

ATOMISTIC SIMULATION OF INTERACTION BETWEEN Cu PRECIPITATES AND EDGE DISLOCATION IN BCC Fe CRYSTAL

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Abstract. The interactions between a $1/2\langle 111 \rangle\{110\}$ edge dislocation and spherical Cu precipitates of diameter $D = 2-8$ nm in bcc Fe have been investigated. A new interatomic potential that will allow performing atomistic simulations of coherent Cu precipitates in α -iron by the embedded atom method has been developed. A rapid growth of the dislocation-precipitate interaction energy is due to structural instability of the particles of diameter $D > 4.2$ nm initiated by dislocation.

1. INTRODUCTION

The effect of fine Cu precipitates on the core structure and the slipping behavior of dislocations is very important for understanding of the alloying behavior in these materials. A considerable increase in the hardness results from thermal aging of steels with an extremely low Cu concentration. Experimental evidence strongly suggests that this property changes due to the formation of initially small bcc Cu precipitates (~1 to 2 nm in diameter). As Cu precipitates grow, they undergo complex structural transformations $bcc \rightarrow 9R \rightarrow fcc$. These transformations are accompanied by changes in the volume and the shape of Cu precipitates. The presence of coherent precipitates affects the slipping behavior of dislocations, and, hence, the mechanical properties are altered. At present, the relation between

the structural state in Cu nanoparticles and changes in the strength of materials containing fine bcc Cu precipitates is not clearly understood.

According to results of simulation [1], Cu atoms randomly distributed in the Fe matrix can have a considerable effect on the motion of dislocations, leading to the solid solution hardening. The motion of edge and mixed dislocations with the Burgers vector $a/2\langle 111 \rangle$ in the $\{110\}$ slip plane was studied [1,2] moving across the spherical coherent precipitations of Cu 3-4 nm in diameter. The phase instability of a particle was noted [2] when it was cut by a dislocation moving in the field of a shear stress applied; however, no considerable effect of a dislocation on the precipitate structure was found in [3]. Therefore, the role of the phase instability in hardening has been an open question.

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2. RESULTS OF COMPUTER SIMULATION AND DISCUSSION

By the molecular dynamics (MD) method it is possible to perform a numerical experiment involving a large number of atoms. This is necessary to explore phenomena developing at the atomic level during the interaction between a dislocation and a precipitate. Here, of principal importance is the choice of the interatomic interaction potentials properly describing the properties of a system under study. We used N-body potentials constructed by the embedded atom method (EAM) [4], in which the energy of an alloy is expressed as

$$E = \sum_i \left\{ \sum_j V_{\text{Fe-Fe}}(R_{ij}) + V_{\text{Cu-Cu}}(R_{ij}) + V_{\text{Fe-Cu}}(R_{ij}) \right\} + F_{\text{Fe}}(\rho_i) + F_{\text{Cu}}(\rho_i), \quad (1)$$

where $V_{\text{Fe-Fe}}(R_{ij})$, $V_{\text{Cu-Cu}}(R_{ij})$ and $V_{\text{Fe-Cu}}(R_{ij})$ are functions describing the pair interaction of Fe and Cu atoms; $F_{\text{Fe}}(\rho_i)$ and $F_{\text{Cu}}(\rho_i)$ are the so-called embedded functions; ρ_i is the total electron density produced on the i -th atom by all its neighboring atoms,

$$\rho_i = \sum_j \rho_{\text{Fe}}(R_{ij}) + \rho_{\text{Cu}}(R_{ij}), \quad (2)$$

where $\rho_{\text{Fe}}(R_{ij})$ and $\rho_{\text{Cu}}(R_{ij})$ are electron densities in the vicinity of Fe and Cu atoms. The potential [5], which describes well the equilibrium properties of bcc Fe, was taken for the Fe-Fe interactions. The potential [6], which was constructed from results of first-principles calculations, was chosen for Cu. This potential correctly predicts the lattice instability of bcc Cu and provides a proper relationship between the energies of the bcc and fcc phases.

