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Influence of Glide Dislocation Motion on Self-Diffusion in b.c.c. Fe. A Molecular Dynamics Study

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The interaction of glide dislocations with own interstitial atoms in α-Fe is studied. As a method of investigation the molecular dynamics simulation is used. The modelled sample is deformed with a rate close to the deformation rates under pulsed laser treatment. Mass transfer parameter for b.c.c. Fe under laser pulse irradiation is calculated. As established, the core of moving dislocation is a trap for interstitial atom. The influence of temperature and deformation rate on mass-transfer coefficient is studied.

Key words: dislocation motion, interstitial atom, pulsed loading, molecular dynamics, mass transfer.

Вивчено взаємодію крайових дислокацій з власними міжвузловими атомами в α-Fe. Дослідження було виконано за допомогою методу молекулярної динаміки. Змодельований зразок піддавався деформуванню зі швидкістю деформації, близькою до швидкостей деформації внаслідок імпульсної лазерної обробки. Розраховано коефіцієнти масоперенесення для ОЦК-заліза в умовах імпульсного лазерного оброблення. Встановлено, що ядро рухомої дислокації є пасткою для міжвузлового атому. Досліджено вплив температури та швидкості деформації на коефіцієнт масоперенесення.

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Ключові слова: рух дислокації, міжвузловий атом, імпульсне навантаження, молекулярна динаміка, масоперенесення.

Было изучено взаимодействие краевых дислокаций с собственными междоузельными атомами в α-Fe. В качестве метода исследования было использовано молекулярно-динамическое моделирование. Смоделированный образец подвергался деформированию со скоростью деформации, близкой к таковой при импульсной лазерной обработке. Рассчитаны коэффициенты массопереноса для ОЦК-железа в условиях импульсного лазерного излучения. Установлено, что ядро движущейся дислокации является ловушкой для междоузельного атома. Изучено влияние температуры и скорости деформации на коэффициент массопереноса.

Ключевые слова: движение дислокации, междоузельный атом, импульсная обработка, молекулярная динамика, массоперенос.

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1. INTRODUCTION

It is well known that diffusion processes are temperature activated. Future studies [1] showed that not only temperature but different defects of crystal structure can make an influence on diffusion processes in solids too. For example high rate of deformation speeds up the diffusion [2–4] that can be caused by formation and motion of glide dislocations. Mostly, mass transfer in metal occurs by vacancy mechanism, but at high-energy irradiation, pulsed influence and ion implantation the transport of self-interstitial atoms takes a place [3, 5, 6]. That is why the computer simulation technics of self-interstitial migration and interaction of edge dislocations with impurities are wildly supported by US Department of Energy [5, 7–9].

The acceleration of atoms mobility in pure iron at room temperature after pulsed laser influence was studied before [10]. The obtained coefficient of self-diffusion was $1{,}6 \cdot 10^{-2}$ sm^2/s that is many orders of magnitude higher than the diffusivity in equilibrium conditions at temperatures up to the melting point. The obtained result of accelerated mass transfer is described by the realization of own interstitial atoms migration under high-speed plastic deformation.

This study uses the molecular dynamics (MD) simulation to investigate how to do the dislocations interact with own interstitial atoms in α-iron under pulsed influence.

2. MATERIALS AND METHODS

As a research sample a rectangular object of pure iron consisted of 26255 atoms was modelled. The modelling was done at three tempera-

TABLE 1. The modelled deformation rates depending on rate of motion of two upper fixed planes.

Rate of motion of fixed planes, m/s	Deformation rate, s^{-1}
23.9	$2.78 \cdot 10^9$
11.9	$1.39 \cdot 10^9$
2.4	$2.78 \cdot 10^8$

tures (77 K, 300 K, and 900 K) and three deformation rates (Table 1). At each temperature of this investigation iron has b.c.c. modification. As it is known the densest packing direction in b.c.c. lattice is [111] and the glide planes are (112) and (110) [11]. Because of this for better visualization of dislocation motion process a system which X direction responded to [111] direction of b.c.c. lattice, Y responded to $[11\bar{2}]$ direction of b.c.c. lattice and Z responded to $[\bar{1}10]$ direction of b.c.c. lattice was built. The dislocation line coincided with Z direction of modelled system.

To create the dislocations the sample was conditionally divided into two equal parts in Y direction and six half-planes from the underside of modelled crystal were removed and other atomic planes were shifted in such way to fill up the obtained emptiness. As a result, two complete dislocations with Burgers vectors $(a/2)111$ were obtained. The dislocation density was $6.6 \cdot 10^{15}$ m^{-2}. The glide plane was $(11\bar{2})$.

