Two-dimensional model of the ordered alloy for the investigation of martensitic transformations

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Two-dimensional model of diatomic crystal is proposed in the present work for the investigation of martensitic transformation under thermomechanical treatment, i.e. the proposed modell allows to simulate temperature effect as well as external loading, like tension, plastic deformation, ets. The model, based on the Morse potential, which are used for the simulation of the diatomic crystal of NiTi type, which is well known as an alloy with the martensitic transformation. This model allows one to define the main characteristics of different phases as the function of one of the potential parameter at 0 K. Potential parameters for the realization of forward and reverse martensitic transformation at finite temperatures are found by the careful checking of all the values. The appearance of one preferable martensite phase is shown despite there are two possible martensite phases. The appearance of the domain boundaries is shown for the martensite phase because of the realization of two opposite direction of martensite growth. The starting and finishing temperatures of the martensitic transformation are obtained. The effect of external stresses on the course of the martensitic transformation is investigated. The potential present in this work can be perspectively used for the investigation of such processes as phase hardening in diatomic crystals.

Keywords: martensitic transformation, molecular dynamics, phase transformation kinetics.

1. Introduction

The alloys with the shape memory effect and superelasticity are successfully used in the production of various smart-systems and sensors. The foundation of such systems is the martensitic transformation, i.e. the phase transition of the first order from highly-symmetric high-temperature austenite phase to the martensite phase with the lower symmetry during cooling (forward transformation) and vise-versa during heating (reverse transformation) [1,2]. In the course of thermocycling the multiple forward and reverse transformations caused and numerous alloys show the phase hardening which in its turn leads to the structure and properties degradation. One of the possible ways to change and increase functional and operational properties of such alloys is the severe plastic deformation which leads to the grain refinement to the nanoscale [3]. The grain refinement cause the decrease of the maximal size of the phase domains and subsequently to the decrease of the deformation of the crystal structure by the inconsistency of the shape and size of the primitive cells of austenite and martensite phases. The investigation of the mechanisms of phase hardening is relevant and interesting subject nowadays. Simulation methods [4-9] can be considered as a powerful tool for the investigations of the mechanisms of martensitic transformation on atomistic level, studying of the microstructure and mechanical properties at various conditions.

In the present work, the development of the new two-dimensional model for the simulation of the martensitic transformation is presented with the careful description of the parameters choice. The results for forward and reverse transformation are obtained.

2. Atomistic model of the ordered alloy for the simulation of martensitic transformation. Simulation details

It is well known that results, produced by molecular dynamics simulation, are considerably depends on the chosen interatomic potentials. Existing potentials can be divided into two main groups – pair and manybody potentials. The application of pair potentials is based on the assumption that the interaction of two considered atoms is independent on the presence of other atoms. Such assumption is not always well-proved, thus in many complicated issues the application of manybody interatomic potentials is required, for example, for metals and alloys potentials produced from embedded atom method are widely spread [10]. However, in the present study for the investigation of two-dimensional crystal it is worthwhile to use simple pair potential among which the potentials of Born-Mayer, Lennard-Jones, Morse, to name a few. For example, Lennard-Jones pair potential was successfully used for investigation of effect of ultrasound and annealing on the structure of nanocrystalline material

[11] and studying of plastic deformation [12-17].

Lennard-Jones function is a two parametric potential which allows one to reproduce the experimental data, for example, for interatomic potential and bonding energy, however, the rigidity of the bond will in its turn dependent on these parameters. For Morse potential,

$$\varphi(r) = D\left(e^{-2\alpha(r-R)} - 2e^{-\alpha(r-R)}\right), \qquad (1)$$

there are three parameters which allows to independently choose required parameters: distance, energy and bond rigidity. Equation (1) defines the interaction energy of the pair of atoms, φ, as the function of the distance between atoms, r. Here D is the energy of bond breaking, R – equilibrium bond length, α is the width of the potential well (bond rigidity). In Fig. 1, Morse potential is shown for $D=R=1$, $\alpha=3$ (black curve) and $\alpha=5$ (blue curve). It is seen, that for bigger α the bond rigidity, defined by the curvature near the potential minima, is higher. It also can be noted, that with the increase of α potential becomes more short-range and at $\alpha=5$ it is enough to take into account only three first coordination spheres.

