

A genetic algorithm for generating grain boundaries

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Abstract.

Generation of realistic Grain Boundaries (GBs) in bicrystals for atomistic simulations requires a search in a multidimensional space for a configuration with the atoms at the GB organized in such a way that the energy of the whole system is minimized. This paper presents a genetic algorithm that allows to find low energy GB configurations by optimizing three main criteria: the local arrangement of the atoms, the relative translation between the two grains that compose the GB and an overall expansion/contraction of the system. It is designed to make a wider and more effective search through the energy landscape compared to other traditional methods, giving access to more configurations and increasing the possibility of finding the global minimum in energy.

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1. Introduction

A Grain Boundary (GB) can be simply defined as the region where two adjacent crystals with different crystallographic orientation meet. Apart from very few exceptions, GBs are always present in crystalline materials and have an important influence on their behavior.

In order to uniquely define a planar GB between two grains three groups of data are needed:

- The misorientation between two adjacent grains, which can be described using five Degrees of Freedom (DoF's) [1–3]. For example, in the *interface-plane* scheme [1] this misorientation is expressed in the following way:

$$\{(hkl)_1, (hkl)_2, \varphi\} \quad (1)$$

where $(hkl)_1$ and $(hkl)_2$ indicate the sets of lattice planes in each grain which are parallel to the GB and φ is the relative rotation of the two crystals around the

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axis normal to the GB. Note that since $(hkl)_1$ (and $(hkl)_2$) can be expressed in a normalized form, only two DoFs are used to describe the orientation of each crystal. Similarly, in the *misorientation* scheme [1], which contains the same information as the previous one, the crystal misorientation is expressed as:

$$\{\theta, \langle UVW \rangle, (hkl)_1\} \quad (2)$$

where θ and $\langle UVW \rangle$ are the angle and axis of misorientation, respectively, around which one of the crystals is rotated with respect to the other.

- The relative positions of the two crystals, which are defined by three more DoF's (T_x, T_y, T_z) that represent rigid translations of one grain with respect to the other starting from a given reference position.
- The local arrangement of the atoms, which refers to the way in which atoms are organized in the GB plane after relaxation.

For a given set of misorientation parameters (5 DoF's) there can be an infinite number of configurations with different relative positions (3 DoF's) and resulting local organization of the atoms near the GB. Each of these atomic configurations could potentially have a different energy and it is generally assumed [4] that real GBs have the tendency to form in such a way that the energy of the system is minimized. As a result, efficient search strategies in atomistic modeling such as Molecular Dynamics (MD) are needed to explore these configurations in a multidimensional parameter space so as to generate an accurate GB structure in a reasonable amount of time. There exist various algorithms used to generate such initial conditions for MD and they can be roughly classified into four categories:

- The first category is composed of the methods that use only geometrical tools to generate a GB. In some cases, a GB is built by overlaying two crystals with a specified rotation angle and then deleting all excess and overlapping atoms [5–7]. In some other cases the GB is formed in such a way that the atoms coincide with a given theoretical model, like the Coincident Site Lattice (CSL) [8] or the Structural Unit Model (SUM) [9]. Additionally, in some other approaches, relaxation of the system using some energy minimization method is performed [10]. These methods are convenient because no search through energy space has to be done; nonetheless they have the drawback that they are only suitable for a limited number of very simple GBs and that the manual positioning of the atoms near the GB plane can be tedious.
- The second category comprises methods that start with two misoriented crystal slabs separated by a region filled with randomly placed atoms emulating the liquid phase. This system is subsequently cooled down using MD until it solidifies and the GB is formed [11]. The idea of these methods is to mimic the natural process of solidification of a GB and aims to obtain a real structure. However, there is an aspect inherent to the MD method that can cause the relaxation of the system to get trapped in local minima: the short time scales that can be reached in a simulation

enforce the use of extremely high cooling rates [12]. In addition, there are also some parameters in the initial configuration (number, position and velocities of the atoms in the “liquid region”) and in the simulation set up (pressure, cooling rate, time-step) that can lead to different results in the final arrangement (and hence energy) of the atoms in the system.

