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PREPARATION OF DATA FROM EBSD MEASUREMENTS FOR CELLULAR AUTOMATON MODELING OF ANNEALING PHENOMENA IN HEXAGONAL MATERIALS

OPRACOWANIE DANYCH Z POMIARÓW EBSD DLA MODELOWANIA Z UŻYCIEM AUTOMATÓW KOMÓRKOWYCH ZJAWISKA WYŻARZANIA W MATERIAŁACH O SYMETRII HEKSAGONALNEJ

Annealing is used to soften and restore plasticity to metallic materials, that were hardened in cold working processes, and to modify the final product structure. Together with plastic forming, it is a crucial element of all thermomechanical processing procedures. While the mechanisms of plastic forming have been rather well understood, the understanding of the annealing processes (as recrystallization or grain growth) and the possibilities of controlling them and introducing expected modifications in technological processes is still considerably limited. The phenomenology of the process and its energetic causes are known and were examined long ago. However, not all relevant physical mechanisms controlling nucleation and growth of grains are clear. The modeling of the annealing processes requires the input data in the form of a possibly complete quantitative microstructure description of a material, both in the state of deformation and of different stages of recrystallization and grain growth. Such description to be used in the model is based mainly on the data gathered from crystallographic orientation sets, obtained in systematic local measurements of a sample, that underwent a specific deformation and annealing process. Advanced data processing, consisting in removing errors and wild spikes, calculating of misorientation axes and angles, grain size characteristics etc., are crucial in the process of creating the simulation.

Wyżarzanie wykorzystuje się by przywrócić plastyczność metali, które we wcześniejszej fazie zostały poddane procesowi walcowania na zimno oraz do modyfikacji struktury końcowego produktu. Wraz z metodami odkształcenia plastycznego jest elementem dominującym we wszystkich termomechanicznych procesach technologicznych. Podczas, gdy mechanizm odkształcenia plastycznego został dość dobrze poznany i zrozumiany, wyżarzanie i możliwości jego kontrolowania do uzyskania zadanych modyfikacji w procesie technologicznym wciąż skrywają wiele niewyjaśnionych zagadnień. Fenomenologia procesu i jego energetyczne skutki są znane i były badane od dawna. Jednakże nadal brakuje jasnego fizycznego opisu mechanizmów kontrolującego zarodkowanie i wzrost ziaren. Modelowanie wyżarzania wymaga danych wejściowych, które są jak najlepszym odwzorowaniem mikrostruktury w fazie deformacji jak i rekrystalizacji oraz wzrostu ziaren. Takie dane uzyskiwane są głównie z lokalnych pomiarów orientacji krystalograficznych. Dane te muszą być poddane zaawansowanym procedurom przetwarzania i analizy danych. Są one związane z usuwaniem błędów indeksacji, obliczaniem osi i kąta dezorientacji, charakterystyką statystyczną rozmiaru ziaren itp. Metody te są nieodzowne w procesie tworzenia modelu.

1. Introduction

To create a reliable description of a phenomenon, a scientist must couple theoretical and experimental efforts. The ideal situation is to have sufficient funds and time to design and carry out a big number of experiments. The situation is almost impossible, especially when the experiment time is long and costs are high. Fortunately, we can model virtual experiments thanks to rapid development of computer hardware.

Even a home class PC has enormous computational power and makes it possible to create computer models with a high level of complexity. Modeling already has gained recognition not only in scientific work, but also in the industry. There are many examples of modeling used in crash tests, fluid dynamics simulations, prediction of mechanical response of tools and constructions (crack analyzing etc.), traffic jam simulations. In the recent years, we can observe a fast development of computer models in Material Science: modeling of annealing,

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magnetic, electrical, mechanical properties of materials. Modeling can be used not only for creating virtual experiments, but also for creating technological procedures, for example, aimed at achieving desired properties of material.

Computer simulations are an unmatched tool for the verification of theoretical assumptions. It is less expensive than experiments. By implementing a theory in computer code, we can carry out a number of tests and examine the influence of changing input parameters. This procedure can be a proof not only of correctness of our predictions, but it can also provide an assessment of the utility limits of a theory. Even if, at the beginning, we cannot create a model, that correctly reproduces experimental results, it can be an invaluable tool for verifying a theoretical description of a phenomenon.

Of course experiments, are the final confirmation of predictions made in theories and models. Thanks to simulations, we can determine the most important parameters to achieve the desired purpose of the experiment. Modeling can also be used to interpret experimental results, for example, of connecting the Kikuchi patterns with crystallite orientation, diffraction patterns or spot patterns. Modeling makes it possible to interpret automatically a large amount of data. But whenever we use that kind of interpretation, we should be aware of the limitations of used algorithms.

By combining these three methods: theory, modeling and experiment, we can create a sufficient and reliable description of a phenomenon.

Modeling of annealing usually uses three principal simulation schemes: Monte-Carlo simulations [1, 2], vertex model [3] and cellular automaton (CA) [4, 5, 6]. All of these approaches have their advantages and disadvantages, and their application depends usually on individual preferences.

