CHEMICAL COMPOSITION OF (310) [100] SYMMETRICAL TILT GRAIN BOUNDARY IN Ni_3Al

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ABSTRACT

Structure of Σ5 (310) [100] symmetrical tilt grain boundary in ordered intermetallic alloy Ni_3Al was constructed and relaxed by Monte Carlo method using pair L-J – type interatomic potential. Three modified grain boundary structures were tested. They differed in chemical composition and in relative grain boundary energy. The configuration with the lowest grain boundary energy was enriched on nickel.

KEYWORDS

Ni_3Al, grain boundary structure, Monte Carlo method

INTRODUCTION

Mechanical parameters of structural materials are the primary characteristics determining their applicability in technical practice. It is known that parameters characterizing brittle behaviour, corrosion, kinetics of atoms redistribution in the material, e.g., may be connected with the presence of grain boundaries (GBs). GBs act as paths of rapid diffusion [1] and they facilitate phase transformation for they are sites of an easy nucleation [2]. They also influence the movement of dislocation and provide sites of easy segregation of alloy components or its impurities [3].

The GB characteristics manifest itself in macroscopically observable processes. Following examples can be given: superplasticity [4,5], recovery due to annihilation of excess vacancies generated by plastic deformation [6] or by irradiation damage [7,8], rapid grain boundary diffusion [9-11], etc.

It is well known that GBs have relative high degree of symmetry. Its structure can be decomposed in discrete structural units that are linked to form repeated patterns [12]. The period of those motifs is higher for high-angle GBs and shorter for low-angle GBs. The variety of structural components in general high-angle GBs is relatively high, whereas it is extremely simplified in case of special GBs. The structure of some special GBs nickel – aluminum intermetallics was studied in detail in papers by Farkas and her coworkers [12-20]. The most deeply understood are low-sigma symmetrical tilt GBs of the family Σ3 (112) [110] and Σ9 (114) [110] in Ni_3Al [15] . The structure of GBs in NiAl was studied in detail in [12, 16]. Diffusion in the structure of GBs was studied, e.g. in [9,10,12,20]; the generation of vacancies by the non-conservative movement of GBs was investigated, e.g., in [21].

The aim of the present work is to simulate the structures of special low-sigma ($\Sigma = 5$) symmetrical tilt GB (310) [100] in Ni_3Al compound, which is a promising structural intermetallic, and to vary the GB chemical composition. Estimation of relative energy σ of generated relaxed structures will enable an estimation of the most probable structure and tendency of the system to GB chemical enrichment on either Ni or Al.

SIMULATION TECHNIQUE

The simulation of the GBs structure in Ni_3Al was carried out by the Monte Carlo technique. Pair potential of L-J type was used for the structure relaxation [22]. The size of the cluster was about 22 000 atoms and the area of the GB was ca 1.2×10^{-17} m^2. Fully symmetrical tilt GBs of the type (310)[100] with $\Sigma = 5$ only were studied; no rigid body translations were searched and/or applied.

RESULTS

The relaxed structure of GB obtained as a geometrical construction and Monte Carlo relaxation without any chemical modifications is shown in Fig.1.

