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Influence of addition elements on the stacking-fault energy and mechanical properties of an austenitic Fe–Mn–C steel

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Abstract

We present a thermochemical model of the stacking-fault energy (SFE) in the Fe–Mn–C system with few percent of Cu, Cr, Al and Si in addition. Aluminium strongly increases the SFE, contrary to chromium, while the effect of silicon is more complex. Copper also increases the SFE, but strongly decreases the Néel temperature. The SFE is the relevant parameter that controls mechanical twinning, which is known to be at the origin of the excellent mechanical properties of these steels. Using this model, copper containing Fe–Mn–C grades were elaborated with SFE below 18 mJ/m^2, in the range where ε-martensite platelets form instead of microtwins during plastic deformation. This substitution of deformation modes, confirmed by X-ray diffraction, does not significantly damage the mechanical properties, as long as the SFE is greater than 12 mJ/m^2, which avoids the formation of α'-martensite.

Keywords: Fe–Mn–C; Stacking-fault energy; Martensitic transformation; Strain hardening

1. Introduction

The $Fe_{22}Mn_{0.6}C$ fcc steel developed by Arcelor exhibits mechanical twinning in addition to dislocation gliding when deformed at room temperature [1–3]. The fine microtwins formed along with plastic deformation act as strong obstacles, such as grain boundaries, and lead to a “dynamical Hall and Petch effect”, a high strain hardening rate and consequently both excellent elongation to fracture (>50%) and ultimate tensile strength (>900 MPa). The relevant parameter for twinning is the stacking-fault energy (SFE) which depends on temperature and composition.

The best hardening rate is obtained at room temperature in this steel, where its SFE is intermediate ($\approx$20 mJ/m^2) [1,3]. At higher values, twinning tends to disappear, while below 18 mJ/m^2 microtwins are replaced by hcp ε-martensite platelets. In an alloy design approach, it is necessary to predict the temperature and composition dependence of the SFE, in order to adjust an alloy’s grade to its forming or service conditions.

We first present a thermochemical model based on the one previously developed for the Fe–Mn–C system, in order to predict the effect of adding few percents of copper, chromium, aluminium or silicon on the SFE. An example of the influence of the SFE on the mechanical properties and deformation microstructure, in connection with the model’s prediction, is presented in the second part in the case of copper.

2. Thermochemical modelling of the stacking-fault energy

In fcc structures, twinning is due to stacking faults (SFs) extending in parallel adjacent dense planes. Extending them every two planes leads to the formation of ε-martensite. A stacking fault can be modelled by two atomic layers of ε-martensite within the dense planes. This allows to write the SFE as [4]:

$$\Gamma = 2\rho\,\Delta G^{\gamma\to\varepsilon} + 2\sigma^{\gamma/\varepsilon} \qquad (1)$$

with $\Delta G^{\gamma\to\varepsilon}$, the free molar enthalpy of the transformation $\gamma\to\varepsilon$, ρ the molar surface density of atoms in the $\{1\,1\,1\}$ planes and $\sigma^{\gamma/\varepsilon} = 8$ mJ/m^2 [1] the energy per surface unit of a $\{1\,1\,1\}$ interface between γ and ε.

According to the simplified previous model for the Fe–Mn–C system [3], the free molar enthalpy of martensite formation can

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be written as follow:

$$\Delta G^{\gamma\to\varepsilon} = \Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX}} + x_{\mathrm{c}}\,\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX/C}} + \Delta G^{\gamma\to\varepsilon}_{\mathrm{mg}} \qquad (2)$$

Using the regular and subregular solution model, $\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX}}$ is the chemical contribution of all the elements in substitution in the fcc lattice. The Fe–Mn excess term is taken into account but the others involving the addition elements are neglected because of the little quantities considered, except for silicon:

$$\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX}} = \sum_i x_i\,\Delta G^{\gamma\to\varepsilon}_i + x_{\mathrm{Fe}}x_{\mathrm{Mn}}[C + D(x_{\mathrm{Fe}} - x_{\mathrm{Mn}})] + x_{\mathrm{Fe}}x_{\mathrm{Si}}[E + F(x_{\mathrm{Fe}} - x_{\mathrm{Si}})] \qquad (3a)$$

$$\Delta G^{\gamma\to\varepsilon}_i = A_i + B_iT, \quad i = \text{Fe, Mn, Cu, Cr, Al, Si} \qquad (3b)$$

with x_i the molar fraction of element i, T the temperature and $\{A_i\}$, $\{B_i\}$, C, D, E and F fitting parameters.

