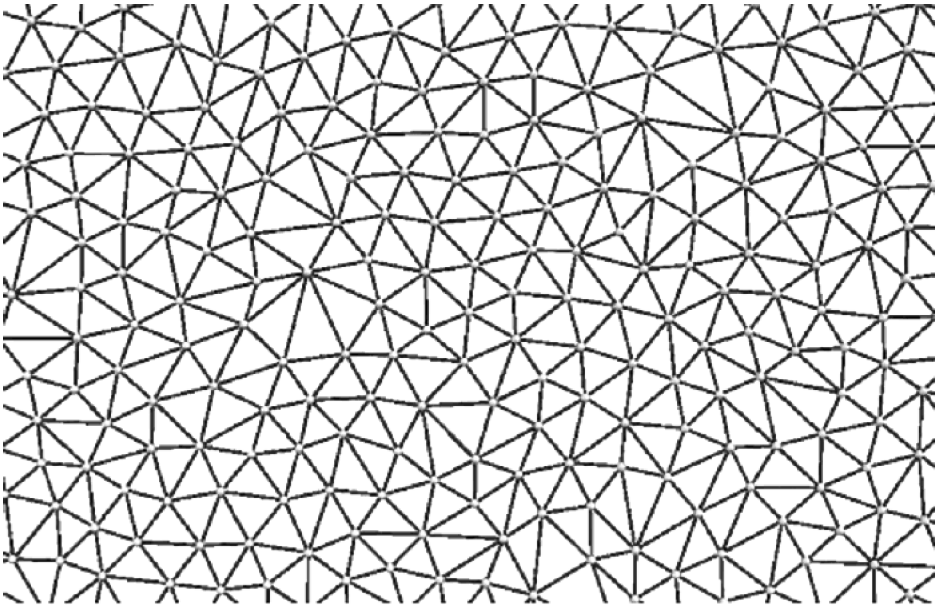

Figure 1. Two-dimensional illustration of the Delaunay tessellation

Thus, **simplex** is supposed to be formed of **vertices** that stand for atoms in MD simulation and **edges** that connect these atoms and in terms of physics define the closest neighbors of an atom.

2.2. Model system. The MD underlying a Cellular Automata (CA) model construction was chosen to be two-dimensional and to consist of 2500 atoms placed in the periodic boundary conditions with constant pressure.

An experimental model was prepared by heating ($\sim 10^5$ steps at a temperature of ≈ 4000 K) to form a disordered state and quenched afterwards. This non-equilibrium system was used to compute a number of states and transitions. When heated to 600 K, the structure slowly relaxes to a less strained state.

Choosing a time step. The time step for MD simulation at the stage of Structure and Transitions Analysis was chosen to be $5 \cdot 10^{-16}$ s at 600 K. Though MD requirements allowed a time step increase to about $\sim 10^{-15}$ s, it was not appropriate for a proper transition generation. Increasing the time step would lead to the formation of clusters of transitions which require a different and complex analysis.

For simplicity and efficiency let us assume that there is only one transition occurrence for a given structure fragment for a single time step. It can be roughly estimated to be about 5–10 transitions per 1000 vertices.

The time step depends on temperature in invectively proportional manner.

2.3. The CA states. To build CA model of the system and to simplify a structure analysis, we have to transform a continuum model representation into a discrete set of states.

This can be done by the edge length discretization and further assigning this discrete measure to the vertex state.

Lengths diagram. We performed several MD runs at different temperatures to obtain distribution of edge lengths and its dependence on the temperature. The model system was heated to a desired temperature and analyzed for some 10^5 steps to obtain the length distribution (Figure 2).

Specific $l_{\max}$ and $l_{\min}$, that are the minimum and maximum supposed lengths of an edge in the system, were chosen to be 4.1 and 2.1 A, respectively. This corresponds to the maximum and minimum lengths to meet at 800 K, the 200 K higher temperature than that of the analyzed model.

Let us note that $l_{\max}$ and $l_{\min}$ should be chosen to be as close as possible to avoid excess of unused states. On the other hand, the selection of too close $l_{\max}$ and $l_{\min}$ may lead to an improper state definition. Moreover, the most versatile structure fragments usually make up these utmost states. So, a proper attention should be given to the choice of $l_{\max}$ and $l_{\min}$.