The first Fe-Cu interaction function $V_{\text{Fe-Cu}}(R_{ij})$ was built up as a superposition of the contributions from individual elements in the form [7]

$$V_{\text{Fe-Cu}}(R_{ij}) = h(x) * (V_{\text{Fe}}(R_{ij}) + V_{\text{Cu}}(R_{ij})). \quad (3)$$

This scheme describing the interaction between components of an alloy is a procedure frequently used for modeling of solid solutions [8]. The function $h(x)$, which depends on the alloy concentration x , is chosen as an expansion into power series in x , while the expansion coefficients are determined so as to ensure the best agreement between calculated and experimental values of the equilibrium parameters of an alloy. In this study, $h(x)$ was chosen from a comparison with results of the first-principles calculations [9] of the concentration depen-

dence of the lattice parameter, the elasticity moduli, and the mixing energy. An analysis showed that the function $h(x)$ remained constant up to $x \sim 0.7$ and increased monotonically at $x > 0.7$. Therefore, later we assumed $h(x) = k$ to be a constant, which varied within the limits $0.3 < k < 0.7$. An optimal value of k was found from a comparison of the calculated concentration dependences of the equilibrium parameters of an alloy with results of the first-principles calculations.

Fig. 1 presents a dependence of the mixing energy E_{mix} on the Cu concentration in the solid solution of a Fe-Cu alloy with a bcc lattice. The curves correspond to the Fe-Cu pair potentials at $0.3 < k < 0.7$. At the copper concentration $0 < x < 50\%$ and $k = 0.56-0.58$ the dependence of the mixing energy $E_{\text{mix}}(x)$ agrees well with the dependence of the potential proposed in [8] and results of calculations performed in terms of the electron density functional theory [9]. The E_{mix} value is large and positive (the maximum $E_{\text{mix}} \sim 120$ meV at $k = 0.56$), pointing to a well-defined tendency for decomposition in the Fe-Cu system.

According to modern representations, hardening with fine precipitates is due to a resistance experienced by a dislocation as it moves across particles of the second phase. The extent of hardening is determined by the size of precipitates, their volume fraction, and the energy ΔE , which is consumed

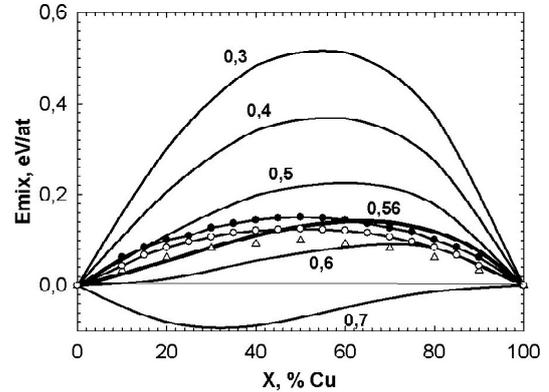


Fig. 1. Dependence of the mixing energy on the Cu concentration in the solid solution of a Fe-Cu alloy with a bcc lattice at the values of the parameter k ranging between $0.3 < k < 0.7$. The triangles correspond to the E_{mix} values calculated at the potential proposed in [8]; the circles, to the values calculated in terms of the electron density functional theory [9] for the ferromagnetic (full) and paramagnetic (open) states.

for cutting a single precipitate by a dislocation. To establish the mechanisms by which the energy changes as a dislocation moves across a particle, we performed the MD simulation of a bcc Fe crystallite containing a dislocation and a spherical Cu precipitate. An edge dislocation with the Burgers vector $1/2[\bar{1}11]$ gliding in the (110) plane was considered. The OX axis of the model crystallite was parallel to the Burgers vector of the dislocation, the OY axis coincided with the normal to the slip plane, and the OZ axis was directed along the dislocation line $[\bar{1}1\bar{2}]$. Fixed boundary conditions were chosen along the OX and OY directions; and periodic boundary conditions, along OZ. A Cu precipitate of a preset size was placed at the center of the crystallite. The size of the crystallite was sufficiently large (the number of atoms in the crystallite was $\sim 3 \cdot 10^5$) in all the three directions so as to exclude the effect of the boundary conditions. The dislocation-precipitate interaction energy ΔE was defined as the work (per unit length) required to move the dislocation from its distant position to a distance X from the center of the precipitate,

