OPTIMIZATION OF FE[100] SYMMETRIC TILT GRAIN BOUNDARIES BY GENETIC ALGORITHM

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1. Introduction

Most of iron based construction materials are polycrystalline alloys. Two adjacent grains are connected by grain boundaries (GB). The geometry and chemistry of GB play important role in the macroscopic physical properties of polycrystalline materials. Understanding the influence of GB properties on material behaviour is essential for material engineering.

Direct observation and experimental study is limited by the lack of resolution of experimental techniques. Computer technology underwent significant development in last few decades. The development enables to solve a variety of complex problems numerically. Computer simulations are therefore effective complementary tool for grain boundary research these days. Important step, which is necessary for simulations of GB properties, is to find an optimized grain boundary structure. It is possible to use various optimization methods, like simulated annealing, molecular dynamics or gradient methods [2-5]. Genetic algorithm (GA) is global optimization method. GA optimization strategy is based on analogy with evolution and adopts its principles. Only the strongest and the best adapted individuals survive and raise offspring. The biggest advantage of GA is efficiency to overcome energy barriers and thus not get stuck in local extreme. Therefore it tends to be good candidate for GB structure optimization [6]. The aim of this work is to apply GA optimization on bcc-Fe symmetric tilt [100] grain boundaries. In particular Σ5(210), Σ5(310), Σ17(410) and Σ13(510).

This paper is arranged as follows. We will describe developed genetic algorithm in sec. 2. In sec. 3 we will present results and comparison with simulated annealing (SA) and in sec 4 we will conclude the results.

2. Methodology

Four supercells with grain boundaries Σ5(210), Σ5(310), Σ17(410) and Σ13(510) were prepared. Two ideal crystals were rotated in opposite direction by the same angle around x axis. The angles are listed in table 1. Exceeding atoms were deleted. Simulation supercell of atoms contains two grain boundaries: one in the middle of the cell and second is from geometrical reasons split between the top and bottom of the cell (fig.1). Embedded atom method (EAM) and periodical boundary conditions were used to compute the whole cluster energy. Only middle grain boundary was optimized by genetic algorithm. Outer boundary was excluded from optimization process. Geometry of computational cell is shown in fig.1.

Important optimization parameter is GB energy. The energy is defined as

$$E_{gb} = \frac{2E_1 - E - NE_c}{2s_x s_y} \tag{1}$$

where E_1 is energy of cluster with two geometric grain boundaries, E is energy of cluster with one optimized and one geometric grain boundary, N is total number of atoms in cluster, E_c is cohesive energy and s_x, s_y are dimensions of cluster in x and y direction. Summarization of simulation supercells parameters is in table 2. Results were obtained by Mendelev[1] potential. Lattice parameter was set up to optimal value given by chosen EAM potential.

Tab. 1. *Characteristic rotating angle for used grain boundaries.*

grain boundary	Σ5(210)	Σ5(310)	Σ17(410)	Σ13(510)
angle	26.565°	18.435°	14.036°	11.31°

Tab. 2. *Parameters used for simulation supercells. In particular: N - total number of atoms in a cell, s_x, s_y, s_z -dimensions of a cell in x, y, and z direction, N_{ga} - number of atoms inside GA-zone, s_{ga} - dimension of GA-zone in z direction.*

	N	s_x[Å]	s_y[Å]	s_z[Å]	N_{ga}	s_{ga}
Σ5(210)	128	5.71	6.384	40.858	62	$s_z/2$
Σ5(310)	168	5.71	9.028	37.92	84	$s_z/2$
Σ17(410)	224	5.71	11.771	38.777	54	$s_z/4$
Σ13(510)	280	5.71	14.558	39.193	68	$s_z/4$

