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APPLICATION OF THE MOLECULAR DYNAMICS METHOD FOR MODELLING OF MASS TRANSFER ON THE BORDER OF NI-AL BIMETAL

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Abstract. *One of the basic issues of examination of process of interaction of two-component alloys is the study of the mass transfer process in the presence of dot flaws: internodal atoms and vacancies. The study of this process in real experiments is impossible; therefore it is reasonable to apply computer modelling. The authors present a model of Ni-Al bimetal diffusion process produced by the method of molecular dynamics.*

Keywords: *method of computer modelling, diffusion process, vacancy, method of the molecular dynamics, internodal atom, crystalline lattice, mass transfer*

Zastosowanie metody dynamiki molekularnej do modelowania transferu masy na granicy bimetalu Ni-Al

Streszczenie. *Jednym z podstawowych zagadnień analizy procesu interakcji stopów dwuskładnikowych jest badanie procesu wymiany masy w obecności defektów punktowych: atomów międzywęzłowych i wakansów. Badania tego procesu w rzeczywistych eksperymentach jest niemożliwe, dlatego uzasadnione jest zastosowanie modelowania komputerowego. Autorzy przedstawiają model procesu dyfuzji w bimetalu Ni-Al stworzony metodą dynamiki molekularnej.*

Słowa kluczowe: modelowanie komputerowe, proces dyfuzji, wakans, metoda dynamiki molekularnej, atom międzywęzłowy, sieć krystaliczna, transport masy.

Introduction

Now, a new class of materials called intermetallics gets increasing application in the industry. Intermetallics have a complicated crystalline structure which determine their unique physic-mechanical properties (high thermal stability, low density, low deflagrability in oxygen, high wear resistance, hardness). A special part in creating materials with the given properties is played by the diffusion processes, which occur in the conditions of high temperatures and speeds of reactions. An examination of diffusion processes at microscopic (atomic) level in real experiments is not always possible and effective, since it demands considerable expenses of time, resources and manpower. The possible solution of this problem is computer modelling of structurally-energetic changes in metals.

Computer modelling allows exploring the dynamics of both fast and long-term processes at an atomic level. Computer modelling is an addition to known experimental and theoretical research techniques, frequently acting as a link between them. The computer model can serve as a mean of approbation of theoretical conceptions, and, on the contrary, to explain or predict the phenomena which earlier have been not fully covered by the theory and experiments.

One of the basic issues of examination of two-component alloys interaction process is the study of the mass transfer process in the presence of dot flaws: internodal atoms and vacancies. [1-3, 8]. Besides, the processes related to mass transfer arise in the presence of the set of other flaws: interstices, flaws of replacement and introduction, dislocations, flaws of packing, boundaries of grains and phases [6].

1. Modelling

In this paper, we attempt to reveal the dependence of the velocity of mass transfer on the distance between flaws. As flaws, intermodal atoms (IA) and discrepancy dislocations (DD) on the boundary of Ni-Al bimetal are considered.

The formation of border of metals with discrepancy dislocations is caused by the distinction in value of constants of lattice Ni and Al [4,5].

The crystal lattice Ni-Al was modelled by a method of the molecular dynamics where atoms interacted by means of potential of Morze. Experiments were carried out with the use of the program [7].

The way of creation of an initial configuration of an estimated cell, as it is proposed in [4], included three stages: construction, primary relaxation and cooling.

The boundary in Ni-Al bimetal passed through the middle of a cell containing 3200 particles (40*80 particles). The cell represented a plane {111}. The choice of this plane for the study is caused by that diffusive processes, as a rule, develop in close-packed directions to which planes {111} correspond in a usual face-centered cubic crystal [2]. Boundary conditions for an estimated cell were set as follows: on axis x - periodic, on axis y - free. The initial temperature of cells was set equal to zero Kelvin.