$$\Delta E = \frac{E_{d+p}(x) - E_d - E_p + E_0}{L}, \quad (4)$$

where E_{d+p} is the energy of the crystallite containing a Cu precipitate and a dislocation; E_d , E_p , and E_0 denote the energy of the crystallite with a dislocation, the crystallite with a Cu precipitate, and the bcc Fe crystallite, respectively; L is the length of the crystallite along the Z axis. The structural relaxation was effected, the total energy was measured, and displacements of atoms in the matrix and the precipitates were determined at each position of the dislocation axis in the slip plane.

Fig. 2 shows the interaction energy ΔE as a function of the distance between the dislocation and the center of the Cu precipitate (the center of the particle is marked with a vertical dotted line). The curves 1-9 correspond to an increase in the precipitate radius R from 1.25 to 3.50 nm (the number of the Cu atoms ranged between 511 and 10890). The penetration of the dislocation into the precipitate is accompanied by an energy gain, which increases nonlinearly with growing size of the precipitate. Depending on R , three regions, in which the mechanism of the interaction between the dislocation and the precipitate is qualitatively different, can be recognized.

If particles are small ($R < 2.2$ nm, curves 1-4), the interaction energy changes fairly little as the particle size grows. In this case, a decrease in the

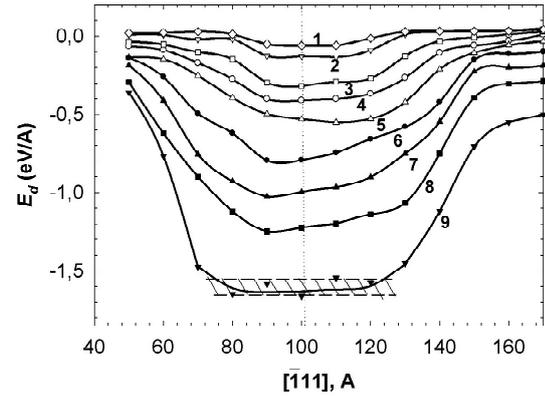


Fig. 2. Energy of the interaction (per unit length) between a dislocation and a precipitate. The radius of the precipitates is $R = 1.25\text{-}3.50$ nm (curves 1-9).

dislocation energy is due to the relaxation of elastic stresses in the precipitate, in which the shear modulus is 40% smaller than it is in bcc Fe (at the interatomic potentials used in this study the Voigt averaged shear moduli are $\mu_{Fe} = 0.859 \cdot 10^{11}$ Pa and $\mu_{Cu} = 0.499 \cdot 10^{11}$ Pa). In the absence of a dislocation, a particle placed in the Fe matrix causes radial displacements, which are due to the concentration expansion resulting from different equilibrium values of the lattice parameter of bcc Cu and Fe. The penetration of the dislocation into the particle is followed by elastic strains localized near the particle core, but copper precipitates retain their bcc structure.

In the case of coarser precipitates with sizes in the range $2.2 \text{ nm} < R < 3.1$ nm, the energy ΔE increases sharply with growing R . In this range of sizes, if a dislocation is absent, a Cu particle in the Fe matrix also retains its bcc structure (Fig. 3a). However, the introduction of a dislocation into a particle leads to a structural instability in the particle (Fig. 3b). For particles with $R > 3.1$ nm, their equilibrium configuration has, even in the absence of a dislocation, the bcc-9R structural instability with the distribution of displacements similar to the one shown in Fig. 3b. The introduction of a dislocation into a particle causes an increase in displacements and the formation of additional regions of shear strain, with the last factor leading to a nonmonotonic dependence of the energy ΔE on the position of the dislocation line in the bulk of the particle (Fig. 2).