Carbon in insertion is simply introduced as a disturbance of the former fcc solid solution [5]. An empirical law has been improved since [3], to account for an increasing carbon effect with manganese content:

$$\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX/C}} = \frac{a}{x_{\mathrm{C}}}(1 - \mathrm{e}^{-bx_{\mathrm{C}}}) + cx_{\mathrm{Mn}} \qquad (4)$$

where a, b and c are fitting parameters according to Ref. [1].

$\Delta G^{\gamma\to\varepsilon}_{\mathrm{mg}}$ is a magnetic term, due to the Néel transition (paramagnetic to antiferromagnetic) of each phase φ:

$$\Delta G^{\gamma\to\varepsilon}_{\mathrm{mg}} = G^{\varepsilon}_{\mathrm{m}} - G^{\gamma}_{\mathrm{m}} \qquad (5a)$$

where

$$G^{\varphi}_{\mathrm{m}} = RT\ln\left(1 + \frac{\beta^{\varphi}}{\mu_{\mathrm{B}}}\right) f\left(\frac{T}{T^{\varphi}_{\mathrm{N}}}\right), \quad \varphi = \gamma, \varepsilon \qquad (5b)$$

with β^{φ} and T^{φ}_{N}, respectively, the magnetic moment and Néel temperature of phase φ, μ_{B} the Bohr magneton and f a polynomial function which expression can be found in Ref. [6].

ρ, $\Delta G^{\gamma\to\varepsilon}_{\mathrm{Fe}}$, $\Delta G^{\gamma\to\varepsilon}_{\mathrm{Mn}}$ and $T^{\varepsilon}_{\mathrm{N}}$ are unchanged compared to Ref. [3]. β^{γ}, β^{ε} have been improved in Ref. [1] to take the effect of carbon into account (additional elements in substitution are neglected):

$$\beta^{\gamma} = \beta^{\gamma}_{\mathrm{Fe}}x_{\mathrm{Fe}} + \beta^{\gamma}_{\mathrm{Mn}}x_{\mathrm{Mn}} - \beta^{\gamma}_{\mathrm{FeMn}}x_{\mathrm{Fe}}x_{\mathrm{Mn}} - \beta_{\mathrm{C}}x_{\mathrm{C}} \qquad (6a)$$

$$\beta^{\varepsilon} = \beta^{\varepsilon}_{\mathrm{Mn}}x_{\mathrm{Mn}} - \beta_{\mathrm{C}}x_{\mathrm{C}} \qquad (6b)$$

with β^{φ}_i the contribution of element i in phase φ and β^{φ}_{ij} the excess i–j term. An empirical expression of T^{γ}_{N} has been fitted to data of literatures [7–10] and measurements conducted on our FeMnCuC alloys. $T^{\varepsilon}_{\mathrm{N}}$ is given in Ref. [3]:

$$T^{\gamma}_{\mathrm{N}} = 250\ln(x_{\mathrm{Mn}}) - 4750x_{\mathrm{C}}x_{\mathrm{Mn}} - 222x_{\mathrm{Cu}} - 2.6x_{\mathrm{Cr}} - 6.2x_{\mathrm{Al}} - 13x_{\mathrm{Si}} + 720\,(\mathrm{K}) \qquad (7a)$$

$$T^{\varepsilon}_{\mathrm{N}} = 580x_{\mathrm{Mn}}\,(\mathrm{K}) \qquad (7b)$$

Table 1
Summarised parameters of the model from Refs. [1,3] and the present work for addition elements (T in K)

