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The influence of aluminium content to the stacking fault energy in Fe–Mn–Al–C alloy system

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Four Fe–30Mn–0.9C–*X*Al alloys are employed to investigate the influence of aluminium content to the stacking fault energy in Fe–Mn–Al–C alloy system. The range of aluminium content is zero to 8.47 wt%. Based on the thermodynamic model, the stacking fault energy can be obtained through calculation. Increasing the aluminium content will make the stacking fault energy of Fe–30Mn–0.9C based alloys increase at 300 K.

Introduction

In addition to the research of corrosion resistance, the study of the mechanical behaviour of the Fe–Mn–Al–C alloy system is also an important topic. In the past years, literature on the mechanical properties such as the high strength, high toughness and high work hardening rate have been reported for the Fe–Mn–Al–C alloys with austenite single phase [1–4]. However, a detailed and systematic investigation on those basic parameters which are always playing important roles in the mechanical behaviour of the Fe–Mn–Al–C alloy is still incomplete. In general, a full austenite Fe–Mn–Al–C alloy with zero aluminium content is quite similar to a high manganese steel or Hadfield steel except it has much higher manganese content. For Fe–30Mn–0.9C–*X*Al based alloys, as the aluminium content changes from zero to 1.44, 5.09 and 8.47 wt %, the lattice parameter of austenite phase increases from 0.3631 to 0.3644, 0.3662 and 0.3674 nm, respectively [5]. From Zuidema *et al.*'s report [6], the addition of aluminium content was also related to the strain induced twinning in regular high manganese steels such as Hadfield steel. Besides, Zuidema also suggested that the strain induced twinning is correlated to the stacking fault energy of the alloy.

It is well known that the stacking fault energy is deeply involved with the mechanical behaviour of most alloys. However, the measurement of stacking fault energy is quite difficult and is not very accurate. The present work is trying to obtain the stacking fault energy of Fe–Mn–Al–C alloy with different aluminium content through calculation.

2. Previous related studies

According to Remy's report [7], the kinetics of deformation twinning in fcc alloys are concerned to be enhanced by the low intrinsic stacking fault energy of the alloys. Remy [7] suggested that the nucleation of a twin in fcc alloys can be considered as being achieved by the propagation of stacking fault in neighbouring plane. Sipos *et al.* [8] proposed that a twin nuclei could be initiated by three layers of microtwin. Such effect is evolved from the interaction of two perfect dislocations with the following reaction.

$$\tfrac{1}{2}[1\,0\,1] + \tfrac{1}{2}[1\,1\,0] \rightarrow 3 \times \tfrac{1}{6}[2\,1\,1]$$

The reaction as above can be generally governed by the nucleation of three layers of microtwin in the fcc crystal.

From the various model, a fcc alloy which has a low stacking fault energy, the perfect dislocation $\frac{1}{2}[1\,1\,0]$ generally can split into two. Shockly partial dislocations with $\frac{1}{6}[2\,1\,1]$ and $\frac{1}{6}[1\,2\,1]$. The intrinsic stacking fault can be formed by the motion of a single Shockley partial dislocation $\frac{1}{6}[2\,1\,1]$ on the (1 1 1) close packed plane. Based on the thermodynamic analysis, the intrinsic fault energy can be written in the following way:

$$\gamma_I = 2\varrho_A \Delta G^{\gamma-\varepsilon} + 2\sigma^{\gamma-\varepsilon} \quad (1)$$

γ_I is the stacking fault energy of the alloys; $\Delta G^{\gamma-\varepsilon}$ is the molar free energy difference between fcc and hcp phase; ϱ_A is the planar packing density of a close packed plane; $\sigma^{\gamma-\varepsilon}$ is the coherent interfacial energy between fcc and hcp.

According to Adler *et al.* [9], the calculated stacking fault energy can fit quite well with the measured composition and temperature in transition metal alloys.

3. Calculation and discussion

The chemical composition of the present used alloys are shown in Table I. The following stacking fault energies changed with different aluminium content are calculated from thermodynamic model which has been proposed by Olson *et al.* [10].