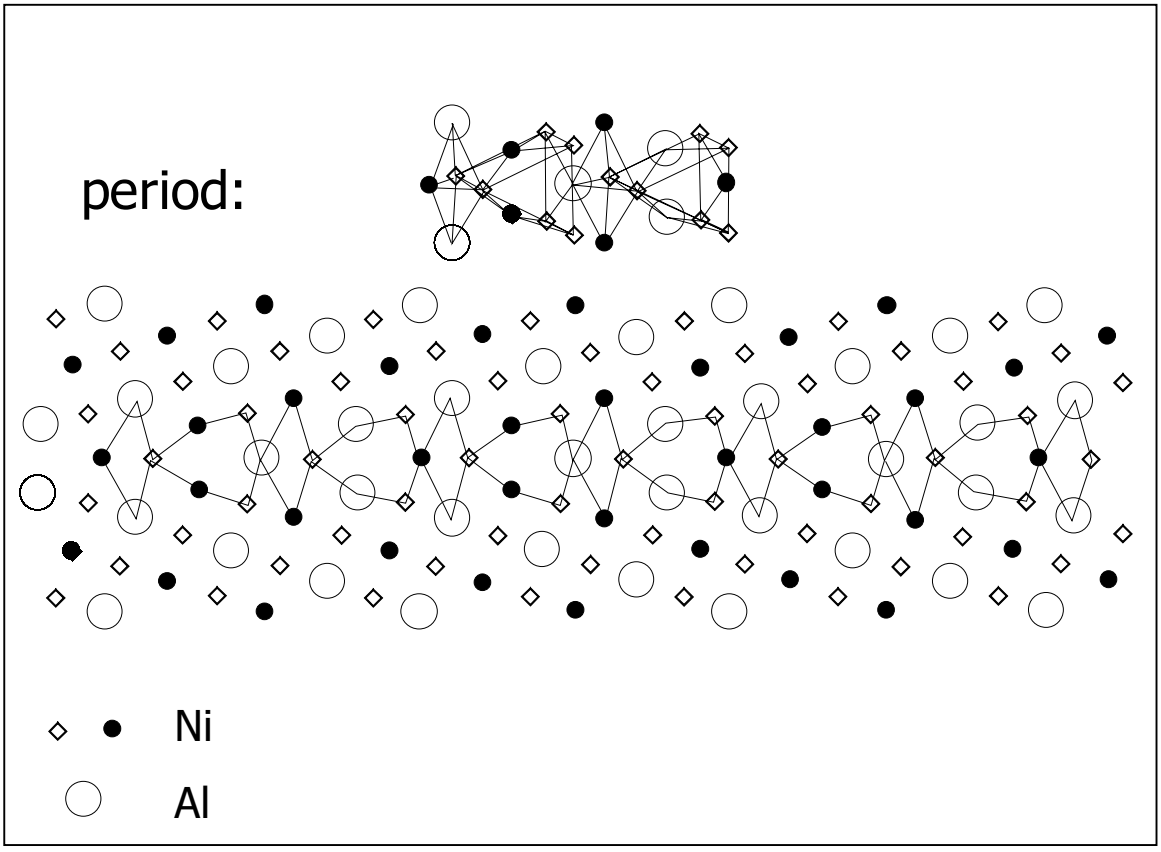

Fig.1 Relaxed structure of symmetrical (310)[100] tilt GB in Ni_3Al

Other three structures were obtained by a modification of this basic structure in a way that is schematically illustrated by the following scheme.