ρ	$2.94 \times 10^{-5}\,\mathrm{mol\,m^{-2}}$	[3]
$\sigma^{\gamma/\varepsilon}$	$8\,\mathrm{mJ\,m^{-2}}$	[1]
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Fe}}$	$-2243.38 + 4.309T\,\mathrm{J\,mol^{-1}}$	[3]
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Mn}}$	$-1000.00 + 1.123T\,\mathrm{J\,mol^{-1}}$	[3]
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMn}}$	$C = 2873\,\mathrm{J\,mol^{-1}}$; $D = -717\,\mathrm{J\,mol^{-1}}$	[1]
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeMnX/C}}$	$a = 1246\,\mathrm{J\,mol^{-1}}$; $b = 24.29\,\mathrm{J\,mol^{-1}}$; $c = -17{,}175\,\mathrm{J\,mol^{-1}}$	[1]
$\beta^{\gamma}/\mu_{\mathrm{B}}$	$0.7x_{\mathrm{Fe}} + 0.62x_{\mathrm{Mn}} - 0.64x_{\mathrm{Fe}}x_{\mathrm{Mn}} - 4x_{\mathrm{C}}$	[1]
$\beta^{\varepsilon}/\mu_{\mathrm{B}}$	$0.62x_{\mathrm{Mn}} - 4x_{\mathrm{C}}$	[1]
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Al}}$	$2800 + 5T\,\mathrm{J\,mol^{-1}}$	
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Cr}}$	$1370 - 10T\,\mathrm{J\,mol^{-1}}$	
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Cu}}$	$2273\,\mathrm{J\,mol^{-1}}$	
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{Si}}$	$-560 - 8T\,\mathrm{J\,mol^{-1}}$	
$\Delta G^{\gamma\to\varepsilon}_{\mathrm{FeSi}}$	$E = 2850\,\mathrm{J\,mol^{-1}}$; $F = 3520\,\mathrm{J\,mol^{-1}}$	

A current assumption [11,12] is that the ε-martensitic (and the reverse austenitic) thermal transformations occurs when $\Delta G^{\gamma\to\varepsilon} \approx -100$ J/mol (respectively, +100 J/mol; we find that +80 J/mol gives better results). The parameters for FeMnC have been obtained first [1]. Then, the parameters concerning the addition elements are fitted to give the best accordance with 120 transformation temperatures of different compositions with less than 5 wt.% of alloying elements. All data have been found in Refs. [6,7,11,13–23]. The set of parameters which give the best estimation of the transformation temperatures over the whole database is summarised in Table 1 (results from Refs. [3,1] and the present paper).

Fig. 1 shows the result when adding each element to the $\mathrm{Fe_{22}Mn_{0.6}C}$ steel. Petrov measured the SFE by loss-energy method and deduced the influence of chromium [23], which is rather weak; our model is in good agreement with his results. Copper and even more aluminium increase the SFE, contrary to chromium. Copper is shown to strongly decrease T_{N}. Silicon have a complex effect on SFE, increasing SFE for small quantities and decreasing it at higher ones. Previous studies on silicon effect showed that Si decreases the SFE but their range of validity is over 4 wt.% [21,24].

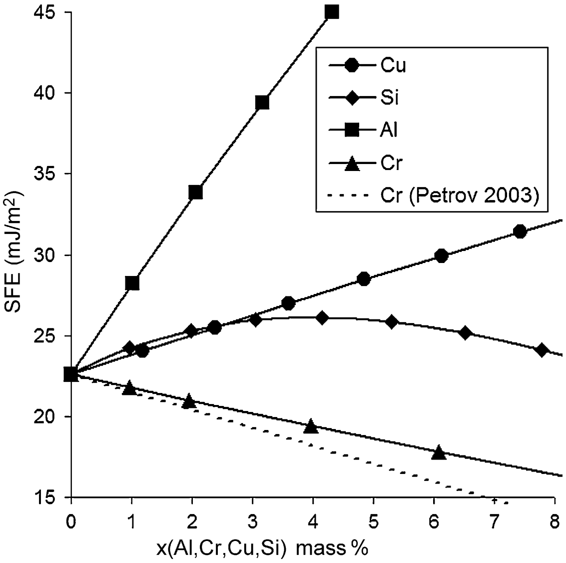

Fig. 1. Predicted influence of alloying elements on the SFE of the $\mathrm{Fe_{22}Mn_{0.6}C}$ reference.