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Thermodynamic calculation of the probability of stacking fault formation in b.c.c. Fe–Zn alloys

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Abstract

An X-ray study of faulting in Fe–Zn alloys was carried out. A correlation between X-ray data and thermodynamic calculations can be used to explain the deformation stacking faults.

1. Introduction

The study of structural imperfections of b.c.c. alloys sheds light on the mechanism of physicochemical interaction of the components. X-ray diffraction methods of investigation of the faulting of the crystal structure in metals and alloys allow the determination, from the broadening of the diffraction maxima, of the particle size, the microstrains of the crystal lattice and the probability of formation of stacking faults. The change in these structural characteristics with alloy composition suggests conclusions on the influence of doping on the formation of the dislocation structure determining the behaviour of the alloys upon their application.

The stacking fault energy is the parameter characterizing the dislocation structure. Owing to its relatively high values in the b.c.c. structure, direct methods of electron microscopy are inapplicable to the determination of stacking fault energy. The present study aims at the determination of stacking fault energy by the stability difference of b.c.c. and f.c.c. (or h.c.p.) lattices.

2. Thermodynamics of zinc-doped ferrites

It is known [1] that the thermodynamic potential of the α phase in the Fe–Zn state diagram is defined by

$$G^{\alpha}_{Fe-Zn}=xG^{\alpha}_{Zn}+(1-x)G^{\alpha}_{Fe}+xRT\ln x + (1-x)RT\ln(1-x)+E^{\alpha} \qquad (1)$$

where x is the atomic fraction of zinc, $1-x$ is the atomic fraction of iron, G^{α}_{Zn} and G^{α}_{Fe} are the standard thermodynamic potentials in the b.c.c. structure and E^{α} is the excess thermodynamic potential.

In the case of a subregular solution, E^{α} is determined by

$$E^{\alpha}=x(1-x)[A^{\alpha}+B^{\alpha}(1-2x)] \qquad (2)$$

where A^{α} and B^{α} are temperature-dependent parameters of the subregular solid solution.

An expression similar to (2) can be used for the thermodynamic potential of the γ phase in the Fe–Zn diagram:

$$E^{\gamma}=x(1-x)[A^{\gamma}+B^{\gamma}(1-2x)] \qquad (3)$$

The difference in the thermodynamic potentials of the α and γ phases or the b.c.c. and f.c.c. structures is given by

$$\Delta G^{\alpha\to\gamma}_{Fe-Zn}=x\Delta G^{\alpha\to\gamma}_{Zn}+(1-x)\Delta G^{\alpha\to\gamma}_{Fe}+\Delta E^{\alpha\to\gamma} \qquad (4)$$

3. Experimental details

Alloys of the Fe–Zn system representing solid solutions of zinc in α-Fe were studied.

Samples were obtained by melting iron of 4N purity and zinc of 6N purity. The alloys were homogenized by thermal treatment and quenched from 1273 K.

Powder specimens were measured by Co Kα radiation under appropriate kinematic conditions. The [110], [211] and [220] reflections were recorded and the method of harmonic analysis [2] was applied to the treatment of the experimental data. The probability of stacking fault formation is represented by

$$\frac{1}{D_{eff}}=\frac{1}{D_r}+\frac{1.5\alpha+\beta}{a(u-b)H_0}\sum_{b}L_0 \qquad (5)$$

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where a is the lattice parameter; b is the number of reflection components broadened by the stacking faults; u is the number of reflection components that are not broadened by stacking faults; $H_0=\sqrt{H^2+K^2+L^2}$, H, K, L are the indices of reflection in normal cubic axes; L_0 is the third index in the orthorhombic axes; D_{eff} is the effective particle size, reflecting simultaneously the effect of the dispersity and that of the presence of stacking faults, D_{r} is the real crystallite size and $1.5\alpha+\beta$ is the probability of formation of deformation and twinning faults.