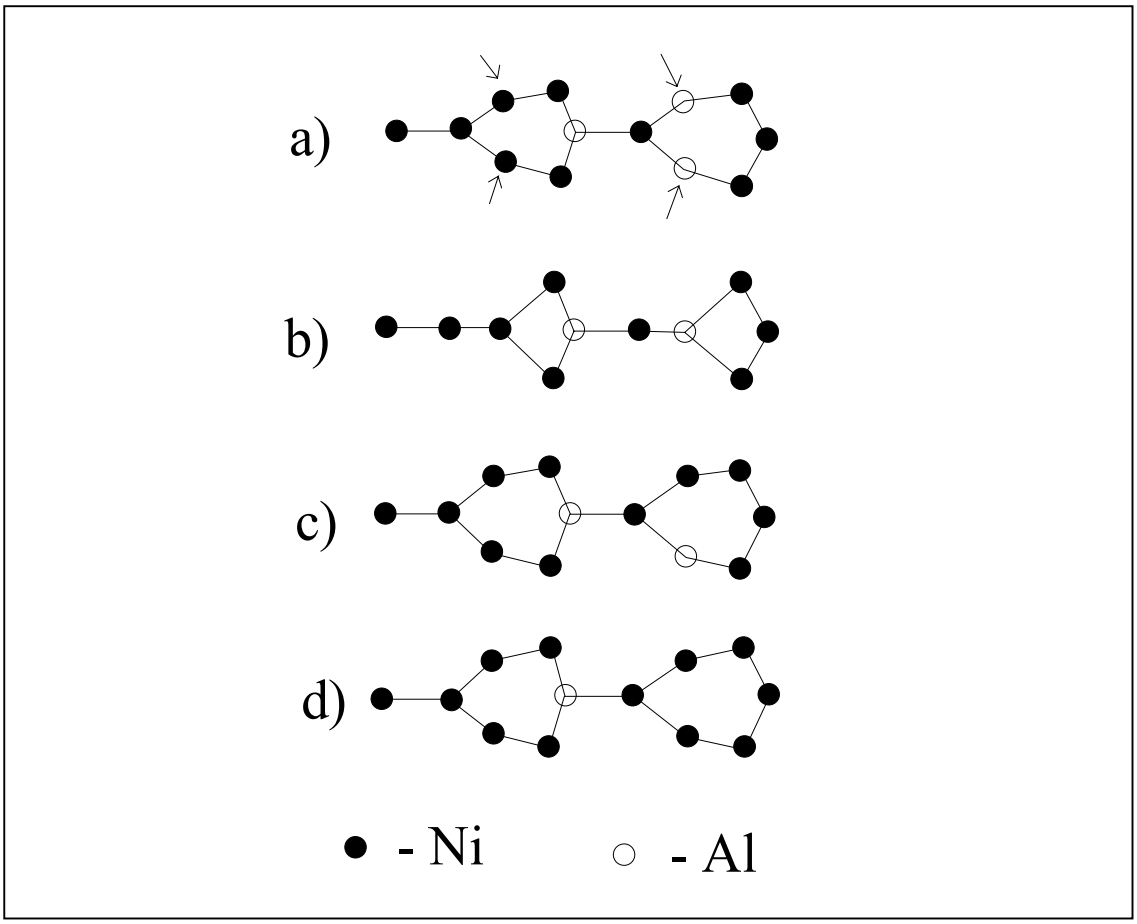

Fig.2 Modification of GB chemical composition – schematically. a) basic structure from Fig.1, b-d) modified structures.

Un-stable atom couples in GB, enhancing most extremely the GB energy σ (indicated by arrows in Fig.2a) were either replaced by a single atom of optimal type (see in Fig,2b; for relevant relaxed structure see in Fig.3) or the atom types were changed. The case with one Al atom in GB replaced by Ni atom (see in Fig.2c) led to a relaxed structure shown in Fig.4, the last tested case with both the Al atoms replaced by Ni atoms (as seen in Fig.2d) resulted in relaxed structure shown in Fig.5.

It is clear that the modification in Fig.2c disturbs the symmetry of GB. With respect to the fact that the interaction radius has been set to first two coordination spheres, however, this structure can be taken equivalent to an imperfect symmetrical GB (reflexion + shift by one period in the direction perpendicular to the tilt axis).

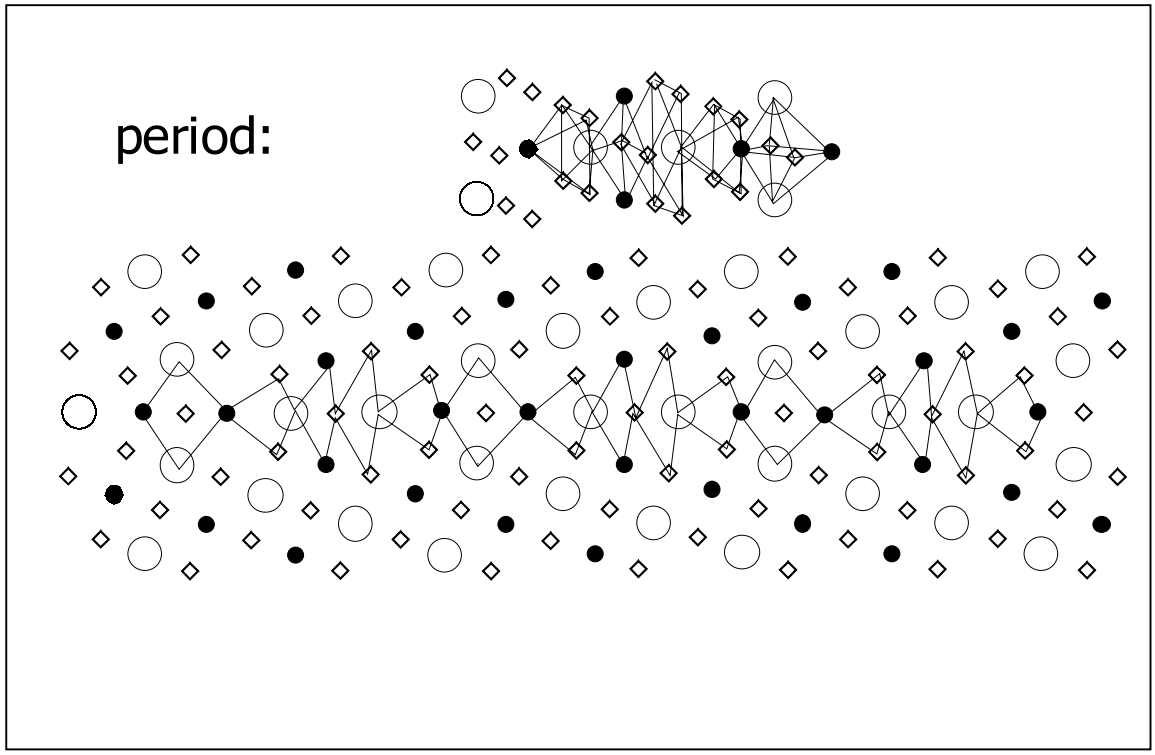

Fig.3 Relaxed structure of (310) [100] tilt GB modified as shown in Fig.2b.

