Variation of the alloying elements effect on the stacking fault energy with temperature

Hamza ESSOUSSI¹, Saïd ETTAQI¹, El Hachmi ESSADIQI².

¹ Laboratory of Materials, Metallurgy and Process Engineering, ENSAM, Meknes, Morocco.
² Aeronautic Laboratory of International University, Rabat, Morocco.

Abstract:
Good mechanical properties of high manganese steels are related in first order to the presence of different mechanisms of deformation, in the other hand the activation of each mechanism depends on the value of stacking fault energy (SFE). With a decreasing value of the SFE, the plasticity of these steels is achieved by: (i) gliding of partial and perfect dislocations, (ii) gliding and mechanical twinning (iii) gliding and ε martensitic transformation, while the variation of SFE value is governed by temperature and chemical composition. The aim of this paper is to highlight the variation of alloying element effect on the SFE with temperature by using the model of Olsen-Cohen.

Keywords: Stacking fault energy, Temperature, Alloying elements, High manganese steels.

1. Introduction
Plastic deformation of austenitic steels is a complex process, mostly heterogeneous, due to the simultaneous effect of several mechanisms of deformation. The dominate mechanism of deformation depends on an external parameter temperature and another internal which is chemical composition.

This paper aimed to show that temperature changes the effect of alloying element on the stacking fault energy is divided in two parts: The first one is focused on the definition of stacking fault energy, the thermochemical model [1] developed to predict the effect of adding few amount of copper, chromium, aluminum or silicon on system Fe-Mn-C. The second part shows the results of modeling.

2. Stacking fault energy definition:
SFE is defined as the energy that measured the stability of hexagonal close packed phase (phase ε) against the faceted centered cubic phase (phase γ) [2], this stability is due to the diminution of free molar enthalpy of martensitic phase formation compared to austenitic phase.

Generally the dissociation of perfect dislocations to partial dislocations is the first generator of stacking fault.

\[ \vec{b} \rightarrow \frac{\vec{a}}{2}[\overline{1}10] + \frac{\vec{a}}{6}[\overline{1}2\overline{1}] + \frac{\vec{a}}{6}[\overline{2}11] \]

The energy of dislocation’s line is proportional to the square of Burgers vector, so the dissociation according to the relationship (1) occurred if:

\[ \frac{a^2}{2} > \frac{a^2}{6} + \frac{a^2}{6} \] (3)

3. Stacking fault energy modeling:
A widely used approach to calculate an ideal SFE was proposed by Olsen and Cohen [2], which defines the required Gibbs free energy to form an intrinsic stacking fault by the movement of a single Shockley partial dislocation occurring on every second plane, a hexagonal close packed (hcp) crystalline structure is formed with thickness of two atomic layers. The core equation to calculate the SFE is:

\[ SFE = 2\rho\Delta G^{\gamma\epsilon} + 2\sigma^{\gamma/\epsilon} \] (4)

Where :
• \(\rho\) : is the molar surface density along \{111\} planes;
• \(\Delta G^{\gamma\epsilon}\) : is the change of molar Gibbs free energy due to the transformation of (cfc) austenite to (hcp) martensite;
• \(\sigma^{\gamma/\epsilon}\) : defines the interfacial energy of the \(\gamma/\epsilon\) interface.

The Gibbs free energy of \(\gamma \rightarrow \epsilon\) phase transformation \(\Delta G^{\gamma\epsilon}\) was intensively discussed in several works in literature like those of S.Allain and P.Dummy [2,3], and its detail expression was divided into magnetic and magnetic contribution.

\[ G^\gamma = G_{\chi m}^\gamma + G_{mag}^\gamma \] (5)

The chemical effect was also divided in two terms one of alloying element and the other is only for carbon (interstitial element) effect.

\[ \Delta G^{\gamma\epsilon} = \Delta G_{FeMnX}^\gamma + x_c\Delta G_{FeMnX/\epsilon}^{\gamma\epsilon} + \Delta G_{mag}^{\gamma\epsilon} \] (6)

With :
• \(\Delta G_{FeMnX}^{\gamma\epsilon}\) : is the contribution of substitution alloying elements within CFC structure, with X= Cu, Cr, Al, Si.
• \(\Delta G_{FeMnX/\epsilon}^{\gamma\epsilon}\) : is the contribution of Carbon in insertion; 
• \(\Delta G_{mag}^{\gamma\epsilon}\) : Is the magnetic contribution due to the Néel transition of each phase.
The detail values of all expressions mentioned above were given in the works [1-4], and the table 1 gives the chemical composition of the tested TWIP steels for SFE calculation.

![Table 1: chemical composition of the tested TWIP steel][4]

### 4. Results & discussions:

**a- Temperature effect:**

In fig.2. We show the total stacking fault energy, chemical and magnetic contributions as functions of temperature. And the value of SFE found at room temperature for this material (TWIP 2) is equal to 20.5 mJ/m² and it is in good agreement with the result referred in [4]

![Fig.2. The predicted effect of temperature on the SFE][5]

We appear clear that the increasing temperature increases also the SFE. That is due in fact to at low temperature the magnetic contribution is the dominate contribution. While, at high temperature the effect of moment magnetic atoms disappear then the chemical effect takes place.

**b- Alloying elements effect:**

It is well known that each alloying element has its own effect on the SFE, while this effect changes with temperature. The temperatures chosen for this study are in the temperature range used for the thermal treatments of these steels as it found in reference [5].

![Fig.3. The predicted effect of Al, Cr and Si on the SFE of TWIP 2 material at room temperature 300K][6]

![Fig.4. The predicted effect of Al on the SFE of TWIP 2 material][7]

![Fig.5. The predicted effect of Cr on the SFE of TWIP 2 material][8]

![Fig.6. The predicted effect of Si on the SFE of TWIP 2 material][9]

Fig.3 shows the result when adding each element (Al, Cr and Si) to the TWIP 2 steel at room temperature. Aluminium increase the SFE, contrary to chromium. Silicon has a complex effect on SFE, increasing SFE for small quantities and decreasing it at higher ones.

Fig.4 shows that Aluminium has a constant effect on the SFE and even if at high or low temperature.

Fig.5 shows that adding Chromium increasing slowly the SFE at low temperature, while this element becomes decreasing SFE at high temperature.

Fig.6 shows the same behavior of Silicon to Chromium.

### 5. Conclusion:

Based on thermochemical modeling and numerous bibliographic data of stacking fault energy we reach to conclude that, there is an indirect effect of temperature on the SFE, which is changing the effect of alloying elements especially the effect of Cr and Si change with temperature.
References