A more elaborate version of this type of method can be found in reference [13], in which two crystals are put together with a given misorientation and several different configurations are generated by removing atoms near the GB. The region containing the GB is then melted, while the rest of the atoms remain attached to their initial positions. Finally, all the atoms are released and the system is successively cooled down and its energy is minimized. This method has been used to find ordered structures of silicon twist GBs.

- The third category contains methods that perform a “brute force” search for the lowest energy GB within the solution space by generating a large number of initial configurations and selecting the one with the lowest energy [4]. Given two crystals with different misorientations, a set of initial configurations is generated by varying their relative positions (T_x, T_y, T_z) and eventually removing overlapping atoms, in the case that the chosen value for their separation demands it. Thereafter a relaxation of each system is performed using a minimization routine. This method is widely used for the generation of GB in single-element and relatively simple systems, and it has proven able to find low energy configurations which coincide with predictions from the CSL or SUM theories. A drawback of this method is that the number of initial configurations can go up to several tens of thousands [4, 14], depending on the periodicity of the GB, making it computationally expensive and time consuming; also, regardless of the number of initial configurations, there are no assurances that the entire solution space is sampled.
- The fourth and last category is constituted by methods that perform a “smart” search within the energy landscape using heuristic algorithms. Despite the fact that these types of algorithms have been widely used to solve optimization/minimization problems, their application to GB construction is relatively new. To our knowledge only two algorithms have been proposed [15–17], and the obtained results are very promising. The first application of these types of methods [16] uses a Genetic Algorithm (GA) to perform a global structure optimization aimed at the prediction of GB structures in silicon. The second application uses a similar GA to predict the equilibrium structure of interfaces in multicomponent materials [15, 17].

The algorithm presented in this paper belongs to the fourth category as it aims to perform a “smart” search to find low energy configurations of GBs. Here, two new extensions to the earlier used GA are introduced: the relative rigid translations and the expansions/contractions that can occur during the formation of a GB are explicitly included in the minimization procedure (Figures 1b and 1c). This allows the algorithm to have full control over the volume expansion and the GB translations, two parameters

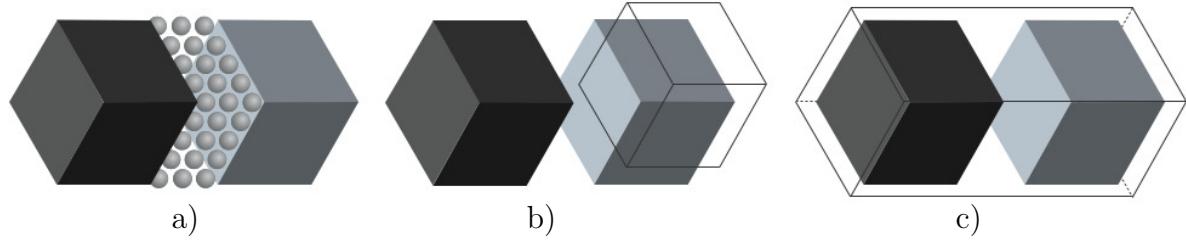


Figure 1. Criteria included in the function to minimize. a)Position of the atoms. b)Relative rigid translations. c)Scaling of the system.

that influence the GB energy. Additionally, a new “reproduction” method for the generation of new candidate solutions –called individuals– is introduced (Section 3.4).

It is important to point out that none of these methods can guarantee that the generated configuration corresponds to *the* global minimum in energy.

2. Energy function

When two mutually misoriented crystals are put together there are a number of parameters, apart from the five macroscopical DoFs, that will influence the geometry and, hence, the energy of the formed interface. The objective of the GA presented here is to find the optimal combination of these parameters that will produce the system with the lowest GB energy (E_{GB}).

The energy to minimize is a function of the following parameters, which are graphically represented in Figure 1:

- **The positions \vec{r} of each of the N atoms in the GB region** [$N \times 3$ parameters]
This corresponds to an array containing the x , y and z , coordinates of all the atoms in the GB region. Their coordinates can be modified by the algorithm.
- **The rigid translations \vec{T} between the two crystals** [3 parameters]
During the formation process of a GB one of the grains can rigidly change its position with respect to the other. In the algorithm this is accounted for by a vector with three components, two of them corresponding to displacements along the GB plane and one to displacements perpendicular to it.
- **The scaling \vec{S} of the system** [3 parameters]
During the process of relaxation, a system containing a GB can expand or contract to evolve towards a more favorable energy state. The algorithm takes this into account by optimizing the contraction/expansion of the system along the \vec{x} , \vec{y} and \vec{z} directions.