To create the interstitial atom (IA) in the pore of crystalline structure one atom from underside was replaced by two atoms in dumbbell configuration. The dumbbell configuration coincided with the direction [110] of b.c.c. lattice (Fig. 1).

The periodic boundary conditions in Z and X directions were used. Two upper and two lower planes in Y direction were fixed to provide plastic deformation of the sample.

Two upper fixed planes were displacing with given rates to provide the dislocation motion. It is the way of realization of plastic deformation in modelled sample. Total displacement in each modelling process (for each temperature and deformation rate) was $2a$ (a = 2.866 Å). The deformation rates in modelled system were close to the deformation rate under the pulsed laser treatment.

The deformation rate was calculated using Orovans equation for deformation value [12]:

$$\varepsilon = \frac{b}{h}, \tag{1}$$

where ε—deformation value, b—Burgers vector, h—the size of the crystal in the direction perpendicular to the glide plane of the disloca-

tion (in the case of this investigation it's a size of crystal in Y direction).

The deformation rate depends on time during which the dislocation will pass all the sample:

$$\dot{\varepsilon} = \frac{b}{h} \cdot \frac{1}{t}, \tag{2}$$

where $\dot{\varepsilon}$ —deformation rate, t—time of dislocation motion through all the sample.

The modelling was done by the MD simulation using the Embedded-Atom Method (EAM) [13] for describing interatomic interactions. Full time of modelling was 1.3 fs, time step was $3 \cdot 10^{-15}$ s.

The coefficient of self-diffusion was calculated to analyse how do the moving dislocations interact with interstitial atom:

$$D_i = \frac{\sum_{i=1}^{N} \Delta^2}{6Nt}, \tag{3}$$

where N—the number of atoms in system, Δ^2—the square of atoms displacement, t—time of diffusion.

In Δ^2 calculations only displacements that are bigger then displacements caused by thermal fluctuations were taken into account. For b.c.c. lattice such displacements in projection on X axis are: $a\sqrt{3/16}$ in [111] direction and $a\sqrt{1/16}$ in two other directions, where a is a lattice spacing. Displacements of atoms in upper side of crystal weren't taken into account because the dislocation motion doesn't mean the motion of mass.

3. RESULTS AND DISCUSSION

3.1. The Interaction of Moving Dislocation with the Interstitial Atom

In the process of heating and relaxation of the system the dislocations and the interstitial atom are fluctuating relatively to theirs equilibrium positions. In compare with f.c.c. lattice [4] the IA doesn't move to the dislocation core if the dislocation stays in place. It is because the distance between neighbour atoms in b.c.c. is more than the same distance in f.c.c. The f.c.c. lattice is more closely packed than b.c.c. and self-interstitial atoms in f.c.c. crystals are more mobile [14].

In the process of dislocation motion and approaching of its core to the position of interstitial atom the stresses around the core initiate the movement of the interstitial atom towards the direction of the near dislocation core. It is caused by tensile stress under the extra half-plane. The dislocation begins to move slowly in the process of ap-

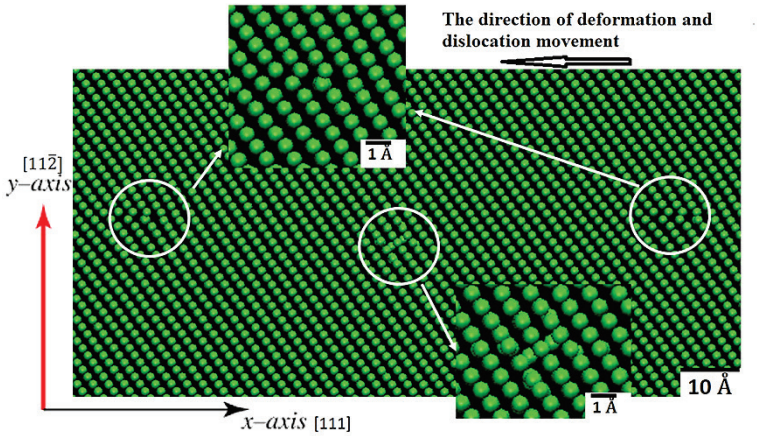

Fig. 1. The part of simulation sell with 2 edge dislocations and 1 self-interstitial atom (in the centre) in dumbbell configuration.

proaching of IA to its core. The interstitial atom is attracted by the core of dislocation and placed under the dislocation in the glide plane (Fig. 2).