A maximum change of the energy ΔE_{max} , which is required for a dislocation to pass a particle (Fig. 4), characterizes the extent of alloy hardening. As can be seen from Fig. 4, the transition from the modulus misfit strengthening mechanism of hard-

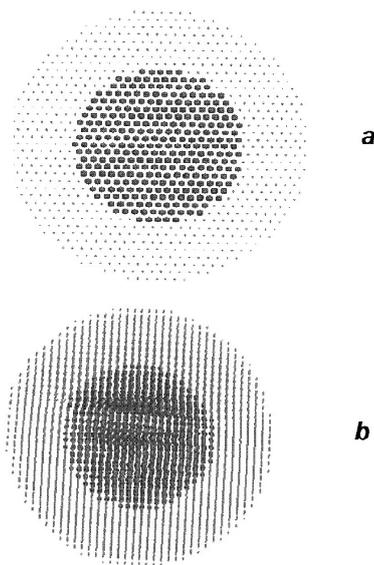


Fig. 3. Fragment of a crystallite containing a Cu particle of radius $R = 2.6$ nm (a) and $R = 3.2$ nm (b) in the Fe matrix.

ening to trapping of dislocations by particles because of a structural instability is followed by a considerable increase in the slope of the dependence $\Delta E_{max}(R)$.

3. CONCLUSIONS

The simulation demonstrated that within a certain range of sizes of copper precipitates in bcc iron the decisive role is played by a specific mechanism of hardening, which results from a structural instability in the particles, with the instability being initiated by introduction of a dislocation. This mechanism is complementary to the commonly discussed mechanism of a modulus misfit strengthening mechanism and hardening caused by elastic fields of the precipitates. The mechanism of hardening with metastable nanoscale precipitates, which has been discussed herein, will be absent in the case of fine ($R < 2.2$ nm) and coarse particles having a stable bcc or 9R/fcc structure¹.

¹ After manuscript submitting paper [10] appears where also presented results of the MD simulations of the interaction between edge dislocation and copper precipitates in iron. Though in [10] considered other regime (Orowan bowing) the results are largely in agreed with obtained in present work.

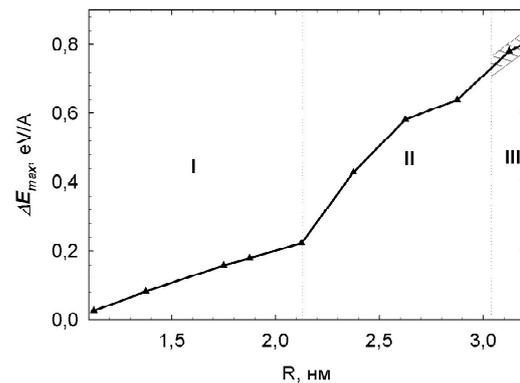


Fig. 4. Energy ΔE_{max} required for a dislocation to pass a precipitate of radius R .

REFERENCES

- [1] K. Topasa, D.J. Bacon and Yu.N. Osetsky // *Modelling. Simul Mater. Sci. Eng.* **44** (2006) 1153.
- [2] S.Y. Hu, S. Schmauder and L.Q. Chen // *Phys. stat. sol. (b)* **220** (2000) 845.
- [3] M. Luwig, D. Farkas, D. Pedraza and S. Schmauder // *Modelling. Simul. Mater. Sci. Eng.* **6** (1998) 19.
- [4] M.S. Daw and M.I. Baskes // *Phys. Rev.* **29B** (1984) 6443.
- [5] V. Shastri and D. Farkas // *Mater. Res. Soc. Symp. Proc.* **408** (1996) 217.
- [6] Y. Mishin, M. J. Mehl, D. A. Papaconstantopoulos, A.F. Voter and J.D. Kress // *Phys. Rev B* **63** (2001) 224106.
- [7] A. Caro, D.A. Crowson and M. Caro // *Alloys. Phys. Rev. Lett.* **95** (2005) 075702.
- [8] A. Caro, M. Caro, E.M. Lopasso, P.E.A Tuci and D. Farkas // *J. of Nucl. Mater.* **349** (2006) 317.
- [9] J. Z. Liu, A. van de Walle, G. Ghosh and M. Asta // *Phys. Rev.* **B 72** (2005) 1.
- [10] D.J. Bacon and Yu.N. Osetsky // *Phil Mag.* **89** (2009) 3333. (Footnotes)