There is, thus, the following function to minimize:

$$E_{GB} = f(\vec{r}, \vec{T}, \vec{S}) \quad (3)$$

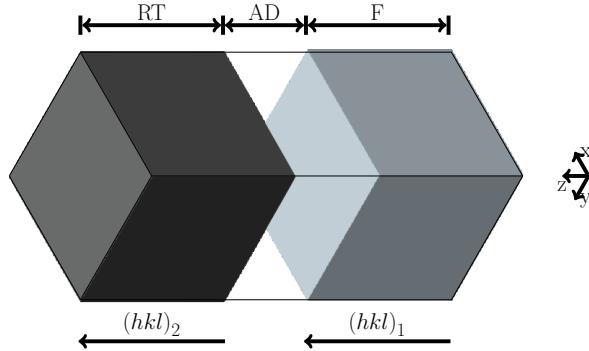


Figure 2. Regions of the grain boundary system. AD is the atomic displacement region; RT the rigid translation region and F the fixed region. $(hkl)_1$ and $(hkl)_2$ indicate the sets of lattice planes in each grain which are parallel to the grain boundary.

Earlier simulations in the literature [15] have shown the importance of changing the number of atoms to access different thermodynamic states; the algorithm presented here can incorporate this feature by allowing for the variation of the number of atoms in the GB region, however, different runs of the algorithm need to be performed.

3. General description of the genetic algorithm

GAs belong to a class of stochastic search methods that work iteratively on a population of candidate solutions to a problem (called individuals), performing a search guided by a fitness function [18]. In the present case this function determines the GB energy (equation 3). In particular the lower the energy, and therefore the higher the fitness, the more the properties (genes) of a solution are likely to be propagated to the next iterations. This Darwinian principle is emulated with specific reproduction, mutation and survival operators, which are applied with stochastic mechanisms that make the GA explore solutions with increasing fitness (lower GB energy).

The implementation of GAs to the GB generation problem offers great advantages, as it does not rely on specific a priori hypotheses (e.g. continuity and convexity), ensuring a wider mapping of the solution multidimensional solution landscape.

3.1. System set-up

To generate the initial system two crystals with the desired relative misorientation are inserted into a molecular dynamics simulation box (see Figure 2), leaving an empty region between them (along \vec{z}) where the interface is going to be located. Periodic boundary conditions are imposed along the GB plane directions (\vec{x} , \vec{y}); perpendicular to it (\vec{z}) periodicity is not enforced so that the bicrystal is bounded by two free surfaces.

This initial system can be divided into three regions: the atomic displacement region (AD), the rigid translation region (RT) and the fixed region (F). The AD region is delimited by the initially empty space between the two crystals. In this unfilled space

atoms are inserted at the start and subsequently modified by the evolutionary algorithm; their positions can evolve individually and as a result of expansions/contractions of the system. The *RT* region contains the atoms of the initial system located towards the positive \vec{z} direction with the *AD* region as reference. The atoms in this region can change their position as a rigid body and due to expansions/contractions of the system. Finally, the *F* region contains the remaining atoms which can only scale their positions when the system contracts/expands.

3.2. Generation of the initial population

Within the GA jargon, a population can be defined as a group of individuals, and an individual as a possible solution to a given problem. In this particular case, every individual is characterized by the three aforementioned parameters, namely \vec{r} , \vec{T} and \vec{S} . As an example, for $N = 250$ atoms in the GB, they comprise 756 adjustable parameter values.

The initial coordinates of the *AD* atoms of all individuals are randomly generated. For these first “solutions”, it is required that the distance between any two atoms is greater than a given value. It is also imposed that all the atoms have to be inside the *AD* region. These requirements keep the atomic positions of the atoms of the initial solutions away from physically unrealistic situations.

In the same way, values for the initial rigid translations and scaling of the system are randomly assigned to each individual.

