ARMA MODELS APPLIED TO PREDICTION OF THE DISLOCATION PATTERNS IN NANOSTRUCTURED MATERIALS

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ABSTRACT

Nanostructured materials by severe plastic deformation have attracted much interest in the last decade due to their size-dependent unique mechanical, physical and chemical properties. During plastic deformation of metals and alloys, dislocations arrange in ordered patterns. When deformed plastically, line defects (dislocations) are introduced into the lattice of each grain. These defects organize into dislocation boundaries separating (nearly) dislocation-free regions with almost perfect lattices, which we term subgrains. Understanding the arrangement of dislocations is essential for science and industry, because their patterns determine many physical and mechanical properties, such as electrical rezistivity of semiconductors or strength anisotropy and fatigue failure of metals. In nanostructured materials, plasticity is caused by the dislocations generated by dislocation sources between grain boundaries. These dislocation spread out, interact with the pre-existing structures, so that an important part of them mutual annihilate each other. Based on the overlapped dislocations concept at the grain boundary frontier, the Hall-Petch relation shows an increase of the restrict flow value when decreasing grain boundaries size.

KEYWORDS: severe plastic deformation, ARMA model, nanostructured materials, molecular dynamics

1. INTRODUCTION

Recent developments in ultra-fine grained materials, which present important improved mechanical properties, have drawn the attention on the use of large-strain plastic deformation for obtaining new microstructures in metals. The formation of homogeneous nanostructures were first developed and applied by Valiev at al. [1991] in the equal-channel angular pressing technique (ECAP) for developing the submicro- and nanometre grain size microstructures.

In nanocrystalline and ultra-fine grain materials (UFG) the plastic deformation appears immediately after a recoverable elastic deformation and is governed by the nucleation and motion of defects in the crystal lattice. In order to investigate the deformation mechanisms at scale smaller than 50nm, researchers have done TEM and HRTEM investigations. In the case of ductile copper there has been discovered the twinning deformation mechanism.

Many material properties (strength, ductility) are directly related to the structure and movement of the line defects (dislocations). It is well known that grain boundaries have an important effect on the mechanical properties of materials leading to the well known Hall-Petch relationship:

$$\sigma = \sigma_0 + kD^{-\frac{1}{2}} \tag{1},$$

where σ is the yield stress, σ_0 is the "friction stress" necessary to move individual dislocations during deformation, k is a constant also called the "Hall-Petch" slope and is material dependent, and D is the average grain size. The relation is no longer available for grain size smaller than 10-30nm [5, 12, 14].

Investigations of the deformation mechanisms and the material properties in nanocrystalline materials with grain size lower than 200nm are based on indirect techniques, which show the appearance

and the interactions of the defects in the crystal lattice. One of the methods used to describe from atomistic point of view the motion of the dislocations is the molecular dynamics (MD) technique. This method considers a small number of dislocations and refers to specific dislocation mechanisms, such as cross slip, dislocation cutting process or dislocation from cracks.

This paper presents the modelling of a dislocation by MD technique in bulk nanostructured and the prediction of the trajectories using Autoregressive Moving Average (ARMA) model.

2. EXPERIMENTAL CONDITIONS

Nanocrystalline and ultra-fine grain materials processed by severe plastic deformation (SPD) methods has been the subject of intense study in the last years for a lot of researchers. One of the most important SPD method is the equal channel angular pressing in 2D (2D-ECAP) because it has the advantage to produce large samples.

In the 2D-ECAP method, the plastic deformation of the material is caused by simple shear in a thin layer at the crossing plane of the channel sections. Due to the non-uniform strain distributions, the amount of equivalent plastic strain generated can be estimated as [14]:

$$\varepsilon = 2/\sqrt{3}\cos\varphi \qquad (2),$$

where ε is the amount of strain and φ is the die channel.

For the case when $2\varphi=90°$, the plastic strain is always $\varepsilon=1.15$. Extrapolation of strength from a strain rate of 10^4 s^{-1} to the one greater than 10^6 s^{-1} becomes problematic, because strain rate cannot be increased without increasing the pressure. The ECAP process usually uses high-capacity hydraulic presses, with the pressing speed between 1-20 mms^{-1}. This pressing speed has no influence on the size of the ultrafine grains because slower speeds produce equilibrate microstructures. During the process, when the pressing speed is increased the yield stress has constant values [12, 14].

