Cluster analysis of atomic structures in amorphous alloys

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Introduction

For amorphous and amorphous-crystalline alloys possess a unique set of physicochemical properties, which attracts the attention of researchers to the search for new materials. The atomic structure with a reduced degree of order, as well as the composition, largely determines the functional properties of the alloys. The absence of long-range order in the atomic structure presupposes the presence of many realizations of the topological and compositional local atomic environment [5]. This causes the presence of many stable configurations of the structure, local minima of the total energy of the system, but which are energetically less favorable than an ordered, crystalline structure of the same composition. This is associated with the degradation of properties with time and with external influences, for example, heating. Often, small changes in the structure lead to significant changes in the physicochemical characteristics of the material. Electron microscopic images of structures are used to determine local order in both materials' science and biological objects. Despite many studies, the authors fail to present universal characteristics of atomic order, as well as a sufficiently complete theory of ordering processes in an amorphous structure. The difficulties are caused by the large number of variants of the disordered atomic structure, the absence of long-range order and the impossibility of describing the local order by crystallographic groups, and the large number of computational resources required for simulating macroscopic measurable volumes of material. In this study, based on the analysis of electron microscopic images of an amorphous structure, a method is proposed for studying local atomic ordering with any kind of symmetry, including non-crystallographic one. It is shown that under thermal action, by the example of the structure of amorphous alloys CoP, CoNiP, NiW, there is a 30% change in the density of atomic clusters with an ordered structure of 1–2 nm in size. It has been shown that, upon heating, both an increase in the degree of order and a decrease occurs.

Experiment

Samples of CoP, CoNiP, NiW amorphous alloys were prepared by electrochemical deposition. We investigate atomic structure of the samples by means of high-resolution transmission electron microscopy on FEI Titan 80-300 at 300 and 80 kV with abberation correction. Samples placed on standart cupper grid have thickness from 2 to 10 nm. Small thickness of the samples allows us to investigate the local atomic structure and show different level of ordering. Series of HRTEM images were obtained at temperatures from 20°C to 300°C.

HRTEM image processing performed by GPU software to have cross-correlation with double-core: $H_{\varphi,r_0}(x,y) = h(x,y) \cdot \sum_{\varphi} h(x - r_0 \cdot sin\varphi, y - r_0 \cdot cos\varphi)$, where $h(x,y) = sinc(\rho/\rho_0) - h_0$. We select r_0 =0.25 nm, ρ_0 = 0.15nm. Parameter h_0 selected from following condition: $\sum_{x,y} h(x,y) \approx 0$. [6]

Results and discussions

We created a software program that can compute large amounts of information in our datasets in order to simulate electron microscopic image studies. The developed app calculates the distance between two points in the Euclidean 2D plane using the electron microscope image pixels as coordinate points [1]. We now need to calculate the distance between two points, so we use Pythagoras' Theorem, which is nothing more than the Euclidean distance [2]. Distance, assume point p have Cartesian coordinates (p_1, p_2) and let q have coordinate (q_1, q_2). Then the distance between p and q is given by [1-4].

$$d(p,q) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2}$$

and finds the nearest neighbor for each point in a dataset within a radius of r=2 nm. Following the determination of nearest neighbors for each point, the program sorts the neighbors in ascending order and prepare the data points for plotting an undirected 2D graph using the nearest neighbor graph algorithm. All nearest neighbors (NN) are calculated for the nearest neighbor search on a two-dimensional Euclidean plane with a specific radius r. After locating the initial coordinate point x, y, the process computes the Euclidean distance for all coordinate points in the dataset.

After computing the distance between two points, the program compares the calculated distances while taking the given radius r into account for each point's computed results and writes the output to a file the nearest points with their coordinates, the distance between the points, and the positions of the coordinates within the given parameter radius. This procedure is repeated for all the coordinate points in a dataset.

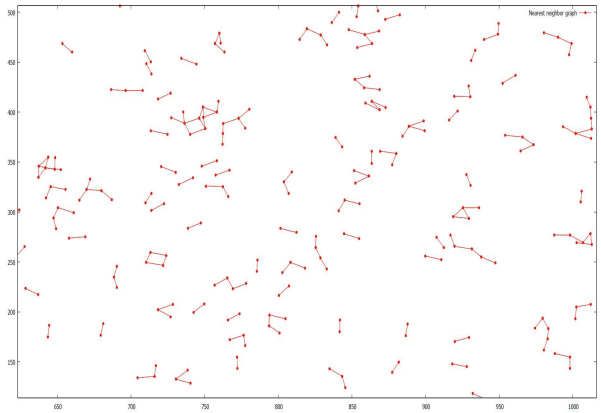

Fig. 1. *A nearest neighbor graph of 2997 points in the Euclidean plane100- 50 interval.*

In our applications of these graphs, the edge orientations are ignored, and the NNG is instead specified as an undirected graph.

Fig. 3. *HRTEM images of Amorphous alloy samples from series4 00001.dm3.*

Conclusions

The results of this study demonstrated the accuracy of the nearest neighbor search algorithm within a given radius using various distance metrics. Experiments were conducted using large datasets derived from electron microscopy images of amorphous and amorphous – crystalline alloy specimens. This allows us to conduct detailed research on the properties of amorphous and amorphous-crystalline alloys. Researchers are still looking for ways to use modern computing software to determine the atomic structure and physicochemical properties of amorphous alloys. We can provide accurate information with much less execution time and resources by using an effective and modern approach to study Cluster analysis of atomic structures in amorphous alloys. More research and innovation are required to fully comprehend the physicochemical properties of amorphous alloys.

References

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