2005 ME Graduate Student Conference
April 9, 2005

MOLECULAR DYNAMICS SIMUATION STUDY OF GRAIN BOUNDARY MOBILITY IN NANOCRYSTALLINE Pd

Shengyu Wang
M.S. Candidate

Faculty Advisor: Dr. Dorel Moldovan

ABSTRACT

We present a new methodology for measuring the grain boundary mobility for curved boundaries using molecular-dynamics simulation of grain growth in a small, specifically tailored Pd nanocrystalline structure. In the model system, the boundaries move under the forces provided by their curvature and in the presence of the triple junctions. The study suggests that during the gain growth, the transfer of the free volume generated in the regions where grains are shrinking to those of growing grains is mediated by grain-boundary diffusion.

Grain growth is an important process, which takes place during annealing of polycrystalline materials and it is mediated by the migration of grain boundaries (GBs). As a consequence of GB migration the boundary area per unit volume is reduced and the mean grain size of grains increases with time [1,2]. The migration of a GB is driven by the presence of a gradient of the free energy across the boundary. Regardless of the detailed nature of the driving force, p, acting on the GBs, more often their migration resembles a continuum viscous movement with a velocity, v, given by an equation of the form:

$$v = mp$$

where m is the GB mobility. Moreover when the GB curvature is the only driving force, p can be written as

$$P = \gamma / R$$

where R is the curvature radius and γ the GB energy, which is a function of GB structure and misorientation.

MODEL AND SIMULATION METHODOLOGY

There has been a great interest and emphasis recently on developing simulation methodology capable of giving not only quantitative but a quantitative description of various types of microstructural evolution. Consequently, determining GB mobility becomes a key issue. However, measuring GB motilities is difficult both in experiments and in atomistic simulation studies mainly because one need to be able to measure simultaneously both the driving force and boundary velocity. Neither one on these properties characterizing the motion of a GB can be measured easily. Most of our current understanding of GB motion is obtained mainly from experiments and simulations on bicrystals. Moreover, given that it is easier to control the driving force and to quantify the motion of a planar boundary, most of these studies focus on planar GBs. The main difficulty in measuring GB mobility of a curved boundary is due to the difficulty in extracting the actual driving force acting on the boundary.

To achieve continuous growth and to minimize the number of different GBs present we focused our study on the model system presented in Fig. 1. Within the periodic-boundary-condition representation, the simulation model consists of two four-sided square grains and two eight-sided octagons. This octagon-square configuration, when replicated in x- and y-directions represents a polycrystal with a bimodal grain-size distribution. One can simplify further the simulation model by choosing the orientations of octagon grains with respect to that of the central grain such that the misorientations, and therefore both GB energy and mobility, have the same values for all four GBs of the central grain. This seems to be a convenient choice since having the same GB energy for all GBs of the central grain will also ensure that there would be no net cumulative torque acting one this grain and therefore no grain rotation, which, otherwise, is known to be a common phenomenon in nanocrystalline metals during grain growth (GG) [3]. Such a highly symmetric configuration can be achieved, for example, by considering a <001> textured columnar microstructure and by appropriate choice of the crystalline in-plane orientations of the four grains. If the orientations with respect to x-axis are: $\theta_1 = \theta_4 = 22.5^o$, $\theta_2 = 0^o$ and $\theta_3 = 45^o$ there will be only two different GBs in the system, i.e. $\gamma_{12} = \gamma_{13} = \gamma$. Accordingly, following the derivation of von Neumann-Mullins (vNM) [4], one can write the relation for the rate of area change of the central four-sided grain:

$$\frac{dA_4}{dt} = m\gamma[2\pi - 4\beta]$$

Which we derived by considering a general value for the dihedral angle β as given by $\beta = \arccos\left(\frac{\gamma_{23}^2 - \gamma_{12}^2 - \gamma_{13}^2}{2\gamma_{12}\gamma_{13}}\right)$ in which $\gamma_{12} = \gamma_{13} = \gamma$ and $\gamma_{12} = \gamma' \neq \gamma$. Obviously one can verify that if all GBs are assumed identical, $\beta = 2\pi/3$, then the equation $dA_4/dt = -2\pi\gamma m/3$ is derived.