At high temperatures (900 K) the interstitial atom is not always attracted by the dislocation core. At deformation rate $1.39 \cdot 10^9$ s^{-1} the IA moves under the dislocation core but it doesn't place in the glide plane and is not attracted by the dislocation core. Besides, the IA approaches one dislocation core or core of another dislocation from time to time. Such behaviour of IA is caused by major influence of temperature at

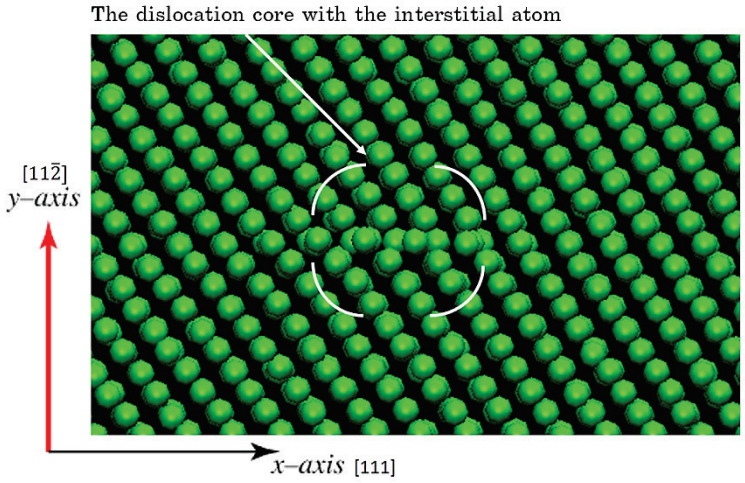

Fig. 2. The position of IA in the dislocation core.

mass-transfer than the influence of mechanical stresses at high temperatures. But at such high deformation rates it's not a frequent phenomenon. After the attracting of IA by the dislocation core, the dislocation continues motion in the glide plane with the initial rate and the IA moves with it.

3.2 The Dislocation Motion Velocity

The velocity of dislocation motion is determined by a lot of factors for example temperature and deformation rate. The described system has two dislocations and one interstitial atom. Only one dislocation interacts with the IA while another one continues its motion without the IA. So, it is appropriate to calculate the motion rate of dislocation with the IA in its core and without it.

The dislocation motion velocity didn't exceed the speed of shear waves in iron (3250 m/s). 10 times increasing of the deformation rate increases the dislocation motion velocity 10 times too. Increasing of temperature causes a small decreasing of dislocation motion velocity. It is connected with the increasing of atom oscillation amplitude and the decreasing of elasticity modulus at high temperatures as it is seen from the Table 2. The presence of IA in the dislocation core almost affects at the velocity of its motion within the limits of measurement error.

3.3. The Influence of Temperature on Mass Transfer in b.c.c. Iron

In this investigation the diffusion by mechanism of random walks in

TABLE 2. The change of motion velocity of dislocation with IA in the core and without it with increasing of temperature and deformation rate.

Temperature, K	Deformation rate, s^{-1}		
	$2.78 \cdot 10^8$	$1.39 \cdot 10^9$	$2.78 \cdot 10^9$
	The motion velocity of dislocation without IA in the core, m/s		
77	90 ± 10	450 ± 50	750 ± 100
300	80 ± 10	250 ± 50	650 ± 100
900	70 ± 10	200 ± 50	650 ± 100
	The motion velocity of dislocation with IA in the core, m/s		
77	90 ± 10	450 ± 50	750 ± 100
300	80 ± 10	400 ± 50	750 ± 100
900	80 ± 10	400 ± 50	650 ± 100

the presence of driving force with the participation of interstitial atom was realized (Fig. 3). Notably, at high-energy impulse loadings the driving force is too high and the random walks are not significant. In this case the directed atoms motion mostly happens. It was established as a result of investigation of concentration profiles shapes [15].

Increasing of temperature from 77 K to 900 K increases the calculated by MD self-diffusion coefficient two times. This increasing is too low in compare with data [17] for non-deformed b.c.c. Fe with the interstitial atoms in concentration $c = 1/2000$. It means that the influence of temperature on mass-transfer process under impulse loading is minor that is in good agreement with data [3, 18].