3.3. Evaluation of the population (fitness function)

Since the final goal of this algorithm is to minimize an energy function, populations are evaluated according to the energy of their individuals. In this work the energy of each individual is calculated as the total energy of the system (including all three regions) via use of an embedded atom method (EAM) [19] potential for aluminum [21] implemented in the MD software CAMELION [20]. It is important to note that the choice of this potential for the calculation of the energy is arbitrary and any other sensible method could be employed.

Once all the individuals of a population are evaluated, they are ranked according to their energy and the best-adapted energy (i.e. the lowest) is used to check for convergence, as will be explained in the following sections.

3.4. Reproduction

The main idea of reproduction is to produce a new population from the individuals of the current, i.e. latest, population. This new population will consist of a new generation of individuals. For this reproduction stage individuals are arranged in couples in such a way that the number of couples corresponds to the number of individuals of the previous population. Note that a given individual can be assigned to more than one couple. A

higher probability for reproduction is assigned to individuals with lower energy so that they reproduce more often than the ones with higher energy. This is done to accelerate convergence by saving the properties (genes) of the best individuals through generations.

Unlike previous research in the literature [15–17] where new individuals (offsprings) are generated by interchanging atoms from a pair of individuals (parents), in the present work to form an offspring the values of the rigid translation, the scaling of the system and the coordinates of each atom from the parents are averaged and assigned to the offspring. For example, if the coordinates of atom i of two parents (father f , mother m) forming a couple are \vec{r}_{fi} and \vec{r}_{mi} , the position of atom i of the offspring (o) will be given by $\vec{r}_{oi} = (\vec{r}_{fi} + \vec{r}_{mi}) / 2$.

3.5. Mutation

The main purpose of the mutation stage is to prevent the algorithm from getting trapped in local minima and to allow it to explore a wider region of the energy landscape. Mutations are random perturbations that are applied to randomly selected individuals of the last generated population. Similarly to reproduction, mutations affect all the variables of an individual: the coordinates of the atoms, the values of the rigid translations and the values of the system scaling. In all cases, mutations simply consist of the addition of random values to the desired properties. For instance, if an individual (offspring o) is chosen to mutate and the coordinates of its atom i are defined by the vector \vec{r}_{oi} , the coordinates of this same atom after mutation (\vec{r}_{oim}) are calculated as $\vec{r}_{oim} = \vec{r}_{oi} + \vec{R}_i$, where \vec{R}_i is a random vector whose length is calculated independently in each cartesian direction.

3.6. Static relaxation

After every new generation of solutions is produced one final step is carried out: the energy of each individual –having still unrelaxed atomic coordinates– is minimized using the relaxation algorithm proposed in reference [22] while keeping the volume fixed. The coordinates of each offspring are then updated and the algorithm returns to the “Evaluation of the population” step (Section 3.3).

This process iterates until energy convergence is reached. Convergence is measured using the individual that has the lowest energy after each iteration.

3.7. Input parameters

The specific operation of a GA is controlled by certain input parameters. In virtually all cases different input parameters of a GA will produce different results. Therefore, to assure and accelerate convergence, different values for these input parameters have to be tried out. In the present work an iterative procedure was developed to evaluate the results of different combinations of the GA parameters. For the problem of finding

low energy configurations of GB, the algorithm was designed to work with the following concrete input parameters:

- **Size of the population:** Number of individuals (configurations) generated in each generation (step).
- **Mutation rate of the population:** Percentage of individuals selected to mutate in each generation.
- **Mutation rate of the atoms:** Percentage of atoms of the individual that is selected to mutate whose positions are modified (mutated).
- **Survival rate:** Percentage of individuals that are kept from one generation to the next without being modified. These individuals are selected on an energy basis, meaning that individuals with lower energy have a bigger probability of being transferred to following generation.
- **Maximum distance for mutation:** Maximum distance that an atom can be displaced during the mutation stage. This same parameter is used for the scaling \vec{S} and the translation \vec{T} .

4. Tuning of the algorithm

The tuning of the algorithm involves the sampling of several value combinations of the previously mentioned input parameters in a system for which the minimum energy configuration is well known: a twin GB. Once the effective parameters for the algorithm are found they can be used for more complicated systems, as will be shown in Section 5.