Another important factor in the ECAP process is the pressing temperature, because it can be easily controlled. For example, during processing pure Al, when increasing the temperature there is an increase of the equilibrium grain size, with the temperature between 0-700° K and the grain size between 0.1-10μm and also an increasing annihilation of dislocations in the grains.

The deformation mechanism of the nanostructured materials is not yet well known. Researchers reported that twinning and grain boundary sliding are the main mechanisms that lead to the deformation. The present paper proposes one new step in understanding how FCC (face-centered cubic) deforms under ECAP conditions by means of the molecular dynamic simulation, particularly for copper.

3. MOLECULAR DYNAMICS SIMULATION

Molecular dynamic (MD) simulations have been used to study the atomic-scale processes that occur during plastic deformation of polycrystalline aggregates of nanocrystalline grains because at this scale no experimental model is able to catch the real deformation mechanism. The simulations suggest that nanocrystalline metals accommodate externally applied loading, by means of grain boundary sliding and the emission of partial dislocations that run across the grains [1,8]. The MD simulations also suggest that grain boundary sliding and the partial dislocation emission are triggered by atomic shuffling and free volume migration in the grain boundaries. For creating our molecular dynamic model we have used the trail representation set up by [2,3,4,5,6,7].

3.1 Creating the geometry

Recent TEM investigations have showed that ductile copper consists of irregular-shaped grains with random orientations. Grain sizes are between 100nm and 1μm, and each grain contains a high density of growth twins of the 111/[112] type. Starting from the trail representation build up by [6,8,] we have created our own molecular models, as shown in figure 1 (a, b, c, d).

For creating the molecular model we use the lattice orientation of the ductile copper, which is a face-centred-cubic (FCC) material. The FCC materials have larger interstitial spaces, being capable of retaining other atoms with atomic radius r=0,146a, where a is the lattice constant. For ductile copper a=3.61Å, the minimal distance between two atoms is 2.556 Å and the atomic radius is r=1.278Å. For the potential energy of the molecules, we use the Lennard-Jones pair potential that shows the r^{-12} and r^{-6} contributions.

3.2 Simulation conditions

The model simulations used for investigating the molecular dynamics simulations were carried out in copper (Poisson's ratio ν = 0.347, b = 0.256 nm, indenter radius r_i=50nm, elastic module E=123GPa and an estimated shear strength of the crystal $G/2\pi$=7.6GPa). The simulation uses number of 149 atoms in a cell size of 6.9x6.9 μm with a time step of 0.5-0.6ns with a shear stress τ_{max}=10.7GPa, in the conditions of a diffusion process. Diffusion is a mechanism that creates thermal activated salts for the atoms. Our MD simulations used periodic boundary conditions with reflecting walls with the temperature between 0.2-2.5° K and the internal pressure between 0.5 and 2 MPa.
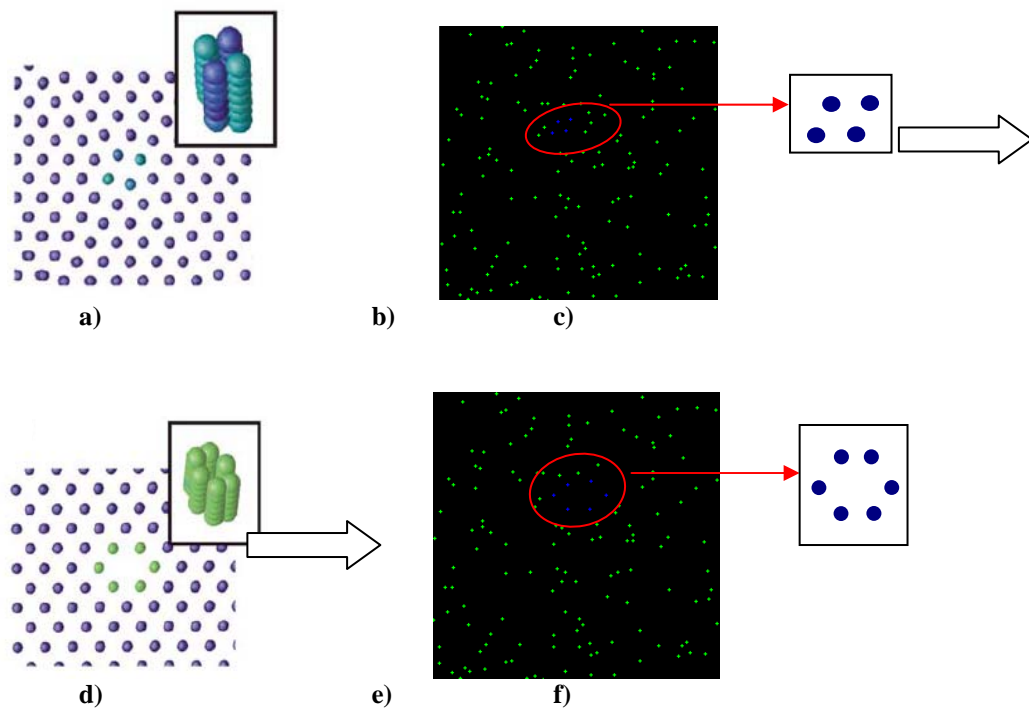
Fig. 1 Schematic model of two dislocation process: a) trail of partial point defects, d) vacancy tube [Buehler et al., 2005], b) trail of partial point defects, e) vacancy tube, our generated models, c) and f) 2D section through the dimensional elastic field for both cases.