The length measure calculation. For each edge in the tessellation, we assign a nonnegative integer measure

$$L_i = \left\lfloor \frac{l_i - l_{\min}}{l_{\text{step}}} \right\rfloor,$$

that stands for the function of its length. Here l_i is a length of edge, $l_{\text{step}} = (l_{\max} - l_{\min})/N_{\text{stat}}$, N_{stat} is the number of discrete edge lengths in the system, and $\lfloor x \rfloor$ is rounding to the nearest integer not exceeding x.

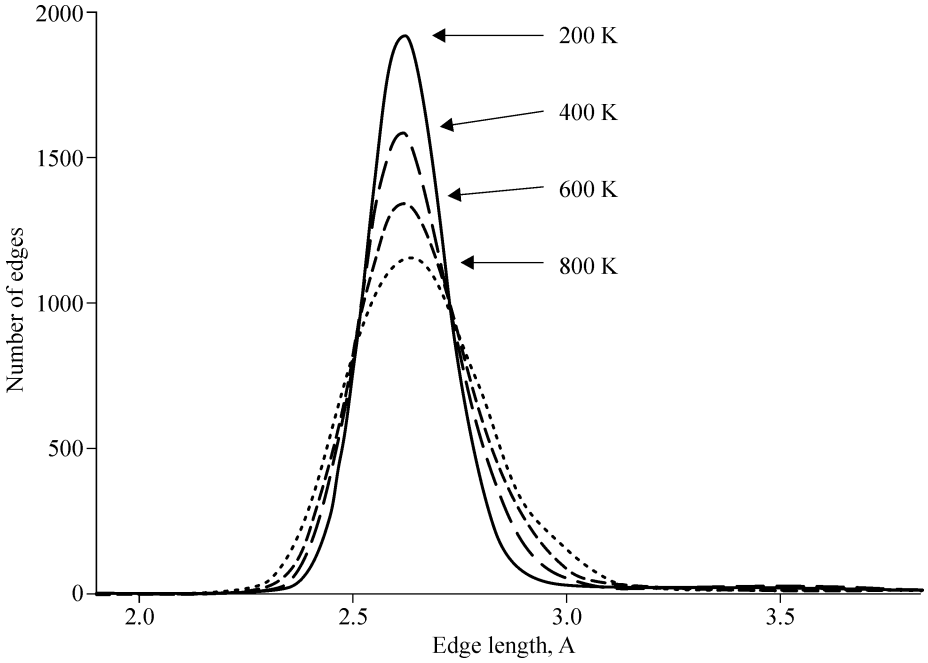

Figure 2. Edge lengths distribution in the model system in different temperature conditions

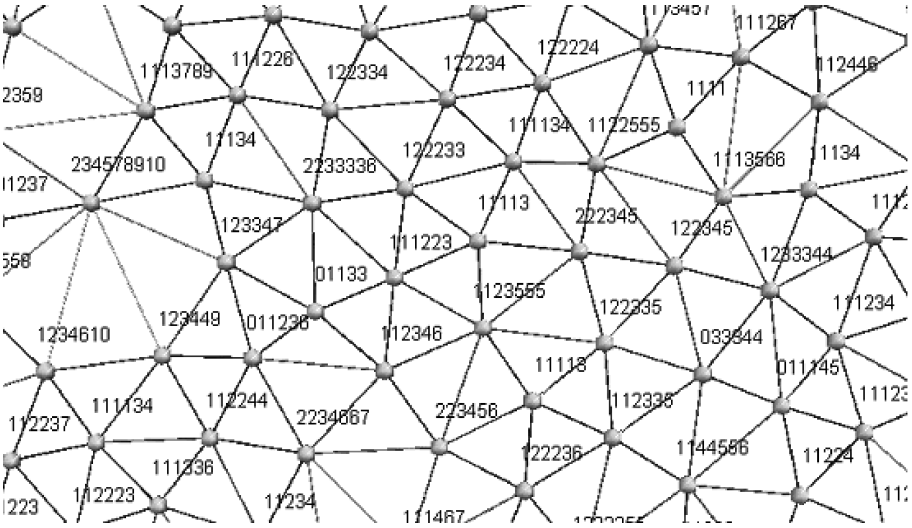

Figure 3. The Delaunay triangulation of the model system with measures assigned to vertices

We divided the interval into $N_{\text{stat}} = 10$ equal parts. So, the length l_{step} of a single part is $(4.1 - 2.1)/10 = 0.2$ (A).