The input parameters are sampled as follows: the size of the population is kept constant at 100 individuals; there are five allowed values for the mutation rates of the population and of the atoms, which are varied from 10% to 90% with increments of 20%; four allowed values for the survival rate, varied from 0% to 15% with increments of 5%, and seven allowed values for the maximum distance for mutation: 0.03, 0.1, 0.3, 0.5, 1.3, 2.0 and 2.7 Å. Altogether these constitute 700 possible combinations for the input parameters. Note that since all the systems have the same number of atoms and their free surfaces are identical, measuring the energy per atom of the whole system reflects the relative value of the GB energy. Each trial optimization runs for 50 iterations. This number of iterations was found to be a good compromise between computational time and convergence. Note that since all the systems have the same number of atoms and their free surfaces are identical, measuring the energy per atom of the whole system reflects the relative value of the GB energy.

To set up the problem two grains with orientations defined by the interface plane scheme as $\{(4\bar{3}0), (\bar{4}30), 0\}$ (twin GB) are put in a simulation box separated by a distance of approximately 8 Å, as seen in Figure 3a. Note that even though the choice of this separation is rather arbitrary, the system will evolve to find the value for this parameter that will minimize the energy. Each crystal has 444 atoms. The initial dimensions of the system are $22.72 \times 20.94 \times 58.56$ Å³ in the \vec{x} , \vec{y} and, \vec{z} directions, respectively. These

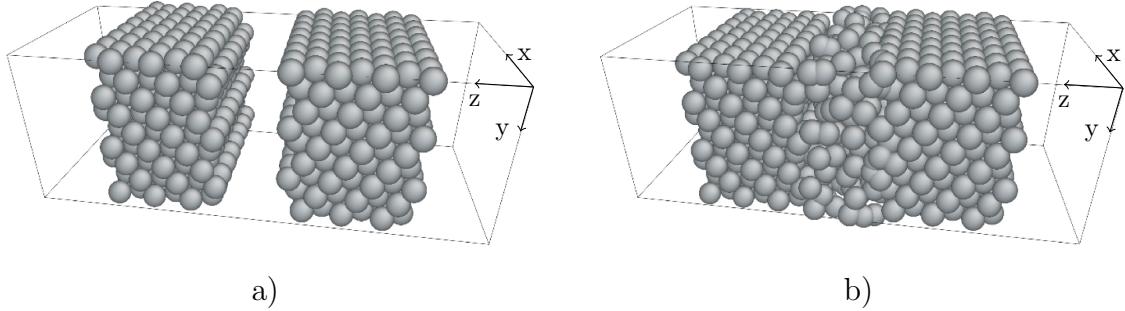


Figure 3. a) Initial position of the crystals for the case of a $\{(\bar{4}30), (\bar{4}30), 0\}$ twin grain boundary. b) Example of an individual of the first generation [23].

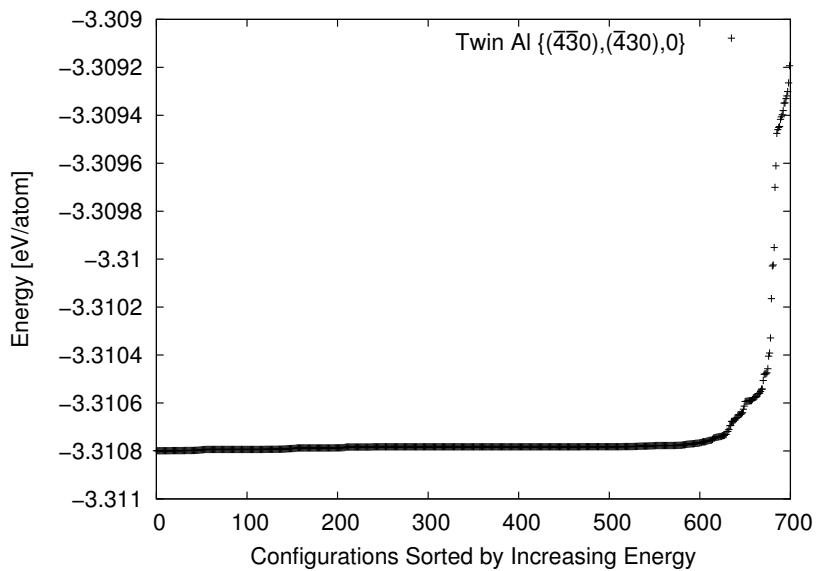


Figure 4. Obtained minimum energy for different sets of parameters used by the genetic algorithm. The results are sorted by increasing energy. Results for a $\{(4\bar{3}0), (\bar{4}30), 0\}$ twin grain boundary.