Artificially created interface of metals was exposed to the relaxation procedure during which boundary atoms occupied the equilibrium position. As a result of relaxation, the rise in temperature of a cell to several tens Kelvin was observed. The time of relaxation of a cell made 100 ps, 10 ps has been given for a cooling stage. Such time framework of the experiment is enough for the cell has had time to get rid of excessive free volume which arose on the border of metals at the moment of creation of initial structure [4]. As a result the boundary with characteristic discrepancy dislocations caused by distinctions of constant lattices (Fig.1) was formed.

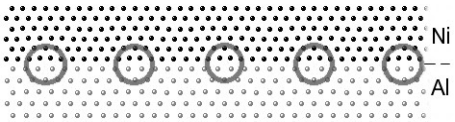

Fig.1. The boundary of Ni-Al bimetal with highlighted discrepancy dislocations.
Rys. 1. Granica bimetalu Ni-Al z zaznaczonymi dyslokacjami niezgodności sieci.

The next stage of the experiment consisted of implantation of IA at various distances from bimetal boundary. The atoms of Ni and Al were implanted by turns in interstitial space of nickel. An example of implantation is presented on Fig.2. Under the further relaxation of a cell there were directed displacements of atoms towards the boundary, according to crowdion mechanism, with the subsequent replacement of atoms from a boundary row to the adjacent metal.

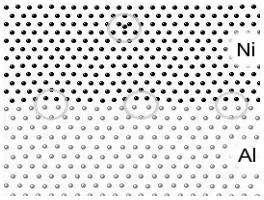

Fig.2. Configuration of a cell after implantation of interstitial atoms with the isolation of implanted atoms and nearest to it discrepancy dislocations on the Ni-Al bimetal boundary.
Rys.2.Konfiguracja komórki po implantacji atomów międzywęzłowych z izolacją implantowanych atomów i sąsiadującez nimi dyslokacjie z powodu różnych stałych sieci na granicy bimetalu Ni-Al.

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As a result of a series of computer experiments it has been established that introduction of the implantation of IA leads to the directed displacement of atoms along the direction of dense packing till the crossing of a close-packed row with a boundary of metals and displacement of atoms from a boundary row to the crystal lattice of the adjoint metal, provided that those displacements of atoms occur towards the nearest discrepancy dislocation. Thus, an original annihilation of flaws to a more favourable energy condition of system occurs. As a result of this sort of relay-race atomic displacements there is a recrawling of a dislocation at one interatom distance deep into the Al lattice. (Fig. 3)

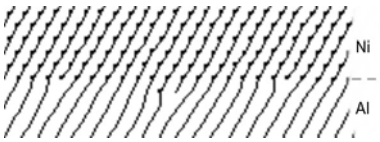

Fig. 3. The boundary of Ni-Al bimetal 0.5ps after relay race atomic displacements. On the centre DN crawled over at one interatomic distance in Al
Rys. 3. Granica bimetalu Ni-Al, 0.5 ps po lawinie dyslokacji. W centrum pełzająca dyslokacja o jedną odległość międzyatomową Al.

At the implantation of a Ni atom, the depth at which IA caused the directed relay race displacements towards the nearest discrepancy dislocation on the boundary of metals has reached 13 - 14 interatomic distances of a lattice from the boundary of metals. It should be noticed that to achieve a similar effect further than the 11th row of atoms from the boundary, it is necessary to heat a cell in addition. For example, to activate atomic displacements from the 12th and 13th row-spacing it was necessary to heat a cell to 100 and 150 K respectively. The further rise of temperature did not lead to the increase of the distance of implantation of an interstitial atom from the boundary border of the metals, leading to the directed displacement of atoms.

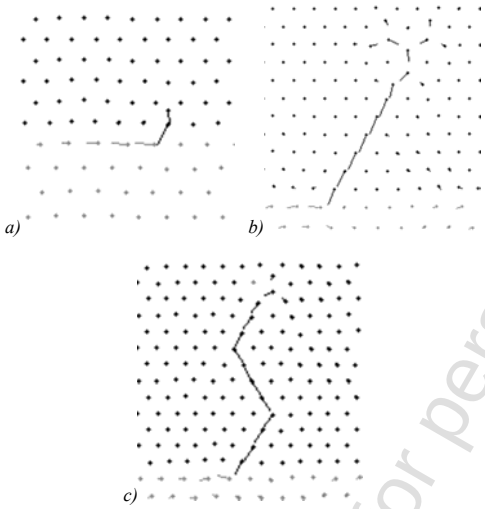

Fig. 4 . Trajectories of relay race atomic displacements.
Fig. 4 . Trajektorie lawinowych przemieszczeń atomowych.