The most advanced simulations of annealing processes have been done for materials with cubic symmetry. These works advanced significantly the understanding of annealing phenomena [e.g.]. Up to now, however, no sufficiently general library has been created, the routines of which could be used to build models for each of the growth and recrystallization problems under consideration. This is caused by a large variety of process-controlling parameters, that have to be accounted in particular cases.

This also depends on the cognitive potential of experiments, because there are still regions which remain unreachable for our scientific eye. What is most depressing is that those regions seem to be the most interesting ones. For hexagonal materials, simulations of annealing are still in a preliminary stage. The biggest efforts are directed at modeling of processes in titanium and zirconium alloys.

2. Data preparation

At the beginning of CA history, this method seemed to be the panacea for modeling complex systems. It was simple to implement, fast to execute and powerful. CA didn't become the answer to all problems, because of a minor inconvenience: it lacked strict rules, which could be used to transform a differential equation into a CA. But if we are aware of the constraints, we can use it for very effective modeling, because it is still a very powerful idea.

A cellular automaton [7] is a discreet system of cells. Every cell can have a number of properties and a set of these properties is the state of a cell. The state of a cell evolves in time. The evolution is determined by a set of rules, that describe the new state of a cell in the next time span. The rules usually use the state of the neighboring (Fig. 1) cells to determine the new state of a given cell. 1D CA is the easiest model to understand. One of the simplest 1D CA models is a line of white and black points (pixels). The neighborhood of a pixel is the closest pixel on right and on the left. If we have only two possible colors, we can create 8 different rules for cell behavior. For example, if a point is black, its neighbor on the right is black and the neighbor on the left is white, the color of the pixel will change from black to white in the next time span. The evolution of this line of pixels in time will create an image (Fig. 2 with), where the width is equal to the number of pixels in the line and height is equal to the number of time spans.

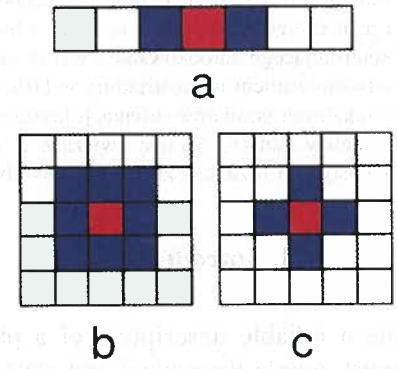


Fig. 1. CA neighborhoods: a) 1D b) 2D Moor c) 2D von Nuemann

In 2D (Fig. 1a and Fig. 1b) cells arrangement usually are used two types of neighborhood: von Nuemann - 4 closest neighbors or Moore - 8 closest neighbors. The main idea of CA is very simple. Its implementation is usually not difficult, but it is most important, that even simple rules of the system behavior make it evolve significantly from static to quasi-chaotic states. Fig. 2

shows different behavior of 1D CA. CA is a simple a line of pixels with a black pixel in the middle. After an evolution, we observe a number of lines which create the presented pictures. The usefulness of the CA has already been proved in simulations of fluid dynamics, self consistent systems, biological simulations etc. This idea is also frequently used for image analysis and processing.

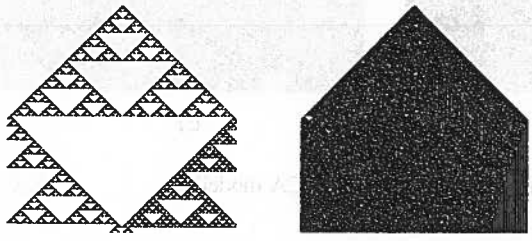


Fig. 2. Behavior of 1D CA

In our model, we create a CA directly from EBSD measurements. An EBSD map is basically a set of points with given coordinates and orientation specified at these points. Every measured point is treated as a cell and the state of the cell is simply its crystallographic orientation. The orientation of a cell can change in time, as the system evolves according to the rules based on the orientation of its neighbors. Of course, not only the orientation describes the state of the crystallite in the polycrystalline material but basically it can be quite good input and output parameter for the simulation, especially that properties of the material are strictly depended on orientation of the crystallites.

The main objective of our model is to describe recrystallization in zirconium alloy. It is a very complicated problem, because experimental are not sufficient, as the measurements of heavily deformed regions in the sample cannot be made by traditional SEM/EBSD.