Martensitic transformation is connected with the transformation of the high-temperature phase into low-temperature phase with lower symmetry which took place during decrease of the temperature below the critical point. It is well-known, that pair one-well potentials like Morse for monoatomic crystals cannot reproduce stable phase besides close-packed. In case of two-dimensional lattice, only triangle lattice will be stable. To model the phase transformation with the help of Morse potential better to consider diatomic ordered alloy with the AB stoichiometry. In this case, for the description of the interatomic interaction it is required to find the parameters of three potential functions for interaction of A-A, B-B and A-B interaction:

$$\varphi_{AA} = D_A \left(e^{-2\alpha_A (r-R_A)} - 2e^{-\alpha_A (r-R_A)}\right), \qquad (2)$$

$$\varphi_{BB} = D_B \left(e^{-2\alpha_B (r-R_B)} - 2e^{-\alpha_B (r-R_B)}\right), \qquad (3)$$

$$\varphi_{AB} = D_B \left(e^{-2\alpha_B (r-R_B)} - 2e^{-\alpha_B (r-R_B)}\right), \qquad (4)$$

As it would be shown further, for the present study the most suitable parameters are $D_{AA}=D_{BB}=1$, $D_{AB}=2$, $\alpha_{AA}=\alpha_{BB}=\alpha_{AB}=5$, $R_{AA}=R_{BB}=1$ with the changeable R_{AB}. Atomic mass of the atoms of both sorts is equal to 1.

It should be noted, that the bonding energy were chosen such as the ordered state of the alloy is preferable. Indeed, the ordering energy is $E=D_{AA}+D_{BB}-2D_{AB}=-2$ and the negative
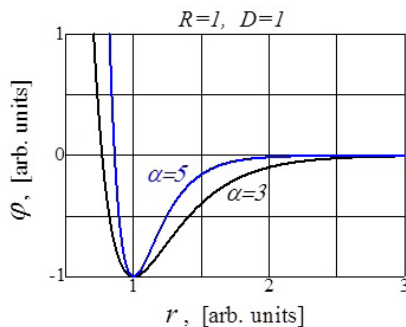
value means that at low temperatures the ordered state would be preferable.

In Fig. 2, the schematic of high symmetric austenite phase (central part) and two martensite phases M_1 (right part) and M_2 (left part) is shown. Austenite phase has the square primitive cell with the lattice parameter a, and two sorts of atoms. Interatomic distance is equal to $a/\sqrt{2}$. The three dimensional analogy to this phase is B2 based on bcc lattice, which is characteristic for intermetallic alloy NiTi.

Martensitic phase M_1 can be obtained from austenite by the shear of close-packed atomic rows alternatively by $a/\left(2\sqrt{2}\right)$ (shown by arrows in the left part of Fig. 2) with the following relaxation. Herewith, red zigzag line in austenite phase transforms to the zigzag line with the lower amplitude in M_1 phase. Tetragonal primitive cell of M_1 contains four atoms and has the lattice parameters a_1, b_1. Martensitic phase M_2 can be obtained from austenite by the shear of close-packed atomic rows by the value multiple to $a/\left(2\sqrt{2}\right)$ (shown by arrows in the right part of Fig. 2) with the following relaxation. Blue straight line in austenite transforms to blue straight line rotated by some angle. Tetragonal primitive cell of M_2 contains two atoms and has the lattice parameters $a_2/2$, b_2. The translational cell with the parameters a_2, b_2, contains two primitive cells and, correspondingly, four atoms.

The stability of tree equilibrium phases shown in Fig. 1 can be investigated by the calculation of the density of the phonon states for different values of R_{AB} [see eq. (4)]. If there is no imaginary frequencies then the considered structure is stable, otherwise – nonstable. The results are presented as the dependence of lattice parameters a and b on R_{AB} (in Figs. 3a,b), dependence of the potential energy E on R_{AB} (Fig. 4, a,b), dependence of the area of the translational cell per atom, S, on R_{AB} (Fig. 4,c,d), and tetragonality (b/a) on R_{AB} (Fig.4,e).

