GENETIC ALGORITHM: GRAIN BOUNDARY SLIDING AND MIGRATION

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1. Introduction

Genetic algorithm (GA) is an optimization method derived from evolution principle in nature, where the weak individuals die and the strong individuals survive and raise offspring. It belongs to the group of global optimization methods [1-3]. The optimization problem is coded into genes and chromosomes, which are usually strings with numerical or symbolic values. The genes and chromosomes are modified during the evolution, by the crossover or mutation operators, in order to find the best parameters of the optimized system. The level of optimization is described by fitness function. The aim of GA is to minimize or maximize the fitness function. One of the biggest advantages of the GA is its flexibility, hence it can be used to solve every multi-dimensional problem, which can be encoded to chromosome and evaluated via specific fitness function. Moreover the GA can be parallelized very well. It should be emphasized, that the aim of the parallelization is not only to accelerate the computer simulation but also to obtain qualitative better results [4]. This fact connected with the huge development of computer power during last decades makes the GA method very attractive and valuable.

Fitting the potentials [5,6] and predicting the structures [7-9] are the main applications of GA in solid state physics. One of the challenging topics in solid states is to understand the process of grain boundary sliding and migration on atomic level [10-13]. The essential part of this study is structure optimization, which is multi-dimensional problem with unknown barriers between local extremes. There are two main methods used for the GB sliding and migration examination, namely: molecular dynamics (MD) [12,13] and simulated annealing (SA) [10,11]. Our aim is to investigate the possibility of the application of parallel GA on this problem. We will use simulated annealing as a comparison method. We will investigate the GB sliding and migration processes of two FCC metals, copper and aluminium.

The paper is organized as follows: The parallel genetic algorithm method used for GB sliding simulation and the initial atomic configurations are described in the Sec. 2, Sec. 3 contains the comparison of the results obtained by simulated annealing and genetic algorithm and finally the results are concluded and discussed in Sec. 4.

2. Methodology

We developed genetic algorithm combined with simulated annealing in order to investigate GB sliding and migration. The simulated annealing is embedded into the GA scheme like special mutation process. We encoded the problem of GB structure optimization to GA terminology as follows: (i) a gene is the position of an atom within the simulation supercell, (ii) a chromosome contains positions of all atoms, except the six fixed atoms in the middle of the upper grain and six fixed atoms in the middle of the lower grain and (iii) a population is a group of 20 supercells (individuals) that have different structures. The fitness function is the total energy of the supercell. For the energy computation, we adopted the

Embedded-atom Method (EAM) [14] and periodical boundary conditions. The used potentials are listed in Table 1.

The new generation is formed as follows: (i) two best individuals are moved directly to the next generation – elitism, (ii) eight offspring are created via single point crossover and (iii) ten individuals are chosen by a tournament selection, annealed and then sent to the next generation. Annealed means that, positions of all atoms are changed within a given radius R_{SA}. The R_{SA} radius is linearly decreasing from 10^{-3} to 10^{-4} nm during the evolution. When the new generation is formed, the mutation is applied on five random individuals from the new generation. Position of ten random atoms is changed within a given radius R_{mut}. After each 1000 generations the R_{mut} radius decreases to 85%. The zero generation contains the initial geometrical structure, derived from coincidence site lattice (CSL) theory, and nineteen structures derived from the initial geometrical structure by randomizing the positions of all atoms (except the fixed ones) within the radius 2.5×10^{-2} nm. The parameters of the initial supercells are in Tab. 1

Tab. 1. *The parameters of the simulation supercells and list of EAM-potentials, which were used in our simulation*

Element	EAM	GB type	Size-x[nm]	Size-y[nm]	Size-z[nm]	Atoms
Cu	Ref. [15]	Σ5(210) - tilt	0.3615	0.8083	5.1734	128
Al	Ref. [16]	Σ5(210) - tilt	0.4050	0.9056	5.7959	128

Our parallel GA adopts multistage hierarchic scheme. The scheme consists of three stages, referred as stage 0, stage 1 and stage 2. Each stage has N^S root populations and N^{S+1} slave populations, where S is the stage number. Each root has its own N slaves. The root population of the stage 0 will be referred as main root population. When the new generation is formed, the slave populations send their best individuals to root populations. Root populations change their N worst individuals for the newcomers. The migration of the individuals starts on the stage 0, then continues to stage 1 and finishes on the stage 2. The logical acceptable range of parameter N is from 2 to 10 populations. If N is lower than 2, basic scheme of the parallel GA is broken. In the case of N > 10, more than half of the population is replaced with the newcomers, and the individuality of each population is questionable. For the simulation it is necessary to have available P processor units

$$P = \sum_{i=0}^{3} N^i \tag{1}$$

The N = 3, was used for the simulation, which implies the use of 40 processors.

All populations have the same GA scheme, described above, except these modifications: (i) each population has different seed for random generator derived from the seed of main root population, (ii) slave populations of the stage 2 have the R_{mut} parameter set to 5×10^{-3} nm and the others to 2×10^{-3} nm and (iii) the best individual of the main root population is excluded from the mutation process in order to achieve monotonic convergence in energy. If the energy of the population get stuck on the same value in 200 consecutive generations a re-initialization process starts. The process differs according to hierarchy of the population. Main root population and stage 1 root population: The coordinates of twelve random atoms are changed within the radius 6.25×10^{-3} nm to five random individuals. The best individual is excluded from this process. Stage 2 root populations: New population is generated from the best individual by randomizing the positions of atoms within the radius 1.25×10^{-2} nm. Stage 2 slave populations: New population is generated from the best individual by randomizing the positions of atoms within the radius 2.5×10^{-2} nm.

