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Stacking fault energy of cryogenic austenitic steels*

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Stacking fault energy and stacking fault nucleation energy are defined in terms of the physical nature of stacking faults and stacking fault energy, and the measuring basis for stacking fault energy. Large quantities of experimental results are processed with the aid of a computer and an expression for calculating stacking fault energy has been obtained as

$$\gamma_{\rm SF}^{300}({\rm mJ\cdot m^{-2}}) = \gamma_{\rm SF}^{0} + 1.59{\rm Ni} - 1.34{\rm Mn} + 0.06{\rm Mn}^2 - 1.75{\rm Cr} + 0.01{\rm Cr}^2 + 15.21{\rm Mo} - 5.59{\rm Si} - 60.69({\rm C}+1.2{\rm N})^{1/2} + 26.27({\rm C}+1.2{\rm N})({\rm Cr}+{\rm Mn}+{\rm Mo})^{1/2} + 0.61[{\rm Ni}\cdot({\rm Cr}+{\rm Mn})]^{1/2}.$$

Keywords: austenitic steels, stacking fault energy, alloying element
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1. Introduction

The stacking fault energy (SFE) of cryogenic austenitic steel is a parameter of great importance, which has an effect on the strength and deformation character of steels, and also has an effect on the critical point, features and products of martensitic phase transformation. The driving force for phase transformation at the $M_{\rm s}$ point is related to the SFE and strain energy of the parent phase.[1] Then, the formation laws of austenitic twins, stacking fault and ε-martensite can be explained by the change of the SFE.[2] The energy is also a key parameter in studying the relationship between the structure and property of an austenitic stainless steel, and also strongly affects the martensitic morphology and substructure formation.[3]

Much fruitful research has been conducted on the SFE.[4,5] But the data obtained are scattered and conclusions often disagree with each other; some are even opposite to each other.[6] The main reasons for this may result from differences in experimental methods, experimental conditions and experimental errors. However, the most important reason may lie in the understanding of the conception and definition of the SFE. The effect of the SFE on phase transformation has been analysed thermodynamically, and a quantitative expression for calculating $M_{\rm s}$ and $M_{\varepsilon{\rm s}}$ has been given.[7] In this paper, we discuss the conception of the SFE and we manage to explore the effect of alloying element and temperature on it.

2. Conception and definition of the SFE

To state briefly, the definition of the SFE described in the literature can be classified as follows.

According to the dislocation theory,[8] both glide planes and twin planes of austenite are $\{111\}_\gamma$. And the burgers vector a perfect dislocation is $1/2 < 110 >$, which can be resolved into two $1/6 < 112 >$ partial dislocations. A stacking fault is built up in the area between the two partial dislocations and the energy change resulting from the abnormal stacking is called the SFE. Stacking faults are formed by partial dislocations spreading, while the SFE is the work done to overcome the resilience interactive energy of dislocation. Then an expression connecting the width of a stacking fault with the SFE is deduced. In most of the literature, data are obtained from this expression by measuring widths of stacking faults.

According to crystallography, the SFE is the energy difference between atoms in the normal structure and those in the stacking fault area. The single stacking fault is like a very thin flake of a twin. A stacking fault is formed between the normal structure and the glide plane of the spreading dislocation. Energy is raised by the abnormal stacking, and the increment of the system energy is the SFE,[9] which is about twice the boundary energy of annealed twins. Furthermore, in Ref.[1] it was agreed that the SFE should include

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the volume energy and surface energy. A stacking fault can spread automatically when the sum of strain energy and chemical free energy (negative) is equal to the surface energy.

In view of the free enthalpy difference of phases, the SFE reflects the energy difference between two crystal lattices of fcc and hcp, and decreases with increasing electronic concentrations.[2] Shi[10] agreed that the SFE of a pure metal is equal to its Gibbs free enthalpy difference of a layer of atoms between fcc and hcp lattices. He also obtained an expression to relate the SFE to $\Delta G_{\mathrm{M}}^{\gamma\to\varepsilon}$, and pointed out that, for alloys, the Suzuki effect should be taken into account. The segregation of solute atoms in a fcc crystal at equilibrium state has been calculated by Dewit and Howard,[11] who stated that the free energy difference between fcc and hcp structures is different from the SFE at the same temperature with the same composition.

Based on the nucleation mechanism of stacking faults,[12] the SFE is equal to the difference between the chemical free energy in the stacking fault area and the sum of strain energy and boundary energy. Only when the SFE attains a certain negative value can stacking faults spread automatically and ε-martensitic phase transformation take place.