The simulation of phase transition at $R_{AB}=0.85$ is discussed hereafter. As it can be seen from Fig. 4,c, the volumetric effect of the transformation is quite low which is typical for NiTi alloy. In Fig. 5, the potential functions with the parameters used for calculations ($D_{AA}=D_{BB}=1$, $D_{AB}=2$, $\alpha_{AA}=\alpha_{BB}=\alpha_{AB}=5$, $R_{AA}=R_{BB}=1$, $R_{AB}=0.85$) are shown. For AA and BB bonds the same parameters are used (black and blue color), while for AB bond the potential with the bigger bonding energy is used to provide the stability of the ordered state and with the smaller
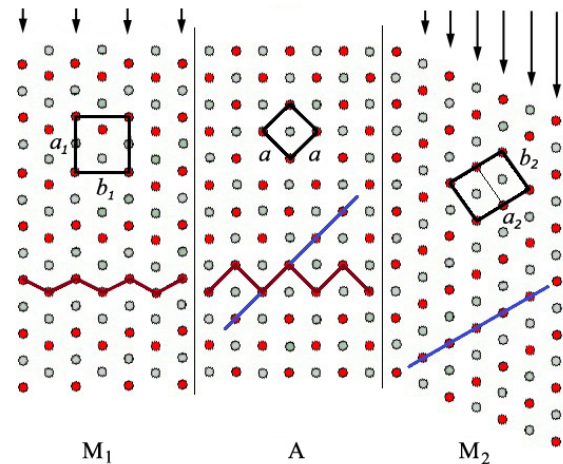

Fig. 1. Morse potential for $D=R=1$, $\alpha=3$ (black color) and $\alpha=5$ (blue color).

Fig. 2. Schematic of the structure: austenite (central part) and martensite M_1 (left) and M_2 (right). Atoms of different sorts are shown by different color.

equilibrium interatomic distance (to provide the presents of both austenite and martencite phases).

The ideal defect-free crystal with the 128×128 translational cells in the each of which two types of atoms are presented is considered for the investigation of the martensitic transformation. The number of atoms is equal to 32768. Periodic boundary conditions are applied. At the initial state all the atoms have zero velocity and get a random deviation from the equilibrium positions. The amplitude of the initial deviations defines the energy transmitted to the system in the initial period of time. The potential P, kinetic K and total T energy of the system and the energy of the phase composition and normal and shear stresses and strains are calculated during $t=300$ time units. Kinetic energy in two cases is calculated: (i) with the initial structure - martensite M_1 and (ii) initial structure – austenite. Thus, in the first case reverse and in the second case – forward transformation is studied.
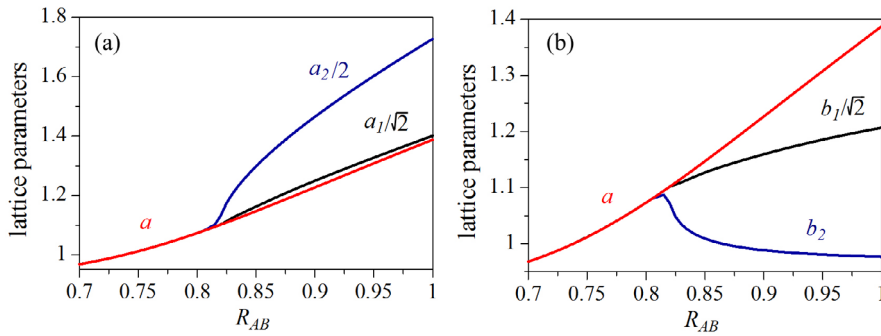