The vertex measure calculation. Having all edges characterized, we can obtain measure for the vertex (Figure 3). It is composed of the surrounding edges measures arranged in a specific order. It is simple and efficient to represent the row of edge's measures in a sorted way. In this case, for example, two vertices with edges $(3, 7, 1, 1, 4)$ and $(1, 1, 4, 3, 7)$, respectively, would have the same state.

2.4. Transitions. If we run MD simulation and monitor the vertices states, we will notice they are changing. There are three types of possible transitions: Edge Length Change (ELC), Edge Disappearance (ED), and Edge Appearance (EA). Each transition is associated with two vertices.

In Table 1, a brief example of a set of transitions is shown. They are encoded in a following manner:

V_1, V_2 are measures of two vertices on the ends of a varying edge. Labels V_1 and V_2 are assigned to vertices as a result of their measures comparison and the least measure in representation of an integer is labeled as V_2. This helps to decrease the number of transitions. Some pairs V_1 and V_2 can take part in several transitions. This should be taken into account when calculating probability of the transitions.

Table 1. Dictionary of transitions obtained by analysis of the model system

Edge Length Change					Edge Disappearance				Edge Appearance			
V_1	V_2	L_0	L_1	P	V_1	V_2	L_0	P	V_1	V_2	L_1	P
112223	112222	1	2	304678	1223346	112226	6	85	122234	11122	6	79
122223	112223	1	2	277084	1223346	111226	6	79	122334	11122	6	79
222222	122223	2	1	272368	1222346	111226	6	75	122235	11222	7	73
222222	122222	2	1	227659	1222346	112226	6	71	122334	11222	6	67
122223	122222	1	2	198473	1222357	112227	7	69	122234	11222	6	61
222223	222222	2	1	197121	1222357	111227	7	66	122235	11122	7	60
112223	112223	1	2	185503	1222367	111227	7	60	122229	12222	9	56
222223	122222	2	1	182089	1222299	122229	9	57	122333	11122	6	53
122223	112222	1	2	181392	1222367	112227	7	55	122236	11222	7	46
222222	122222	2	3	160065	1222356	111226	6	55	122226	11222	7	46
122223	122223	3	2	154703	1122367	112227	7	48	112236	11222	7	46
122223	112223	2	1	133654	1223357	112227	7	45	122235	11122	6	45
112223	111223	1	2	132050	1122367	111227	7	45	112234	11122	6	45
122222	112223	2	1	130627	2223346	111226	6	44	112334	11122	6	43
122222	112223	2	3	121830	1222399	112229	9	43	122236	11122	7	43
122223	122223	1	2	121762	1222356	112226	6	41	122235	11222	6	42
222223	222223	2	1	119680	2222346	111226	6	41	122344	11122	6	42

L_0 is an initial length measure of the changed edge. The edge with this length measure must connect V_1 and V_2 (it is absent for EA transition).

L_1 is the final length measure of the changed edge (it is absent for ED transition);

P is the number of times the transition was detected in the course of analysis, P is used to calculate the probability of the transitions.

3. Analysis of results

3.1. The number of items in the dictionary. Using the vertex measure analysis, we compose a dictionary of transitions for the model system. In Figure 4, the number of transitions collected in the dictionary vs. time step (iteration) is shown.