dimensions are chosen in such a way that the intended periodicity along \vec{x} and \vec{y} can be imposed. Finally, each individual of the first population is generated by randomly inserting 240 atoms without overlap in the *AD* region (see Figure 3b for a typical first individual).

A plot with the energy per atom for the best final individual of each of the combinations of input parameters is shown in Figure 4. The results show that the algorithm performs very well for this problem. The minimum energy found by the

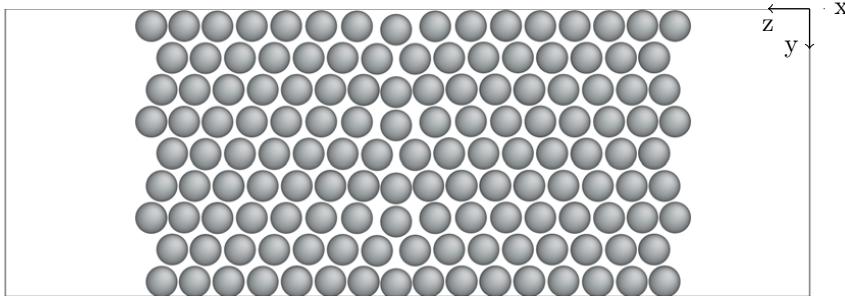


Figure 5. Perfect twin in aluminum obtained after the minimization procedure.

algorithm is indeed equal to the energy of a perfect twin GB in Al, which, in this case, was calculated based on its known structure and using the same interatomic potential as the one used for the GA. From the 700 combinations of parameters that were tried, around 600 were able to converge to the geometry of a perfect twin. A visual inspection of the obtained system confirms that the geometry corresponds to that of a perfect twin (Figure 5).

The following set of parameter values are selected as being optimum for this application of the algorithm. This set is arbitrarily selected from the many sets of parameter combinations that converge to the correct energy:

- Size of the population: 100 individuals.
- Mutation rate of the population: 70%.
- Mutation rate of the atoms: 10%.
- Survival rate: 15%.
- Maximum distance for mutation: 1.342 Å.

Figure 6 shows the convergence behavior of the energy for the selected parameters. Note that only ten generations were needed to reach convergence.

5. Application of the algorithm to an unknown grain boundary

To obtain a minimum energy configuration for a different GB, i.e. $\left\{ \left(24\bar{1}\right), \left(\bar{4}2\bar{1}\right), 0 \right\}$, the same procedure was followed as the one for the twin GB. First, two crystals separated by a distance of approximately 8 Å and misoriented in such a way that the desired symmetric tilt GB is obtained are inserted into a simulation cell (Figure 7) of dimensions $19.71 \times 30.13 \times 53.31$ Å³. Each crystal is composed of 504 atoms and each individual of the first population is generated with 272 atoms in the *AD* region.

Since an effective set of input parameters was already selected in the previous section there is no need to repeat that search. Five independent runs of the GA are performed with the selected parameters in order to monitor the effects of the statistical choices made by the algorithm.