Fig. 3. Parameters of the simulation cell as the function of (a) $a(R_{AB})$, $a_1(R_{AB})/\sqrt{2}$, $a_2(R_{AB})/2$, and (b) $a(R_{AB})$, $b_1(R_{AB})/\sqrt{2}$, $b_2(R_{AB})$ for three equilibrium phases: austenite (red curve), martencite M_1 (black curve) and M_2 (blue curve).
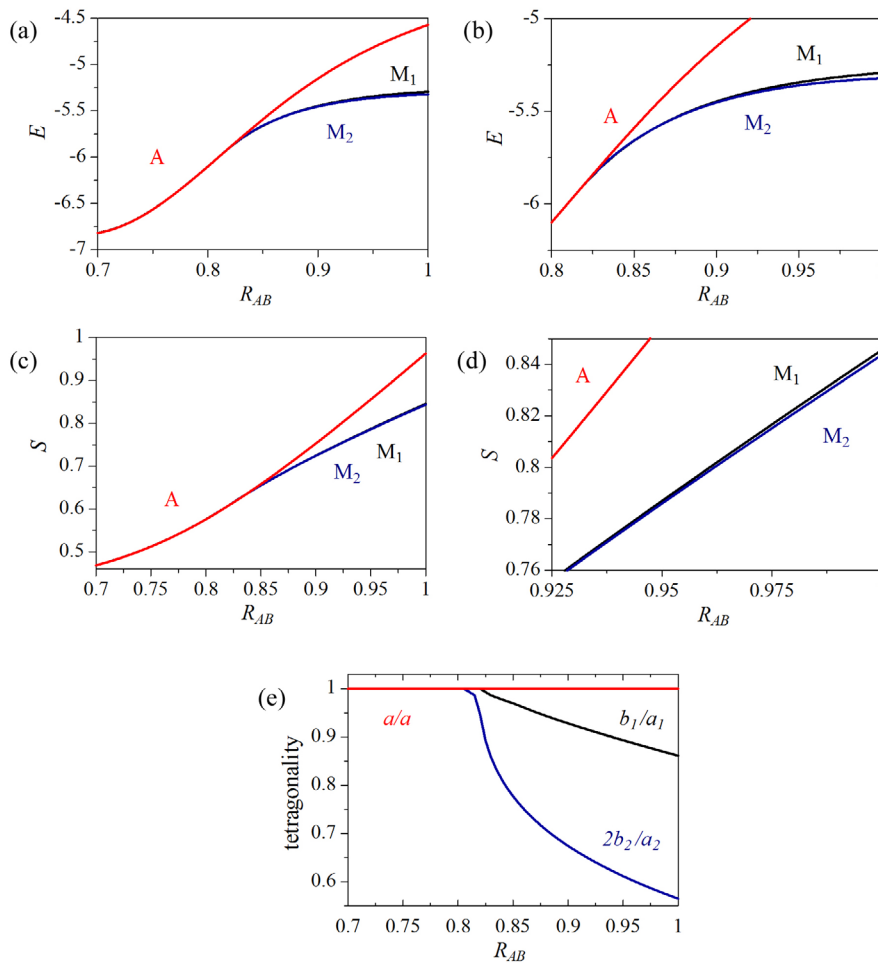

Fig. 4. Potential energy E (a,b), area per atom S (c,d) and tetragonality parameter (b/a) (e) as the function of R_{AB} for three equilibrium phases: austenite (red curve), martencite M_1 (black curve) and M_2 (blue curve). In (b) the same as in (a) but for the point close to the phase transition.
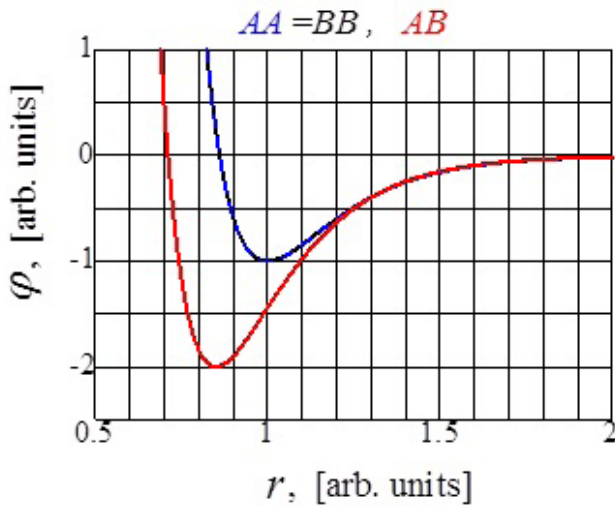
Fig. 5. Interatomic potentials for chosen parameters: $D_{AA}=D_{BB}=1$, $D_{AB}=2$, $\alpha_{AA}=\alpha_{BB}=\alpha_{AB}=5$, $R_{AA}=R_{BB}=1$, $R_{AB}=0.85$.

3. Results and discussion

In Fig. 6, the examples of the phase distribution obtained for different values of the kinetic energy, K, which is the measure of temperature in present model, are shown. Austenite phase is shown by red, martensite M_1 – by blue, martensite M_2 – by green color and undefined atoms – by gray color. In (a-c), the initial phase is M_1 and with the temperature increase the fraction of austenite grows. In (d-f), the initial phase is austenite which transforms to the M_1 during cooling. It should be noted, that only one type of martensite - M_1 - is

observed, while no M_2 is found (Fig. 6,a) despite the energy of the formation of both phases are almost similar at chosen R_{AB} (Fig. 4, b). This can be explained by the appearance of high elastic stresses in case of the formation of M_2. As well as M_1 can be formed by the shift in two opposite directions, there are two types of domains in the structure. The areas with the different orientation are separated by the domain boundaries and by the areas with the undefined state.