3.4 Simulation results

During the simulations, once we increase the temperature and the internal pressure is constant, the kinetic energy also increases. When we decrease the pressure and the temperature is constant, the kinetic energy decreases, bellow the average value. For the second type of dislocation, when we decrease the pressure and the temperature is constant, the kinetic energy does not decrease so much, is still above the average value (Fig.3). The total energy depends both on the temperature and the pressure (Fig.4). When both parameters increase, the total energy also increases. In both cases, when the temperature was constant and we increased the external pressure, the pressure inside the simulation cell increased significantly. The velocity distribution increased once with the temperature, it lost part of its intensity.

The snapshots of the atoms movement under the conditions similar to the ECAP process show that the atoms from the elastic field around the dislocation spread in many directions similar to a diffusion process (Fig.2).
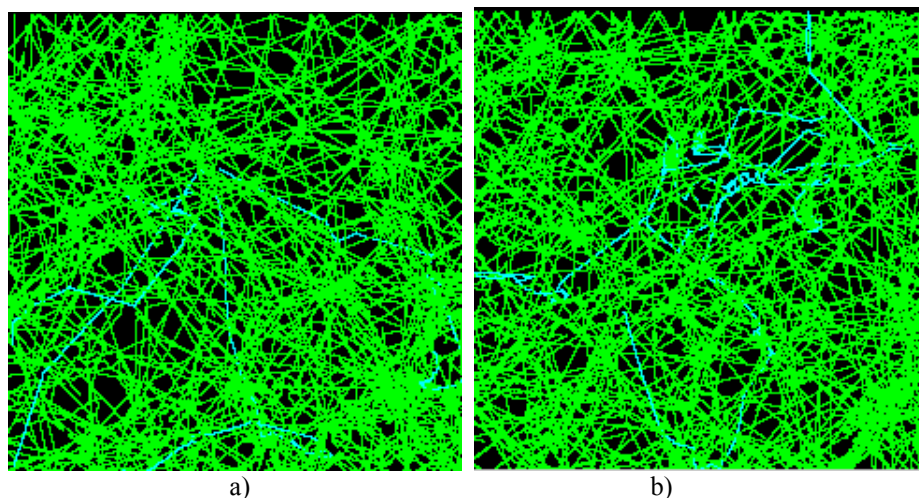