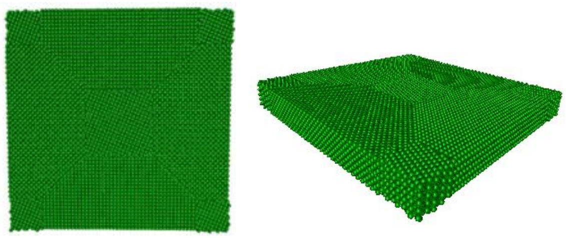

Fig. 1. The initial grain structure.

From the MD simulations γ can be estimated directly as the total excess energy of the system (compared to a perfect crystal at the same temperature) divided by the total GB length (justifiably assuming that γ is practically the same for all GBs present).

The dimensions of the octagonal and square grains were defined by the length of their sides, initially set equal to a = 10 nm. The thickness of the system in the texture direction was set equal to 10(002) planes, resulting in a total thickness of 5 lattice parameters $a_{0,}$ (a_0 = 0.389 nm at 0^oK [5] i.e., about 3 times the cut-off radius, R_c = 1.35 a_0, of the interatomic potential used [5]. With these dimensions, the square grains contain initially around 12,000 atoms each and the octagonal grains contain around 64,000 atoms each.

The simulations were performed at zero pressure and constant temperature (1200K) conditions by using a combined Parrinello-Rahman and Nose-Hoover constant pressure-constant temperature technique [6]. To quantify the GG process, a special procedure for automatic grain identification was developed. The procedure used common-neighbor-analysis (CNA) technique [7] to identify atoms in a crystalline state (fcc, for a perfect lattice, or hcp, in the case of stacking faults or twin boundaries). The atoms that have not been identified as in either an fcc or a hcp state are marked as disordered atoms.

Figure 2, shows the time evolution of the microstructure. One can clearly see the continuous shrinkage of the four sided grain. Since the thickness of the grain is constant, we can derive the area change with respect to time by calculating the number of atoms in the central grain. Knowing the rate of area change of the four sided grain we can extract the mobility of the GBs surrounding this grain which at 1200 K is m = 2.64 x 10^{-8} m^4/Js.

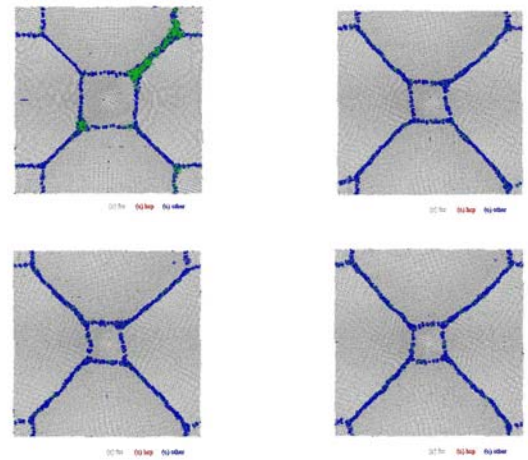

Fig. 2. Four snapshots of the simulated system consisting of two four-sided and two eight-sided grains after: 0.0024ns, 0.17ns, 0.35ns, and 0.51ns.

ACKNOWLEDGMENTS

This work was supported by the Louisiana Board of Regents.

REFERENCES

1. Humphreys F J, Hatherly, M, Recrystallization and Related Annealing Phenomena, Pergamon, Oxford,1995.
2. Atkinson, H.V., "Theories Of Normal Grain Growth In Pure Single Phase Systems" Acta Metal. 1988; 36, 469-491.
3. Haslam A J, Phillpot S R, Wolf D, Moldovan D, Gleiter H, "Mechanisms of Grain Growth in Nanocrystalline FCC Metals by Molecular-Dynamics Simulation," Mat. Sci. Eng. A, 2001; 318, 293-312.
4. Millins W W, "Two-Dimensional Motion of Idealized Grain Boundaries", J. App. Phys. 1956; 27, 900.
5. Foiles S M, Baskes M I, Daw M S. Phys. Rev. B. 1986; 33, 7983.
6. Melchinona S, Ciccotti G, Holian B L "Hoover NPT Dynamics for Systems Varying in Shape and Size," Molecular Physics 1993; 78, 533.
7. Clarke AS, Jonsson H, "Structural Changes Accompanying Densification of Random Hard-Sphere Packings," Phys. Rev. E 1993; 47, 3975-3984.