From Fig. 7, the starting and finishing temperatures of the martensitic transformation can be found. It is seen, that the starting (finishing) temperatures of the reverse transformation under heating are $K=0.2$ ($K=0.3$), while the starting (finishing) temperatures of the forward transformation are $K=0.19$ ($K=0.14$).

4. Conclusions

In present work, the two-dimensional model of the ordered alloy with the martensitic transformation under thermos- or mechanical treatment is presented. The model allows one to study the alloys with both negligible and considerable high volume effect of phase transition. For the case of small volume effect of the transformation, the starting and finishing temperatures of the martensitic transformation are found. Prospectively, this model can be used for the investigation of the mechanisms of phase hardening under thermal cycling.
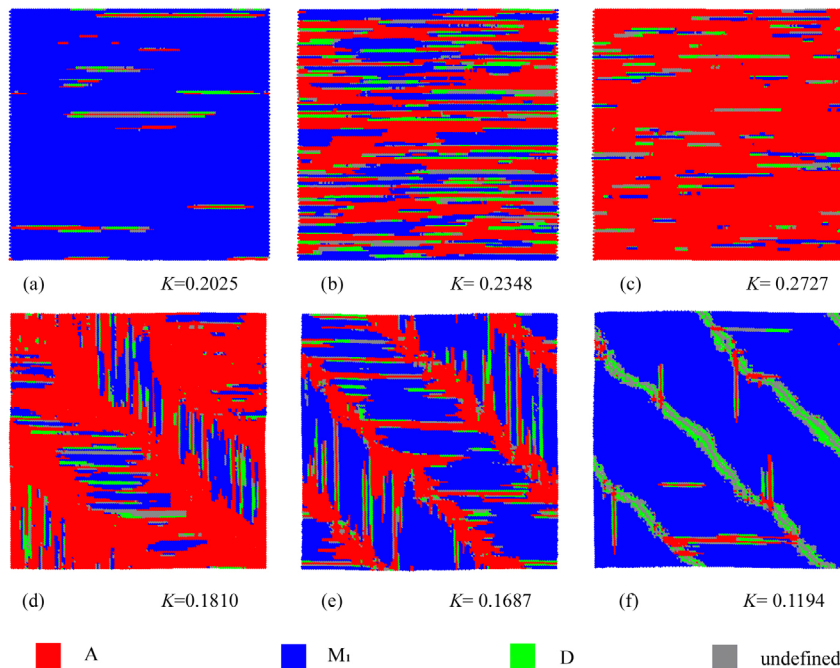
Fig. 6. Phase distribution for different values of kinetic energy K. Austenite (A), martensite (M_1) and domain boundaries are shown by red, blue and green color, respectively. Areas with the undefined structure are shown by grey color.
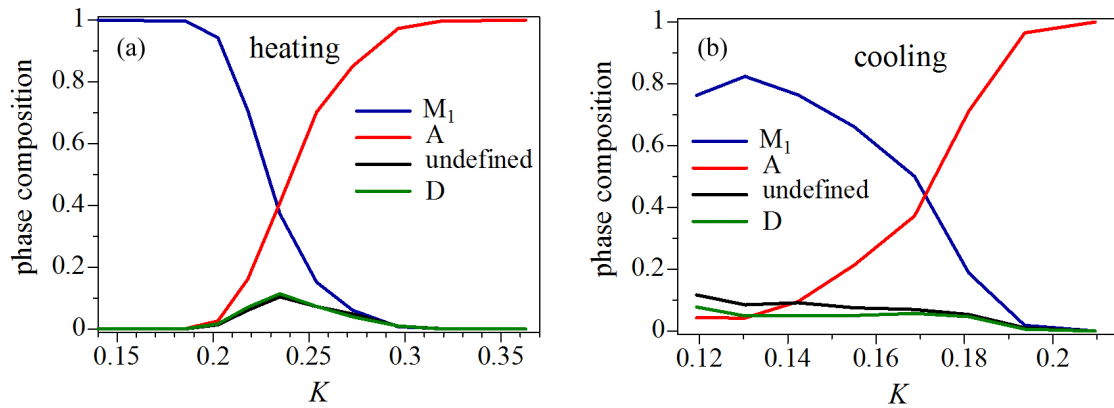
Fig. 7. Dependence of phase composition on kinetic energy K for (a) forward and (b) reverse transformation.

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