Under the implantation of Al atoms the depth, at which IA caused the directed displacements towards the nearest dislocation of discrepancy on the boundary of metals, has reached 11 interatomic lattice distances from the boundary of metals. Unlike the case of implantation of Ni atoms, here the width of the zone in which the temperature acts as the catalyst for activation of atomic displacements is wider by 2,5 times and makes 5 interatomic distances. To obtain such effect for five marginal values, the heating of a cell to 100 - 250 K was made.

The type of the displacement irrespective of the type of an implanted atom is determined mainly by the distance of atom implantation from the boundary of metals. The rectilinear trajectory along the closely packed raw of atoms is peculiar under the implantation at 3 to 8 interatomic distances from the boundary of metals (Fig.4b). Under a closer location of IA to the boundary, it is possible for the displacement to take place not along the closely packed raw, but directly, i.e., at first, the atom is displaced into the adjacent metal, and then a displacement of some of the atoms along the boundary of metals takes place and the nearest dislocation of discrepancy is filled (Fig. 4).

With the more remote location of the implanted atom (8 and more interatomic distances) the broken trajectory of displacement of atoms (Fig. 4) is frequently observed.

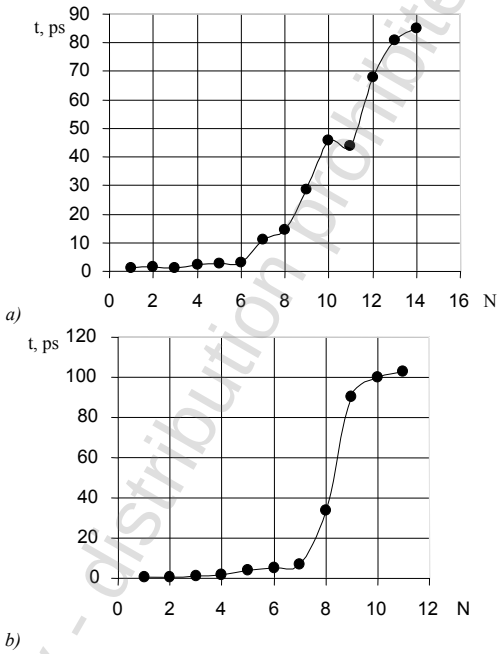

Fig. 5. The dependence of time t of relay race displacements of atoms on the distance of implantation of IA is expressed through the number N of interatomic distances of closely packed raw, between IA and the boundary of metals. a) Ni is implanted Ni, b) Al is implanted.
Rys. 5. Zależność czasu lawinowych przemieszczeń atomowych t na odległości atomów międzywęzłowych, wyrażona przez liczbę odległości atomowych N w sieci pomiędzy atomem międzywęzłowym a granicą metali. a) implantowany nikiel, b) implantowany glin.

Depending on the type of a trajectory, the time, which is required for the displacement up to the boundary of metals and displacement of extreme atom, differed. In the case of a rectilinear trajectory, this process occurs faster in comparison with a broken line trajectory. It is caused, firstly, by the longer way to the nearest dislocation of discrepancy. Secondly, under the change of a trajectory direction of the relay race displacements, there can exist an intermediate steady state.

For more detailed studying of the speed of the process of mass transfer the diagrams of the dependence of the time, for which there are relay race atomic displacements from the distance of implantation to the boundary metals, are obtained and presented in Fig.5. These time dependences include time for the speed of activation of the process of mass transfer, and also the time of mass transfer itself.

The matter is that right after the start of the program, there are no relay race displacements of atoms towards the boundary. For this purpose, some time is required. It is caused by the fluctuations of atoms about the equilibrium position. On the given dependences, the most part of time is spent on the process of initial activation of the relay race atomic displacement.