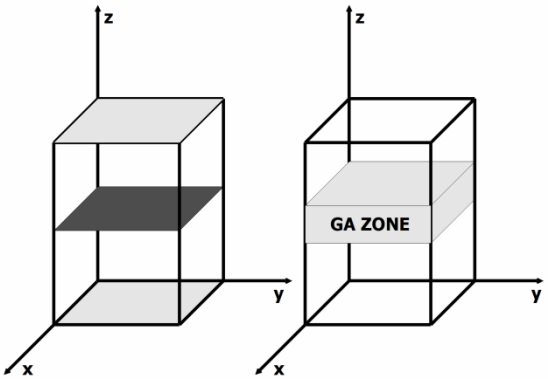

Fig.1: *Geometry of cluster with two grain boundaries. Left panel shows optimized boundary (the plane is in dark grey) and geometric boundary (the plane is in light grey). Right panel shows GA-zone, within which the genetic algorithm is applied.*

Simulation started with "zero-generation" initialization. Our "zero-generation" consists of 20 individuals, which means 20 different GB structures. Randomized positions of atoms within GA-zone were used to obtain the structures. Randomization was limited by radius 0.5Å. Each individual was evaluated by fitness function. Fitness function is equal to GB energy. Lower energy means better adapted individual. Selection, crossover and mutation are basic GA operators [7]. The operators are used to form next generation. In our GA, the next generation was formed as follows: Two best individuals are moved directly to the next generation. Eleven individuals are chosen by tournament selection. Seven structures are obtained via crossover. Two random parents from previous generation form offspring. Parents atoms are sorted according to x, y, or z coordinate. The half of atoms inherits the offspring from one parent and the second half from the second parent. Number of atoms inside GA-zone remains constant. It should be noted that mutation is motive force of GA. Mutation is applied on five random selected individuals from new population. Position of five random atoms is changed within given radius. The radius starts at 0.08Å and decreases to

80% after each 400 steps. In the case of constant energy in 400 consecutive generations, the population is regenerated. The evolution is finished after 50000 generations.

It could be note that it is better to use different method for technique validation than to compare results with other publications. A result of simulation highly depends on used EAM potential. Simulated annealing (SA) was used as a comparison method. Simulated annealing was applied in the same way as GA to ensure the same initial geometrical conditions. Only the atoms inside GA-zone were annealed. The temperature decreases from 350 K to 22 K in 200 steps. At each temperature 1000 optimization cycles were performed. The radius within which the atoms positions were randomized varies from $1x10^{-2}$ to $2.5x10^{-3}$ according to temperature in order to reach acceptance ratio 0.5. Linear or quadratic extrapolation was applied to obtain grain boundary energy at 0K.

3. Results

Grain boundary energies obtained by GA and SA are summarized in table 3. For grain boundaries Σ5(210), Σ5(310), Σ17(410) GA-optimization leads to same results as SA-optimization. Moreover, in the case of GA-optimization, we have physically structures with presented energy, but in case of SA-optimization we do not. The value corresponding with real configuration of atoms is the one at 22K. It is essential to have physical configuration of atoms, corresponding to the lowest grain boundary energy, for further research. Convergence in energy of grain boundaries as a function of temperature (SA) as well as a function of generations (GA) of various GB is shown in fig. 2.