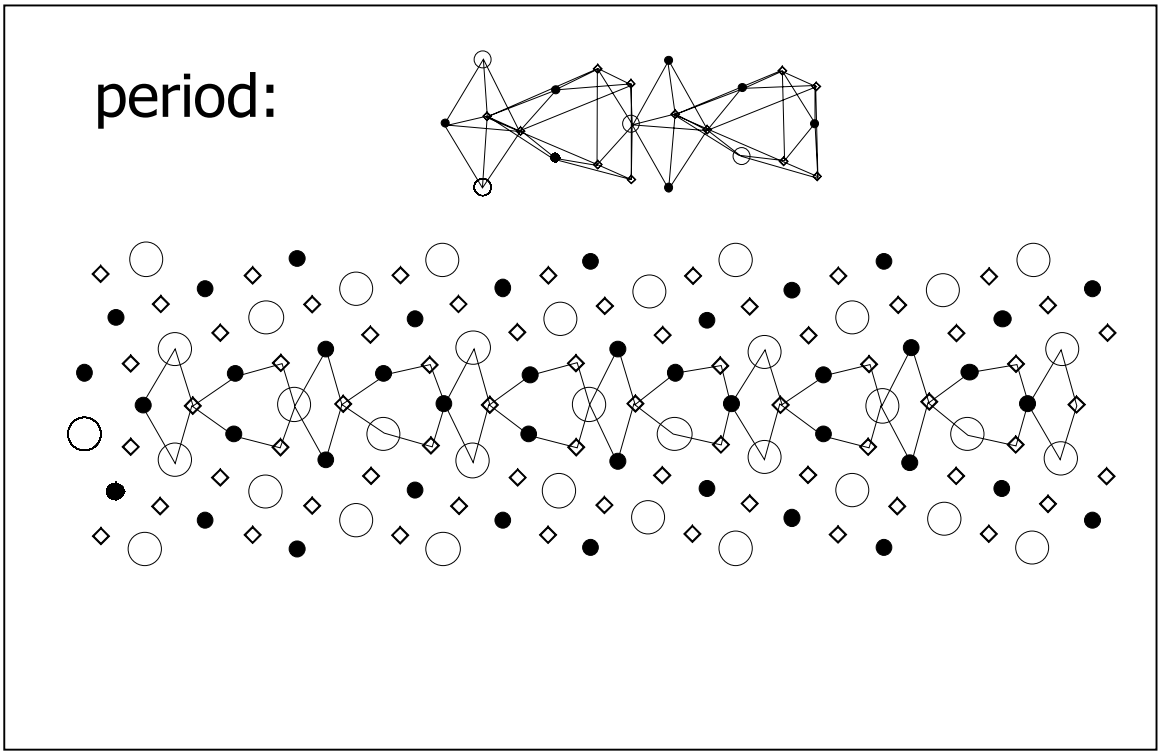

Fig.4 Relaxed structure of (310) [100] tilt GB modified as shown in Fig.2c.