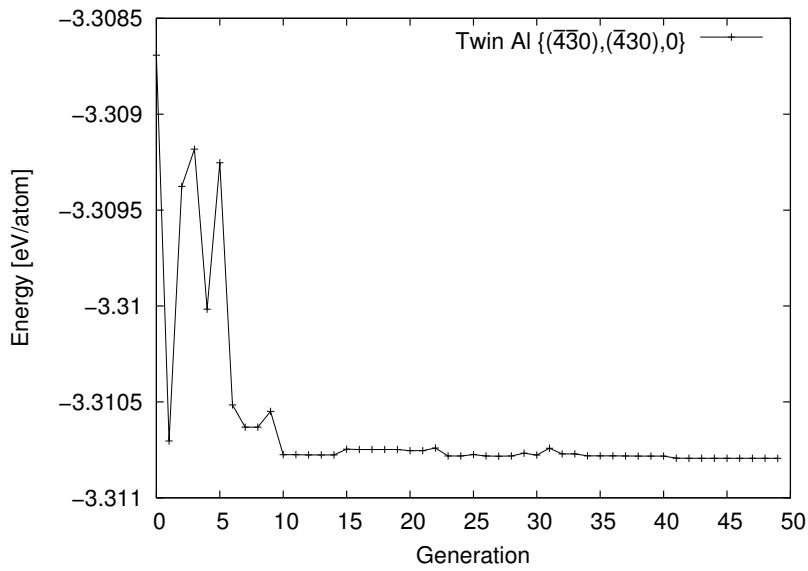


Figure 6. Convergence behavior of the energy, shown for one of the almost 600 combination of parameters of the genetic algorithm that successfully converges to the minimum energy (Figure 4). Results for the $\{(\bar{4}30), (\bar{4}30), 0\}$ twin grain boundary.

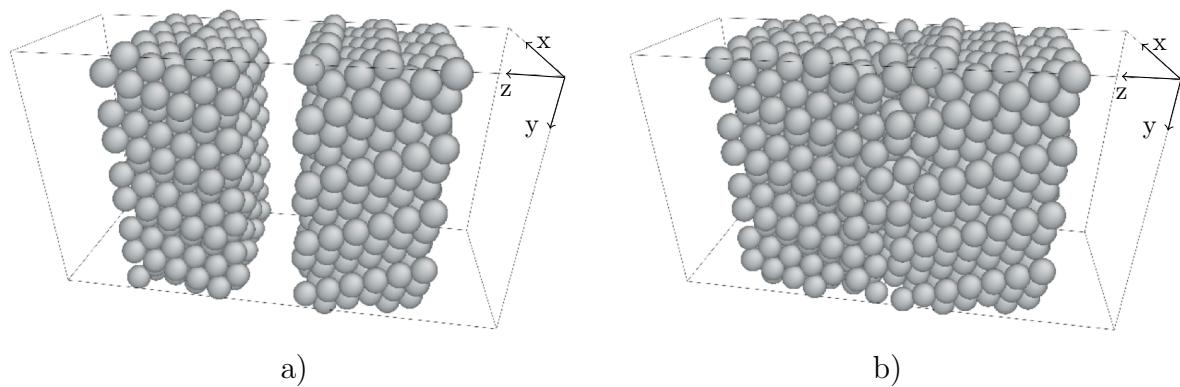


Figure 7. a) Initial position of the crystals for the case of a $\{(24\bar{1}), (\bar{4}2\bar{1}), 0\}$ tilt grain boundary. b) Example of an individual of the first generation.

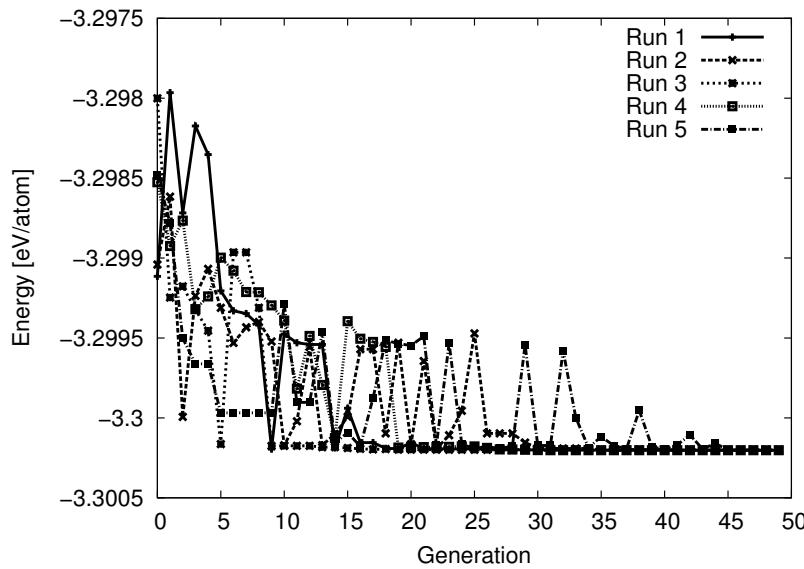


Figure 8. Convergence behavior of the energy presented for the $\{(24\bar{1}), (\bar{4}2\bar{1}), 0\}$ tilt grain boundary. Five independent runs are performed for the selected input parameters. All of them converge to the same energy.