Through adopting a regular solution model, $\Delta G^{\gamma-\varepsilon}$ can be expressed for the present Fe-rich Fe–Mn–Al–C

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TABLE I Chemical composition of the present used alloys

Alloy	Al		Mn		C		Fe	
	wt %	at %	wt %	at %	wt %	at %	wt %	at %
A	0	0	29.15	28.6	0.81	3.6	70.04	67.7
B	1.44	2.8	30.91	29.9	0.88	3.9	66.77	64.4
C	5.09	9.7	30.95	28.8	0.88	3.7	63.08	57.8
D	8.47	15.7	30.06	27.1	0.88	3.6	60.59	53.7

alloys as follows:

$$\Delta G^{\gamma-\varepsilon} = X_{Fe}\Delta G_{Fe}^{\gamma-\varepsilon} + X_{Mn}\Delta G_{Mn}^{\gamma-\varepsilon} + X_{Al}\Delta G_{Al}^{\gamma-\varepsilon} + X_C\Delta G_C^{\gamma-\varepsilon} + X_{Fe}X_{Mn}\Delta\Omega_{FeMn}^{\gamma-\varepsilon} + X_{Fe}X_{Al}\Delta\Omega_{FeAl}^{\gamma-\varepsilon} + X_{Fe}X_C\Delta\Omega_{FeC}^{\gamma-\varepsilon} \quad (2)$$

where X_i and $\Delta G_i^{\gamma-\varepsilon}$ represent the molar fraction and the difference of free energy between fcc and hcp of pure metals. $\Delta\Omega_{ij}^{\gamma-\varepsilon}$ is an interaction energy parameter for components i and j.

The values of the thermodynamic parameters at 300 K have been derived by Stepakoff and Kaufman, [11], Breedis and Kaufman [12], Ishida and Nishiyawa [13] and Adler *et al.* [9] and are shown below:

$$\Delta G_{Fe}^{\gamma-\varepsilon} = -59\,\text{cal mol}^{-1} \quad (3)$$

$$\Delta G_{Mn}^{\gamma-\varepsilon} = 830\,\text{cal mol}^{-1} \quad (4)$$

$$\Delta\Omega_{FeMn}^{\gamma-\varepsilon} = -2590 + 5470X_{Mn}\,\text{cal mol}^{-1} \quad (5)$$

$$\Delta\Omega_{FeC}^{\tau-\varepsilon} = 10167\,\text{cal mol}^{-1} \quad (6)$$

According to the analysis by Ericsson [14] and Hirth [15], the stacking fault energy of pure metal was considered to be almost the same as the free energy difference between the fcc and hcp structure of one stomic layer of the metal. Hence

$$\tau_I = \Delta G_x^{\tau-\varepsilon}/V^{2/3} \times N_0^{1/3} = \Delta G_x^{\tau-\varepsilon}/V^{2/3}(6.02 \times 10^{23})^{1/3} \times 4 \times 18 \times 10^7 \cong \Delta G_x^{\tau-\varepsilon}/2V^{2/3}\,\text{erg cm}^{-2}$$

where τ_I is the stacking fault energy of pure metal, V is molar volume and N_0 is Avogadro's number. The stacking fault energy τ_{Al} is equal to 166 erg cm^{-2} [16] and molar volume of aluminium is about 10 cm^3 mol^{-1}.

Therefore, $\Delta G_{Al}^{\tau-\varepsilon}$ can be calculated as follows:

$$\Delta G_{Al}^{\tau-\varepsilon} = 1541\,\text{cal mol}^{-1} \quad (7)$$

The other values of thermodynamic parameters $\Delta\Omega_{FeAl}^{\gamma-\varepsilon}$ and $\Delta G_C^{\gamma-\varepsilon}$ can be estimated from the following appropriate equation [13]:

$$\Delta G_x^{\gamma/\varepsilon Fe} = \Delta G_{Fe}^{\gamma-\varepsilon} - \left(\frac{\partial}{\partial T}\Delta G_{Fe}^{\gamma-\varepsilon}\right) \times (1 - X_{Mn} - X_x)\frac{\Delta T_0}{X_x} \quad (8)$$

$$\Delta G_x^{\gamma/\varepsilon Fe} = \Delta G_x^{\gamma-\varepsilon} + \Delta\Omega_{FeX}^{\gamma-\varepsilon} \quad (9)$$

where ΔT_0 is the change in $T_0^{\gamma/\varepsilon}$ temperature of Fe–Mn alloys by the alloying of X_x and $(\partial/\partial T\ \Delta G_{Fe}^{\gamma-\varepsilon})$ is estimated 0.99 at 300 K from the thermodynamic data of Stepakoff and Kaufman [11].