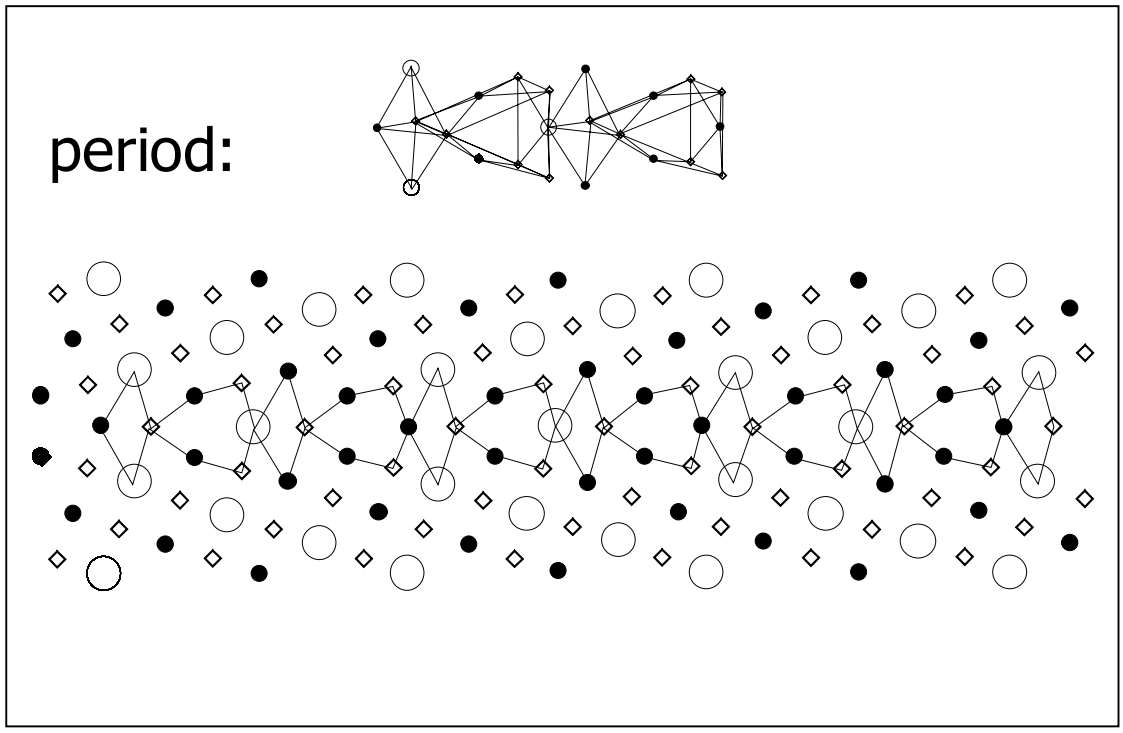

Fig.5 Relaxed structure of (310) [100] tilt GB modified as shown in Fig.2d.

It was obtained that the thickness of the layer close to GB, influenced by the presence of the GB, was about 8 Å which is slightly higher than commonly accepted GB thickness $\delta = 5$ Å [10]. The energy of grain boundary σ was calculated as the difference between the energy E of GB layer and average energy of parallel layer in the bulk. The dependence of calculated energy E on the distance from the grain boundary for the un-modified GB (and for 0K) is illustrated in Fig.6.

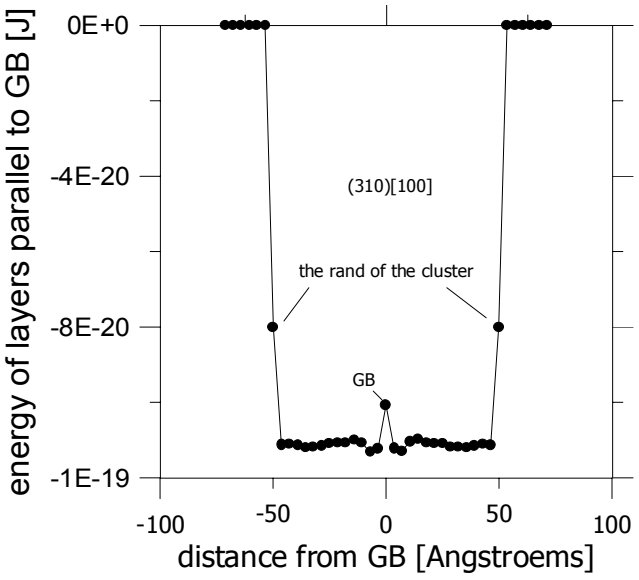

Fig.6 Energy of layers parallel to GB.

The values of σ obtained for all the structures together with the chemical composition of the GB (i.e. the composition of repeating GB period) are listed in the Table 1.

Table 1 Energy of GB σ, and chemical composition of GB period.

GB	Relaxed structure in Fig.	σ J / m^2	N_{Ni} at. % Ni
basic type – see Fig.2a	1	0.29	77.3
modification according to Fig.2b	3	0.23	83.3
modification according to Fig.2c	4	0.28	81.8
modification according to Fig.2d	5	0.29	86.4

CONCLUSION

It can be seen in Table 1 that the proposed type of modification of studied (310) [100] GB structure can lead to a certain reduction in GB energy. The lowest value of σ gave the modification that involves the exchange of some part of Al atoms by Ni atoms in the GB - indicated schematically in Fig.2b. The reverse implication may be also expected, namely, the enrichment of this type of GB on Ni may lead to a lower GB energy.

ACKNOWLEDGEMENTS

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