3.4. The Influence of Deformation Rate on Mass Transfer in b.c.c. Iron

The described model simulates the plastic deformation due to a rapid thermal expansion under pulsed laser treatment. In the case of high-speed deformations a mechanical loading gives the significant contribution to the mass-transfer coefficient (Fig. 4).

With 10 times increasing of deformation rate the self-diffusion coefficient of α-Fe increases 10 times too. It is in good agreement with data obtained in [17] and confirms the assumption of a significant contribution of dislocation motion in mass-transfer processes.

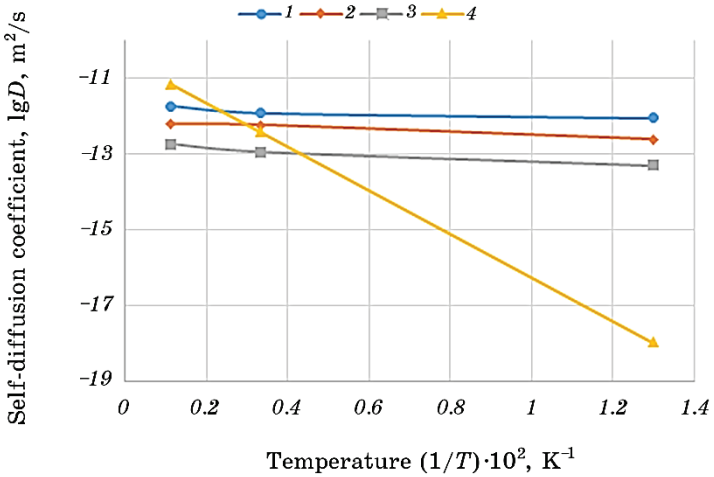

Fig. 3. The dependence of self-diffusion coefficient on temperature for b.c.c. Fe under pulsed loading: *1*—the deformation rate is $2.78\cdot10^9$ s^{-1}, *2*—the deformation rate is $1.39\cdot10^9$ s^{-1}, *3*—the deformation rate is $2.78\cdot10^8$ s^{-1}, *4*—theoretical data for b.c.c. Fe with self-interstitial atoms and without deformation [16, 17], calculated using diffusion equation.

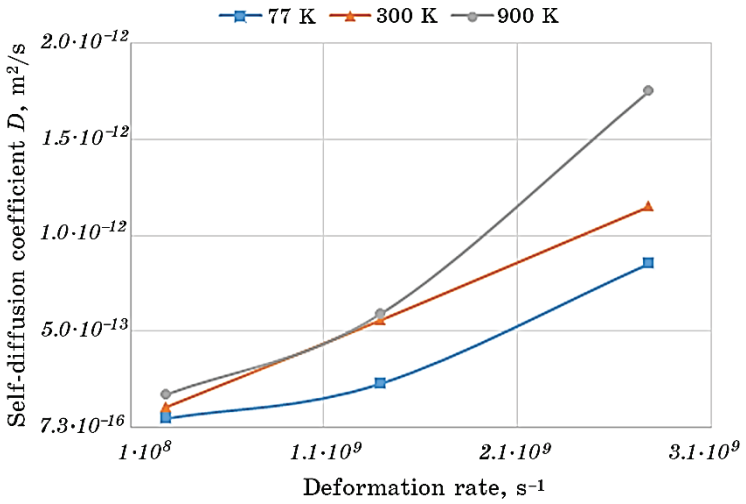

Fig. 4. The dependence of self-diffusion coefficient on deformation rate for α-Fe.

4. CONCLUSIONS

A three-dimensional MD model of b.c.c. Fe with two glide dislocations and one self-interstitial atom showed that the interstitial atom moves to the dislocation core and fixes by the field of its stresses in the process of dislocation motion and its approaching to the interstitial atom. The subsequent motion of the dislocation is carried out together with the interstitial atom in the core. It means that the dislocation is a moving trap for the point defect.

In the case of non-deformed b.c.c. sample while the dislocations stay in place the interstitial atom doesn't approach the dislocation core, unlike the same situation in f.c.c. lattice [4] where the interstitial atom moves to the dislocation core in the absence of dislocation motion. This is due to the more closely packing of f.c.c. lattice in compare with b.c.c. That is why the self-interstitial atoms in f.c.c. lattice are more mobile [14] and the dislocation stress field in f.c.c. extends further.

Increasing of the temperature decreases the dislocation motion rate. It is connected with the decreasing of elasticity modulus.

The results of self-diffusion coefficient (D) study in the presence of interstitial atom showed that the mass transfer processes mostly depend on deformation rate than a temperature.

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