According to our estimations, the dependence of the speed of "pure" mass transfer, i.e. without time for the process activation, under the implantation of IA Ni, on the distance between IA and a discrepancy dislocation, has the form presented in Fig.6 a). Estimations are given under the implantation of IA on the distance from 2 to 13 interatomic distances from the bimetal boundary. The corresponding diagram under the implantation of IA Al is presented in Fig.6. b), the maximum distance of implantation has made 11 interatomic distances.

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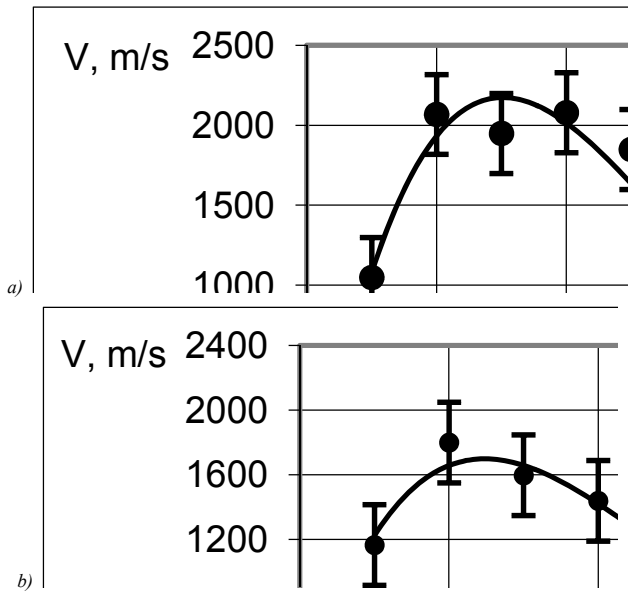

Fig.6. The dependence of the speed of mass transfer on the distance expressed through the number N of interatomic distances of closely packed raw, between IA and the boundary of metals. The dependence is given for a case of implantation of atom a) Ni, b) Al, (approximation is a polynomial function of the 4th degree).

Rys.6. Zależność szybkości transportu masy na odległość wyrażoną jako liczbę odległości międzyatomowych gęsto upakowanej sieci N, pomiędzy atomem międzywęzłowym a granicą metali. Zależność podana dla implantacji atomu a) Ni, b) Al, (aproksymacja wielomianem 4 rzędu).

At the implantation of IA on about 2 interatomic distances from the boundary border, the speed is much lower, than at 3 - 6 for the case of Ni and 3 - 5 in the case of Al. It can be explained that at the given distance the displacement of IA occurs directly into the adjacent metal, while at 3 to 6 interatomic distances for Ni and at 3 to 5 for Al it occurs along the closely packed raw. Further a considerable falling of the speed of the relay race displacements occurs. The reason which has caused the decrease in the speed of displacements is the reduction of the stress of an elastic field of a dislocation.

Some distinctions in numerical values and an inclination of approximating curves in Fig.6 a) and b) are determined by the distinctions in the elastic field created by IA, Ni, and Al.

The estimation of errors was made according to the formula for calculation of indirect reproduced measurements:

$$\Delta F = \sqrt{\sum_{i=1}^{n}\left(\Delta x_i \frac{\partial F}{\partial x_i}\right)^2},$$

where $F(x_i)$=F(x_1, x_2,..,x_n), x_i – are directly measured independent values having an error Δx_i. The error is mainly caused by fixing of the moment of the start of the relay race atomic displacements.

2. Conclusions

In the conclusion it is necessary to note that the given results are similar to the results in [8] where internodal atoms and vacancies were considered as annihilating defects. In [8] the dependence of the speed the mass transfer from the distance between defects has similar form at the distance of more than 3 interatomic distances; however there is no initial decrease in speed at 2 interatomic distances. This effect in our study is caused by the presence of the boundary of bimetal. Besides, in [8] annihilating defects are observed at the distance of no more than 8 interatomic distances. In our case at the implantation of Ni the mass transfer is possible up to 11 interatomic distances without heating of a cell.

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