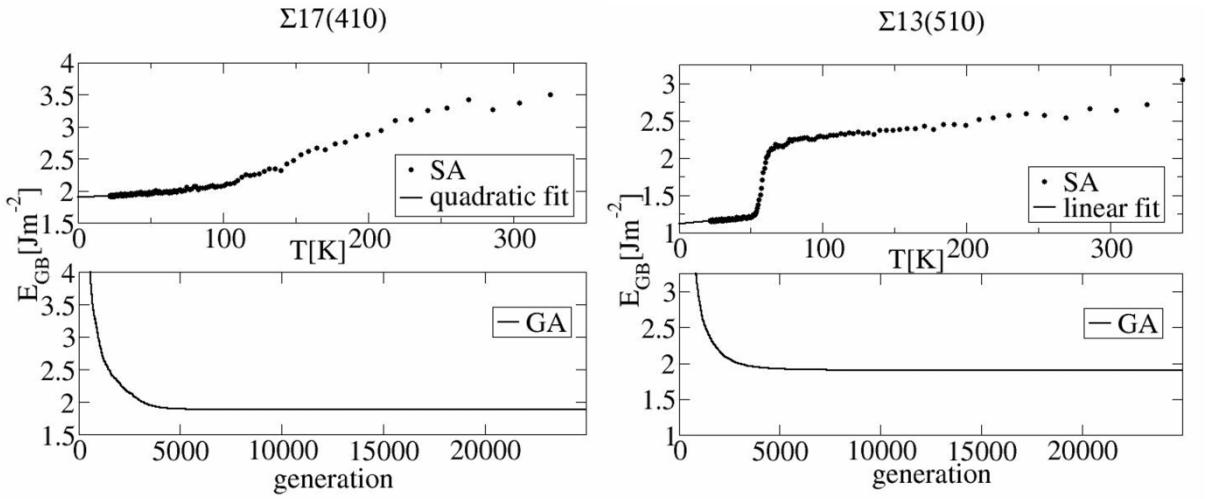

Fig.2: *Convergence in energy of grain boundaries as a function of temperature (SA) as well as a function of generations (GA). Type of the grain boundary is displayed at the top of the panel.*

A big mismatch between SA and GA in energy occurs in the case of Σ13(510). Grain boundary energy obtained by SA is much lower. As it is obvious from SA-convergence in fig. 2, SA-algorithm overcame potential barrier and jumped out from the local minimum around temperature 60 K, while GA could not escape from it. It is confusing because especially genetic algorithms are more efficient for their ability to overcome local extremes. The comparison with results presented by Terentyev [2] indicates, that both methods SA and GA could have got stuck in local extreme in the case of Σ17(410). Good candidate to solve this problem is parallel GA. Two parallel genetic algorithm schemes were tested: one hierarchic and one cyclic with central element. Each parallel scheme consists of 8 slightly modified GA described in previous section. Results are in table 3 referred as GA-par. Parallel

genetic algorithm improved Σ13(510) grain boundary energy and gave result closer to SA-value. Furthermore, it led to big reduction of Σ17(410) grain boundary energy, which no SA nor simple GA could achieve.

Tab. 3. *Comparison of grain boundary energies obtained by simulated annealing and genetic algorithm. Energy unit is* Jm^{-2}.

$E_{gb}[Jm^{-2}]$	SA (0K)	SA (22K)	GA	MD [2]	GA-par
Σ5(210)	1.509	1.572	1.507	1.392	-
Σ5(310)	1.046	1.115	1.045	0.985	-
Σ17(410)	1.898	1.923	1.886	1.12	1.263
Σ13(510)	1.12	1.16	1.9	1.843	1.441

4. Discussion

We verified that genetic algorithm is very effective tool for grain boundary structure optimization. Grain boundary structure optimization is problem with many degrees of freedom. There is a great possibility to get stuck in local extreme. Genetic algorithm is very flexible, consists of various set up parameters. On one hand, it is difficult to write algorithm suitable for concrete problem, on the other hand variability increases diversity and helps to overcome local extremes. Therefore is GA very good candidate for this optimization problem. We have compared genetic algorithm optimization with wide used simulated annealing optimization. Results show, that genetic algorithms are able to solve problem of grain boundaries structure optimization, moreover parallel genetic algorithms have high probability of overcoming local extremes leading to the lower energy structures.

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References:

[1] M. I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun and M. Asta, Phil. Mag. A, **83**, 3977-3994 (2003).
[2] D. Terentyev, X. He, *Open Report of Belgian Nuclear Research Centre*, SCK•CEN-BLG-1072, ISSN 1379-2407, (2010)
[3] S. von Alfthan, K. Kaski, A. P. Sutton, Phys. Rev. B, **76**, 245317 (2007)
[4] P. Ballo, J. Degmová, V. Slugeň, Phys. Rev. B, **72**, 064118 (2005)
[5] I. Dawson, P. D. Bristowe, M.-H. Lee, M. C. Payne, M. D. Segall, J. A. White, Phys. Rev. B, **54**, 19 (1996)
[6] J. Zhang, C. Z. Wang, K. M. Ho, Phys. Rew. B, **80**, 174102 (2009)
[7] M. Mitchell: An Introduction to Genetic Algorithms, A Bradford Book The MIT Press, Cambridge, Massachusetts • London, England (1999)