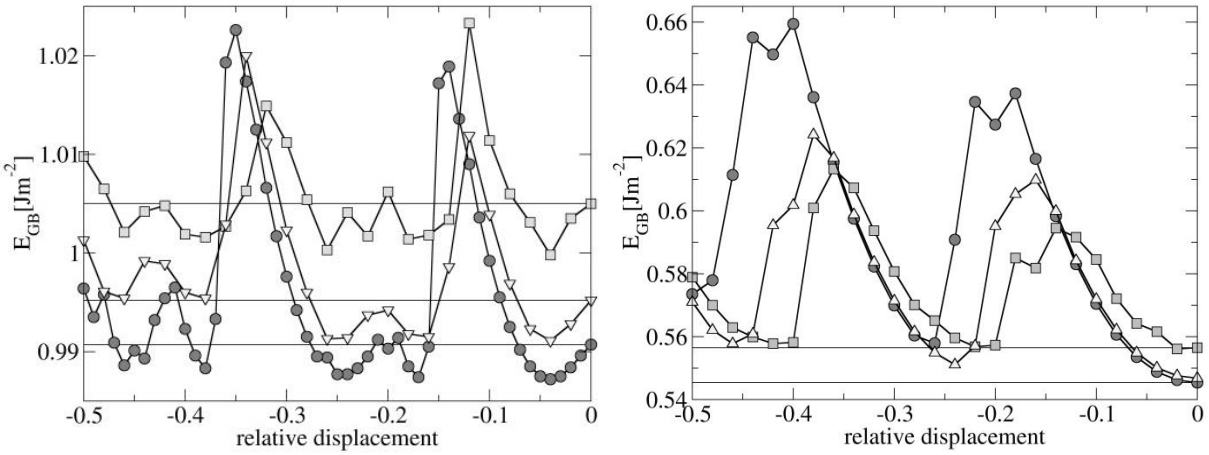
The evolution process ends after 20000 generations. The result of the optimization process is the structure and energy of the best individual of the main root population. The program is written in FORTRAN90 and data flow between populations is provided by Open MPI.

Sliding process is realized by splitting the atoms into two groups: stable and mobile. Each group has the same number of atoms. After the end of evolution the shifting process is applied on the best individual of the main root population. This individual serves as an initial geometric configuration for all populations. The shifting process consists of 26 steps, from 0 to 50% of the period in <120> direction.

The two SA simulations were also performed. One called 0K-annealing, where only the configurations with lower energies were accepted. The initial temperature of the second one (350K-SA) was set up to 350K and the system was cooled to 7.6K by stepwise-exponential decrease of temperature. The amplitude of the atomic displacement varies so that the acceptance ratio remains constant – 50%. The annealing mutation radius R_{SA} of the GA was derived from the amplitude of the atomic displacement used in 350K-SA.

3. Results

The variation of the GB energy during the sliding process of copper Σ5(210) and aluminium Σ5(210) tilt grain boundaries obtained by SA and GA is shown in Figure 1. The GB energy values of the not-shifted grain boundaries and the energy barriers are summarized in Tables 2 and 3. The Tables contain two energy barriers, one located around the 15% displacement referred as 1st barrier and one located around the 35% displacement referred as 2nd barrier.



(a) (b)

Fig.1: *The variation of the GB energy during the sliding of the Σ5(210) tilt GB in copper (a) and aluminium (b). The sliding distance is described relatively to a_{CSL}, of the CSL cell along <120> direction. The circles, squares and triangles correspond to the 0K-SA, 350K-SA and GA simulation, respectively.*

Tab. 2. *The not-shifted grain boundary energy of copper and the maximum energy barrier of copper obtained by simulated annealing and genetic algorithm.*

Cu	SA – 0K	SA – 350K	GA
$(E_{GB})_0$ [Jm^{-2}]	0.9907	1.0050	0.9952
$(\Delta E_{GB})_{max}$ [mJm^{-2}]	28.2 / 31.9 *	18.3 / 10 *	16.7 / 24.8 *

* 1st barrier / 2 nd barrier – specified in the text (Sec. 3)

Tab. 3. *The not-shifted grain boundary energy of aluminum and the maximum energy barrier of aluminum obtained by simulated annealing and genetic algorithm.*

Al	SA – 0K	SA – 350K	GA
$(E_{GB})_0$ [Jm^{-2}]	0.5454	0.5565	0.5468
$(\Delta E_{GB})_{max}$ [mJm^{-2}]	91.9 / 114 *	38 / 56.8 *	63 / 77.4 *

* 1st barrier / 2 nd barrier– specified in the text (Sec. 3)

4. Discussion

It has been found in our simulation that the GA approach leads to reduced energy barriers like SA with elevated temperature. The 350K annealing temperature reduces the barriers by 50% and GA by 30%. However, GA is able to achieve lower GB energies, close to those obtained by zero temperature simulation. The results indicate that, atomic displacements used during SA simulation are valuable input parameter for mutation process during the evolution. All three approaches showed that the process of overcoming the energy barriers is connected with the GB migration and that the migration direction is given by the sliding direction. The connection between the temperature and mutation processes during the evolution is the subject of the further research. Our experiences show, that the parallelization of GA can reduce the probability of the results being affected by choice of the random generator seed. Despite of the higher computational cost of the parallel GA approach, the results indicates that it is worth to use. The energy increase with the higher displacement is connected with the migration of the grain boundary towards the fixed atoms; hence it is reasonable to split shifting process into more separate simulations.

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