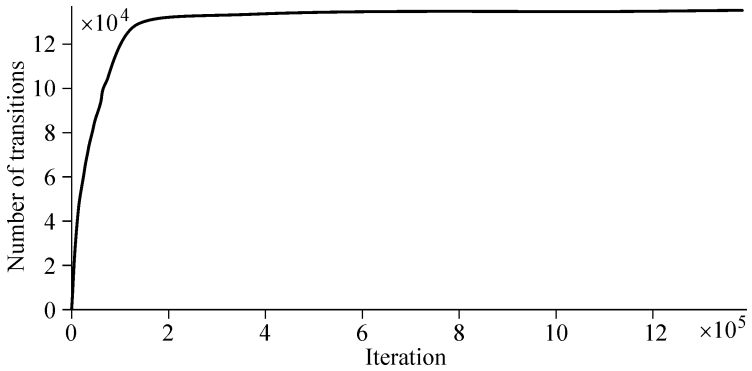

Figure 4. The growth of the dictionary

It can be seen in the diagram that there is a fast growth of the dictionary during the first $2 \cdot 10^5$ iterations, and then it considerably slows almost reaching a constant value at $1.4 \cdot 10^5$. This behavior does not sufficiently depend on structural changes in the model MD experiment. It was verified to reproduce initially from the time steps $5 \cdot 10^5$ and 10^6.

3.2. Transitions. While analyzing over $1.3 \cdot 10^6$ iterations, about $1.4 \cdot 10^5$ unique transitions were obtained. Among them $\sim$ 92 % ELC, $\sim$ 4 % ED and $\sim$ 4 % EA transitions. The total number of transitions analyzed is $\sim 15.4 \cdot 10^6$, where $\sim$ 99.8 % constitute ELC and equally about 0.1 % refer to ED and EA.

As was mentioned above, some different transitions take place with the same vertex pairs. Sets of transitions in the dictionary were analyzed for intersections and the following results were obtained: the first intersection to analyze was the inner intersection, which constitutes $\sim$ 21 % for ELC, $\sim$ 0.7 % for ED, and $\sim$ 26 % for EA transitions. The outer intersections

Table 2. The results of dictionary analysis

Type	Total number of transitions		Unique transitions in dictionary		Intersection of V_1,V_2-sets in dictionary		
	Number	Percent	Number	Percent	ELC	ED	EA
ELC	15437619	99.7891	125902	92.5518	27212	3080	2753
ED	16306	0.1054	5080	3.7344	3080	36	104
EA	16319	0.1055	5052	3.7138	2753	104	1311

were found to be as follows (percentage is given for a set of the least length): ~ 61 % ED vs. ELC, ~ 54 % EA vs. ELC, and ~ 2 % ED vs. EA. A brief representation of introduced data is given in Table 2.

3.3. Distribution of specific states. Figures 5–7 show the distribution of transitions appearance.

Analysis of this diagrams shows that for all three types of transitions, two specific regions can be distinguished. The first one is occupied with diverse transitions that rarely occur. This region is in the vicinity of zero. Another region consists of a few transitions that appear very frequently (some of these transitions are marked in the diagrams). These transitions might be used for structure and properties characterization.

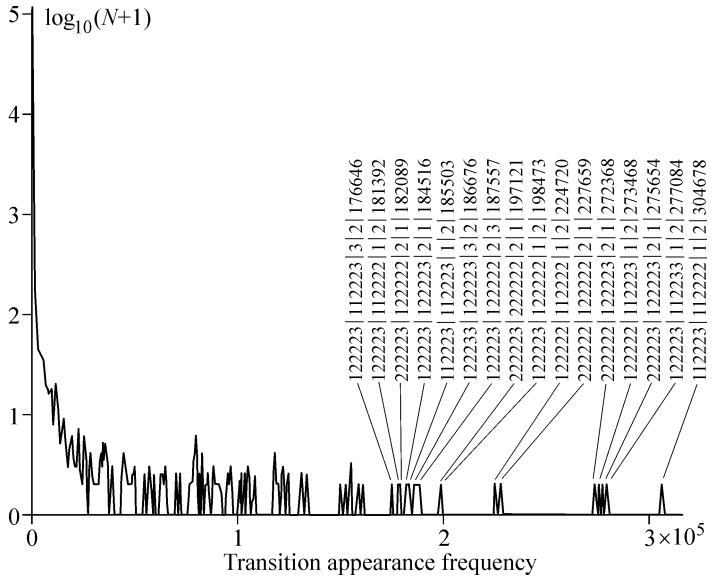

Figure 5. ELC transition appearance frequency. Selected transitions are marked with corresponding transition codes