Fig. 2 Trajectories for a) trail of partial point defects and b) for vacancy tube, in the final stage of simulation
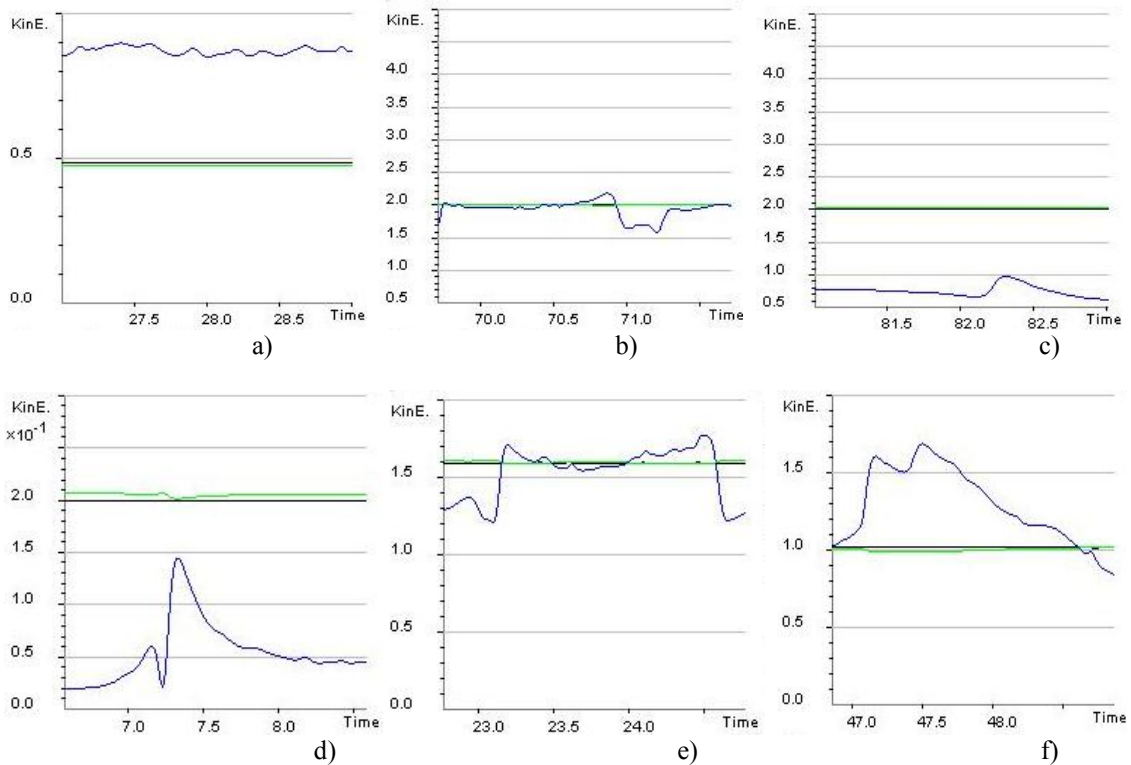
Fig. 3 Histograms of kinetic energy: a), b), c) for the trail of partial point defects;
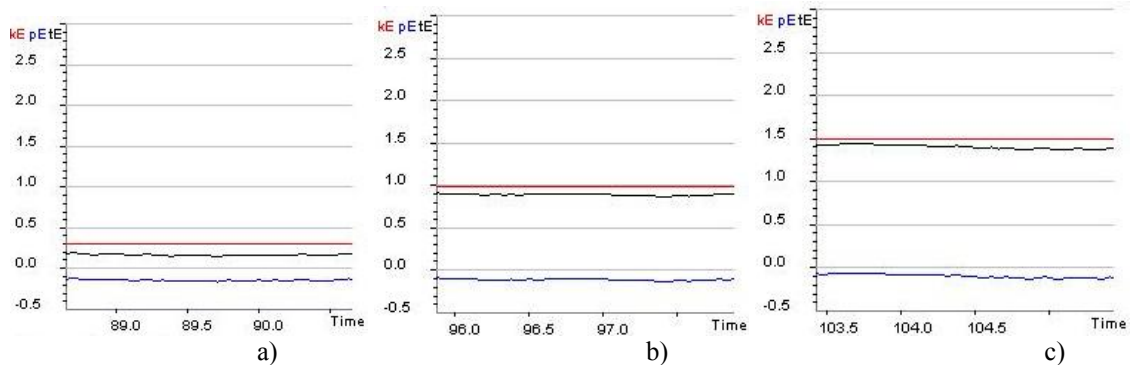d), e) and f) for the vacancy tube