The experimental results are presented in Table 1. The probability of stacking fault formation is the quantity characterizing the tendency shown by the alloys to form faults. The change in this quantity at different compositions determines the influence of the amount and nature of the doping component. The appearance of stacking faults probably depends in inverse proportion on the energy of their formation. The energy values determined by X-ray methods are afflicted by a large error. The thermodynamic data [1] have been used to determine the probability of stacking fault formation (Table 2).

The following values of the subregular solution constants were used: $A^{\alpha}=706.56$ J (g atom)$^{-1}$, $A^{\gamma}=961.0$ J (g atom)$^{-1}$, $B^{\alpha}=258.58$ J (g atom)$^{-1}$ and $B^{\gamma}=0$. The calculated differences in the stability parameters are given in Table 3 as a function of the composition of the alloys studied.

TABLE 1. Structural characteristics of b.c.c. Fe–Zn alloys

Zn (at.%)	$D_{[110]}$ (nm)	$D_{[211]}$ (nm)	D_{r} (nm)	$(1.5\alpha+\beta)\times10^3$
5.6	36.0	24.0	111.0	11.6
9.5	30.0	20.0	111.0	15.0
11.0	28.0	18.0	124.0	16.4
13.0	26.0	16.5	143.0	19.2
15.0	25.0	15.0	250.0	21.7

TABLE 2. Stability parameters of the structure in the Fe–Zn system

Parameter at 1273 K	Fe	Zn
$\Delta G^{\alpha\to\gamma}$ (J (g atom)$^{-1}$)	3.08	−1.009
$\Delta G^{\alpha\to\epsilon}$ (J (g atom)$^{-1}$)	149.23	−225.800

ϵ is the h.c.p. phase.

TABLE 3. Stability parameters of Fe–Zn alloys at 1273 K

Zn (at.%)	$\Delta G^{\alpha\to\gamma}$ (J (g atom)$^{-1}$)	$\Delta G^{\alpha\to\epsilon}$ (J (g atom)$^{-1}$)
5.6	0.68	128.10
9.5	−0.83	113.10
11.0	−2.93	107.86
13.0	−5.02	100.36
15.0	−7.36	92.86

4. Results and discussion

The geometry of stacking faults in the b.c.c. structure in the [211] planes shows that the twinning fault is a structure of atomic layers ordered as in the f.c.c. lattice, while the deformation fault is observed on ordering of the layers similar to the h.c.p. lattice. For this reason it can be assumed that stacking faults are probably formed depending on the difference in the stability of these structures under the experimental conditions. The results are obtained from the study of the structural characteristics of alloys representing solid solutions of zinc in α-Fe with b.c.c. structure, homogenized and quenched from 1273 K. The stacking fault formation in these alloys will depend on the difference in the thermodynamic potential of the alloys crystallized in a b.c.c. lattice and those of the f.c.c. and h.c.p. lattices.

The results of the X-ray studies suggest that the introduction of zinc causes an increase in the microstrains in the lattice of α-Fe at the applied temperature, and hence the dispersity is also increased. This is explained by the influence of the geometric factor. The effect of zinc on the tendency of the alloys to form stacking faults can be explained by taking into account the general rule that the doping component increases the probability of appearance of stacking faults.

As seen from the data presented in Table 3, the change in $\Delta G^{\alpha\to\gamma}$ with increasing amount of zinc introduced leads to a stabilization of the b.c.c. structure, *i.e.* these zinc amounts do not influence the stability of the iron b.c.c. lattice and do not cause the appearance of the f.c.c. structure. The change in $\Delta G^{\alpha\to\epsilon}$ shows that a probability of formation of h.c.p. layers exists and this probability grows with increasing zinc content. The decrease in $\Delta G^{\alpha\to\epsilon}$ suggests a thermodynamic possibility of the appearance of deformation stacking faults.

Since the literature lacks experimental data on the stacking fault energy in Fe–Zn alloys, the change in the thermodynamic potential upon structural transition could be explained by the experimental X-ray data on the probability of stacking fault formation, which depends inversely on the energy. The established correlation between the change in $\Delta G^{\alpha\to\epsilon}$ and the probability of formation of stacking faults proves the influence of the amount and nature of the doping component on the structural characteristics of alloys.

References

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