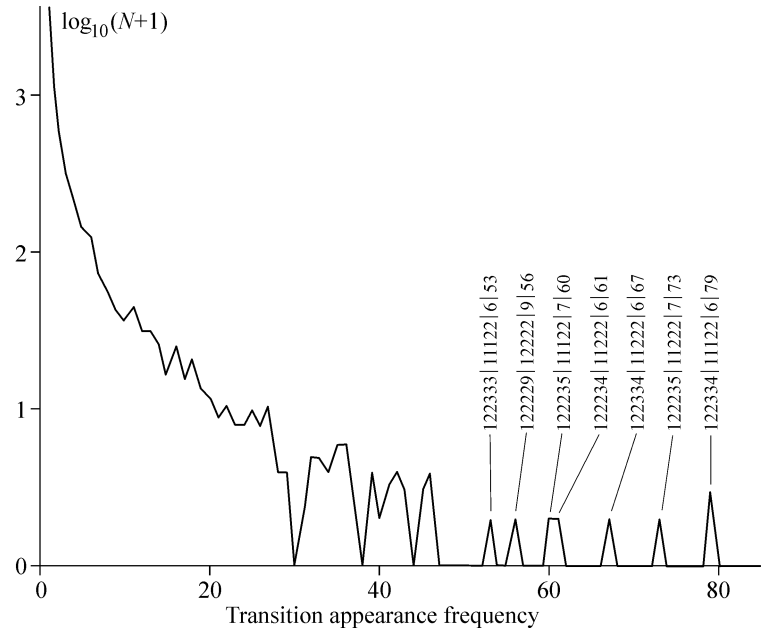

Figure 6. EA transition appearance frequency. Selected transitions are marked with corresponding transition codes

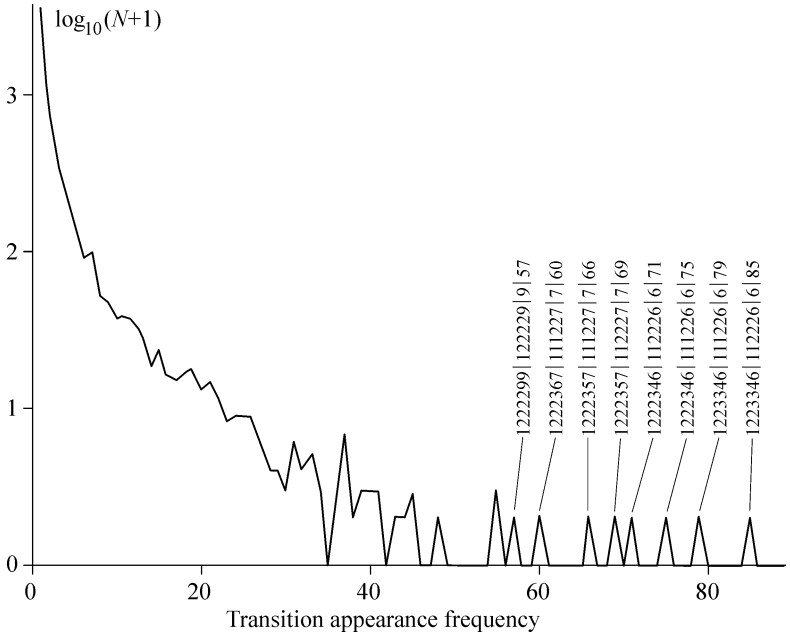

Figure 7. ED transition appearance frequency. Selected transitions are marked with corresponding transition codes

4. Conclusion

The proposed method can be used for a formal description and characterization of disordered amorphous structures in the plane and in three dimensions. A combination of transition templates can be used to describe the evolution of these structures thus leading to CA model construction. The initial data for states and transitions computation may be obtained from any method with appropriate output data. Transitions and states obtained for small clusters can be used to model the larger-scale systems.

Further theory enhancements including second order meshing of data may be used to improve the theoretical efficiency of the method and will be presented in the future.

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