The convergence behavior of the five runs is presented in Figure 8. It can be seen that they all converge to the same energy. This strongly suggests that the obtained value is indeed the global minimum energy for the selected GB. Nevertheless, it is still not possible (by this or any other method) to guarantee a configuration with lower energy does not exist.

In order to check the obtained result the “brute force” method, as implemented in reference [14], was applied to the same GB. The structure of the GBs obtained by the two methods is the same. This structure is shown in detail in Figure 9.

Apart from the fact that GAs are designed to perform a more thorough search through the energy landscape compared to conventional algorithms, the number of iterations required to achieve convergence is usually smaller. For both the “brute force” method and the GA the most time consuming part is that of the relaxation that is done after each configuration is generated. Here is also important to note that the time consumed by the GA itself is negligible compared to the times needed for relaxation.

In the present case, for the $\{(24\bar{1}), (\bar{4}2\bar{1}), 0\}$ tilt GB, the GA converges in approximately 10 to 50 iterations. Although the GBs and materials considered are not the same as in earlier reports [15–17], the GA presented here shows a major improvement in the number of iterations needed for convergence. In the earlier works [15–17], hundreds to thousands of iterations were required.

There is also a performance improvement compared to the “brute force” method, since in that approach the number of initial systems to relax can be as high as 50 000 or more [24]. In the present GA, in each generation there are 100 individuals, giving rise to the need of only approximately 1000 to 5000 relaxations.

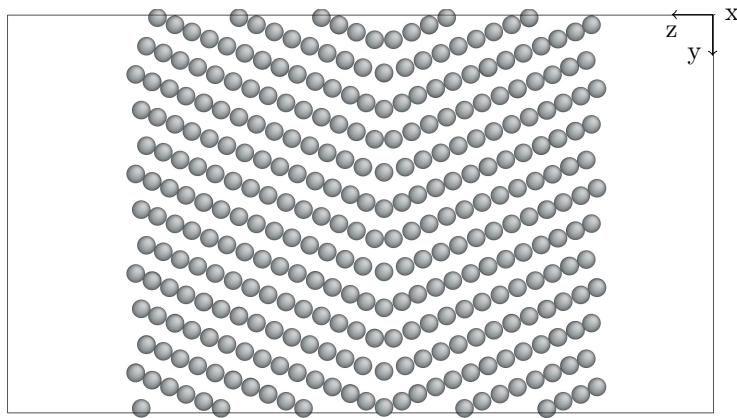


Figure 9. Tilt grain boundary in aluminum obtained after the minimization procedure.

6. Conclusions

An improved Genetic Algorithm (GA) for finding minimum energy configurations of Grain Boundaries (GBs) given the relative misorientations of two adjacent crystals was proposed.

Effective values of the parameters needed as input for the proposed GA were found using a GB for which the minimum energy configuration is well known: a twin GB in Al. Once these parameters were defined, the GA was applied to a more complex system: a tilt GB. The obtained GB energy and structure coincide with those obtained using the “brute force” method, a commonly used manner to solve this kind of problem. It was shown that the current GA has a better performance than the “brute force” method and other existing GAs in the literature.

Unlike previous “smart” algorithms existing in the literature, the current method introduces a new operator of reproduction and allows the simultaneous optimization of three main properties that determine the energy of GBs, namely the local arrangement of the atoms via the modification of their coordinates, the relative translation between the two grains that compose the GB, and the expansion/contraction of the system. Due to the nature of GAs no assumptions need to be made about the shape of the energy landscape, the initial configurations can be randomly generated and the search for a global minimum is more thorough and effective.

Acknowledgements

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