By using the thermodynamic data in Ishida and Nishizawa's report [13] and Equation 8 $\Delta G_C^{\gamma/\varepsilon Fe}$ and $\Delta G_{Al}^{\gamma/\varepsilon Fe}$ can be estimated:

$$\Delta G_C^{\gamma/\varepsilon Fe} = 4283\,\text{cal mol}^{-1} \quad (10)$$

$$\Delta G_{Al}^{\gamma/\varepsilon Fe} = 2336\,\text{cal mol}^{-1} \quad (11)$$

From Equation 9 and Equations 6, 7, 10 and 11, the $\Delta G_C^{\gamma-\varepsilon}$ and $\Delta\Omega_{FeAl}^{\gamma-\varepsilon}$ can be calculated:

$$\Delta G_C^{\tau-\varepsilon} = -5884\,\text{cal mol}^{-1} \quad (12)$$

$$\Delta\Omega_{FeAl}^{\gamma-\varepsilon} = 795\,\text{cal mol}^{-1} \quad (13)$$

From Equation 2 , the value of $\Delta G^{\gamma-\varepsilon}$ for the present four alloys can be calculated to be

$$\Delta G^{\gamma-\varepsilon} = 34.7\,\text{cal mol}^{-1}\ \text{(alloy A)}$$

$$\Delta G^{\gamma-\varepsilon} = 94.9\,\text{cal mol}^{-1}\ \text{(alloy B)}$$

$$\Delta G^{\gamma-\varepsilon} = 230\,\text{cal mol}^{-1}\ \text{(alloy C)}$$

$$\Delta G^{\gamma-\varepsilon} = 387\,\text{cal mol}^{-1}\ \text{(alloy D)}$$

The packing density of the four alloys is calculated from lattice parameter of austenite phase.

$$\varrho = 2.52 \times 10^{-9}\,\text{mol cm}^{-2}\ \text{(alloy A)}$$

$$\varrho = 2.50 \times 10^{-9}\,\text{mol cm}^{-2}\ \text{(alloy B)}$$

$$\varrho = 2.48 \times 10^{-9}\,\text{mol cm}^{-2}\ \text{(alloy C)}$$

$$\varrho = 2.46 \times 10^{-9}\,\text{mol cm}^{-2}\ \text{(alloy D)}$$

The interfacial energy between fcc and hcp is about $10 \pm 5\,\text{mJ m}^{-2}$ for transition metals. Using Equation 1 and the values of $\Delta G^{\gamma-\varepsilon}$, $\varrho^{\gamma-\varepsilon}$ and $\sigma^{\gamma-\varepsilon}$, the stacking fault energy of the present four alloys are calculated as follows:

$$\gamma_I = 27.3 \pm 10\,\text{ergs cm}^{-2}\ \text{(alloy A)}$$

$$\gamma_I = 39.8 \pm 10\,\text{ergs cm}^{-2}\ \text{(alloy B)}$$

$$\gamma_I = 67.7 \pm 10\,\text{ergs cm}^{-2}\ \text{(alloy C)}$$

$$\gamma_I = 99.6 \pm 10\,\text{ergs cm}^{-2}\ \text{(alloy D)}$$

4. Conclusion

1. Based on thermodynamic model, the stacking fault energy for Fe–Mn–Al–C alloy with austenite single phase can be obtained through calculation and the stacking fault energy is calculated which increases with increasing aluminium content.

2. For Fe–30Mn–0.9C–XAl based alloys, the stacking fault energy can be calculated to be changed from 27.3 to 39.8, 67.7 and 99.6 ergs cm^{-2} as X increases from zero to 1.44, 5.09 and 8.47 wt %.

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