Fig. 4 Variation of total energy as a function depending on time

4. ARMA MODEL PREDICTION

Autoregressive Moving Average (ARMA) model is a modelling technique to predict or reconstruct a data sequence. The ARMA [p,q] model or Box-Jenkins model is one of the most traditional techniques in statistical times-series analysis. The model consists of two parts, an autoregressive (*AR-p*) part and a moving average (*MA- q*) part and can be expressed as:

$$X_t = c + \varepsilon_t + \sum_{i=1}^{p} \varphi_i X_{t-1} + \sum_{i=1}^{q} \theta_i \varepsilon_{t-i} \qquad (3),$$

where p is the order of the autoregressive part, q is the order of the moving-average part, $\varphi_1, \ldots, \varphi_p$ are the autoregressive parameters, $\theta_1, \ldots, \theta_q$ are the

moving-average parameters, c is a constant and ε_t denotes the series of errors also called the "white noise".

In order to predict the dislocation trajectories pattern for our two dislocation mechanisms, we used the ARMA model prediction from the MATLAB software.

For both models we picked 10 several points from the trajectories of one molecule of the dislocations. For each point (x,y) we defined 4 anterior points that helped us calculate the prediction of the time series data for x and for y axis. After applying the ARMA model we obtained 20 prediction points that will help us draw the trajectory prediction curve. In figure 3 (a,b) we can see the trajectories prediction curves for one molecule from each model, the first five points in each graph are points used for prediction.

ARMA model was applied for a single molecule that bound the dislocation. In (a) case, the dislocation is belonging to the partial point defects and (b) case is for dislocation type vacancy tubes.

The time of nanostructuring simulated by MD is 7 sec and the ARMA prediction is calculated for 20 sec.

The pattern evolution is different between the two types of dislocations that mean the number of bounding atoms and the space-distribution influence the movement of the trails of dislocation.

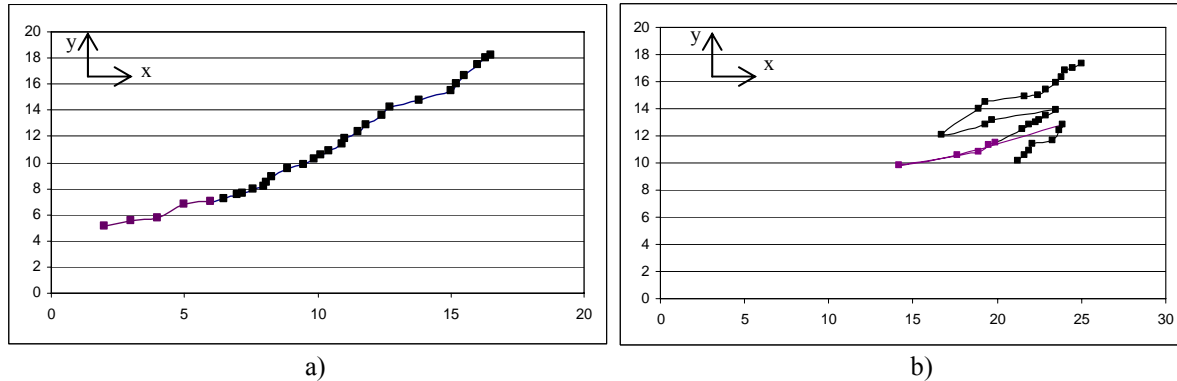a)   b)

Fig. 5 Prediction trajectories curves for a molecule from each dislocation pattern: a) for the trail of partial point defects, b) for the vacancy tubes.

5. CONCLUSIONS

In this paper we have employed the molecular dynamics simulations in order to examine the modelling oh two dislocation mechanisms, trail of partial point defects and the vacancy tubes, in a 2D crystal lattice during the diffusion process. For predicting the dislocation trajectories we used the ARMA model implemented in the MATLAB software.

The results underline the importance of considering the shape of the trajectories of these atoms during the process with the goal of predicting the geometrical loci. If the loci could be known, the macroscale simulation of the ECAP process can be improved by considering within the constitutive model of an internal variable tat describe such nanoscale phenomenon. The results obtained are the first approach for the multi-scale analysis of the ECAP process by finite element modelling.

By combining the patterns obtained by MD and ARMA model could be identified a complex analytical form that best fit the dislocation evolution.

Using ARMA prediction, the number of simulations MD could be diminished that lead to saving computing-time and computer-memory.

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