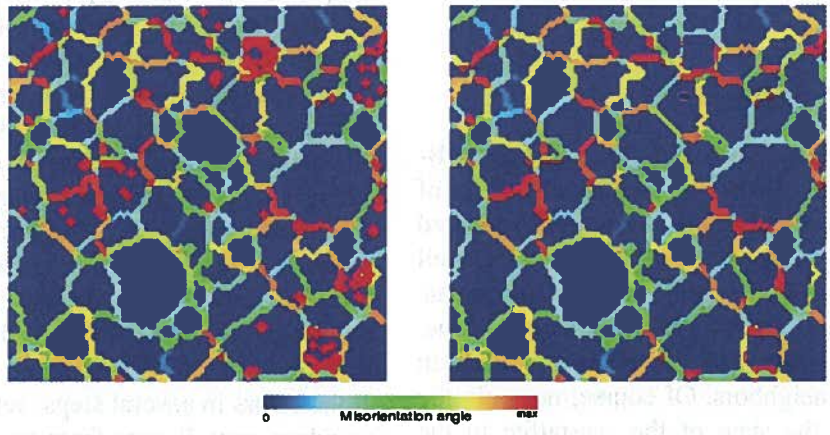
Before we can run the simulations, we need to remove errors from EBSD maps. This involves removing of unindexed points and misindexed points (wild spikes). It is also reasonable to remove very small grains with the area of several measured points. For a CA, every point should have a well defined orientation. The error points usually constitute a significant percentage of the measured map. That's why removing errors is a very important and hard procedure to carry out. Of course, the level of complication is directly correlated with the distribution of error points.

Unindexed points can be classified into tree main groups: a single point or a few unindexed points inside well-defined grains, unindexed points located within grain boundaries, unindexed points grouped into clusters (Fig. 3). The unindexed point appears when Kikuchi pattern can not be interpreted. Such situation can occur, when the contrast of the pattern is to small and the pattern is unrecognized by the algorithm. Removing unindexed points is not a very complicated procedure, if they belong to the first two groups, as we can use CA idea to remove them. In every step of the clearing procedure, the orientation of an unindexed point is chosen from the set of well defined orientations of the neighboring points. The state (orientation) of the error point is changed to the state adopted by the majority of its neighbors. The majority is not so important if we have an error inside a grain. The situation gets more complex if an unidexed point is located within the grain boundary area. The presence of such points influences considerably coarseness of the boundary. If unidnexed points are gathered in small groups, their orientations cannot be determined on the basis of the orientations of all neighbours, because some of them are not indexed either. Therefore, it is necessary to locally reduce the number of neighbours taken into consideration. It is important for the number of neighbours under consideration to remain at a reasonable level. In extreme case, when the orientation of an unindexed point is determined on the basis of a single neighbour, it is possible to remove all the errors in several steps, yet the reconstructed grain boundary may diverge from its actual shape to such an extent, that the boundary behaviour changes during simulation.

Unfortunately, this can also influence the error clusters. By repeating the clearing procedure, we can also remove them but it's should be considered if this is the desired effect. We should be careful with these clusters. Those regions are large and we are making neighborhood grains grow into those regions by repeating the clearing error algorithm. It is dangerous, because this can create big grains that would never exist in real samples. Those grains in the simulation can lead to undesired effects, like abnormal grain growth in the early stage of recrystallization. If we cannot remove them by applying some other criterion, they should stay unaffected. In CA modeling, all errors should be removed, including clusters. Algorithms for removing all errors are time-consuming, because they usually involve manual operations. From the point of view of data analysis, if the error clusters contain only few percent of measured points, clearing them will not affect the results.

a) b) c)

Fig. 3. Data for error removing: a) raw data, b) clusters of errors, c) data for CA modeling.



a) b)

Fig. 4. Wild spikes misorientatoins maps: a) map after errors removing, b) map after removing wild spikes.

Wild spikes pose more difficult problems (Fig. 4). The reason of this error is in the misinterpretation of Kikuchi patterns. This situation can occur, when two different orientations have similar Kikuchi patterns and the indexing procedure cannot distinguish between them. We can usually discover misindexed points by analyzing the misorientation [8] angle and axis [9] profiles with EBSD map points distribution (positions). After this procedure, we can determine the misorientation of a wild spike. Removing those errors is not so simple, because even if we have the knowledge about its misorientation, and it is not a single point with well known neighborhood, it is almost impossible to distinguish between errors and real grain boundaries. Fortunately, it is possible to use a procedure based on finding very small grains inside big ones and if a grain boundary has the misorientation of a misindexed point, we can change the orientation of these points to the orientation of those outside the grain. If a small grain is placed between two grains, we choose the grain, that creates a boundary with the misorientation proper for wild spikes, and take its orientation as the correct one for error points. Of course, we can also choose grains with small areas and change them into unindexed points and, after that, start the procedure for clearing these errors. The influence of a misindexed point is very significant for misorientation profiles. That is why it is crucial to analyze the profiles of misorientation during the removal errors, in order to be aware of the changes.

3. Summary

The output of the simulation strongly depends on the input data. This is why it is important to be extremely careful and aware of the changes, that are made by error removing procedures. We should use several maps to create the most reasonable picture of a microstructure. Removing errors is crucial for creating reliable statistics from a EBSD map. That is why this process should be treated less automatically.

For grain growth simulations, we usually have good results from EBSD, and those methods are sufficient for removing errors. Removing errors in recrystallization simulations is much more complicated, because the most interesting highly-deformed regions are usually pure indexed.

More efficient error removing procedures can be based on the analysis of band contrast, band slopes and orientation contrast. Clearing the results of EBSD measurements can be also achieved by improving the removing errors algorithms. The more advanced algorithms should take into account larger number of neighbors and to have more capacity for adaptation.

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