Summarized from the above, the definitions of the SFE given by different researchers are diverse from each other and rather confusing. It is necessary to reach a common understanding.

Because of the substantial existence of stacking faults in cryogenic austenitic steels, and their important effect on phase transformations, deformations, slips and twins, the SFE and stacking fault nucleation energy can be defined as follows.

To avoid confusion, the SFE can be defined as the energy value that is calculated according to the measured width of a single stacking fault by the expression derived from the dislocation theory. In fact, the SFE reflects the strain energy caused by stacking faults and the Suzuki effect caused by the segregation of alloying elements. This definition is identical to the conventional definition of the SFE. This energy value is denoted by γ_{SF} or the SFE, which has been measured in many works. Thus, the data obtained are meaningful in engineering.

The stacking fault nucleation energy is the variation of the system energy caused by the formation of stacking faults, and is denoted by ΔG_{SFE}. Upon phase transforming, the existing stacking faults can become the cores of phase transformations. The stacking fault nucleation energy roughly means the same as the SFE defined by Cohen, which refers to the sum of three energy values, namely, the decrease of free enthalpy in the area of stacking faults (ΔG^{C}, negative), strain energy (ΔG^{E}, positive), and boundary energy (ΔG^{S}, positive). Of course, the Suzuki effect of solute atoms has been taken into account in the above-mentioned cases.

3. Effect of alloying elements and temperature on the SFE

3.1. Contribution of alloy elements to SFE

Stacking faults in alloyed austenite are certainly escorted by Suzuki atmospheres. The alloying element has different effects on quantities such as ΔG^{C}, ΔG^{E}, ΔG^{S}, and macroscopic effects on γ_{SF} and ΔG_{SFE}, which may also be affected by the contents of the same kind of elements. The effects of the alloying element on γ_{SF} obey the following laws. If the content of the alloying element is not large, then as the content increases, γ_{SF} will decrease to a value of a certain limit and will then increase immediately. In the case of carbon steels, γ_{SF} is reduced by adding such elements as Ni, Cr and Mn. But in the case of Fe–Mn alloys, γ_{SF} is raised by adding a small amount of Cr, Mo or Ni.[3] In cryogenic austenitic steels, $\gamma_{\mathrm{SF}}^{300}$ at room temperature may be expressed as

$$\gamma_{\mathrm{SF}}^{300} = \gamma_{\mathrm{SF}}^{0} + \sum_{i=1}^{n} a_i M_i, \tag{1}$$

where M_i is the alloying element, and a_i is its coefficient. The effect of some alloying elements is nonlinear, and interactions between them may occur. γ_{SF}^{0} is supposed to be the SFE of pure γ-Fe at room temperature. The values of $\Delta G^{\gamma\to\varepsilon}(300\mathrm{K})$ obtained from Refs.[10] and [13] are about $460\sim544\mathrm{J\cdot mol^{-1}}$. The value of γ_{SF}^{0} calculated from the formula in Ref.[14] is about $36\sim42\mathrm{mJ\cdot m^{-2}}$. Here γ_{SF}^{0} is an average value. According to the nature of the alloying element and the results of many researchers, the following expression can be obtained by means of computer processing

$$\begin{aligned}
&\gamma_{\mathrm{SF}}^{300}(\mathrm{mJ\cdot m^{-2}}) \\
=&\gamma_{\mathrm{SF}}^{0} + 1.59\mathrm{Ni} - 1.34\mathrm{Mn} + 0.06\mathrm{Mn}^2 \\
&- 1.75\mathrm{Cr} + 0.01\mathrm{Cr}^2 + 15.21\mathrm{Mo} - 5.59\mathrm{Si} \\
&- 60.69(\mathrm{C}+1.2\mathrm{N})^{1/2} + 26.27(\mathrm{C}+1.2\mathrm{N}) \\
&\times(\mathrm{Cr}+\mathrm{Mn}+\mathrm{Mo})^{1/2} + 0.61[\mathrm{Ni}\cdot(\mathrm{Cr}+\mathrm{Mn})]^{1/2},
\end{aligned} \tag{2}$$

where the symbol for the alloying element represents its weight percentage. The relevant coefficient (R) of the expression is 0.71, and the F test value is 7.65. Hence, it is obvious that γ_{SF}^{300} is strongly dependent upon the content of the alloying element. Figure 1 shows the relevant scattered points of measured and calculated results for γ_{SF}. The applicable ranges for alloying elements in this expression are ~40Mn, ~25Cr, ~23Ni, ~2Mo, ~4Si, ~0.45 (C+N) (weight %). The total amount of alloying elements should be less than or equal to 45 (wt %).

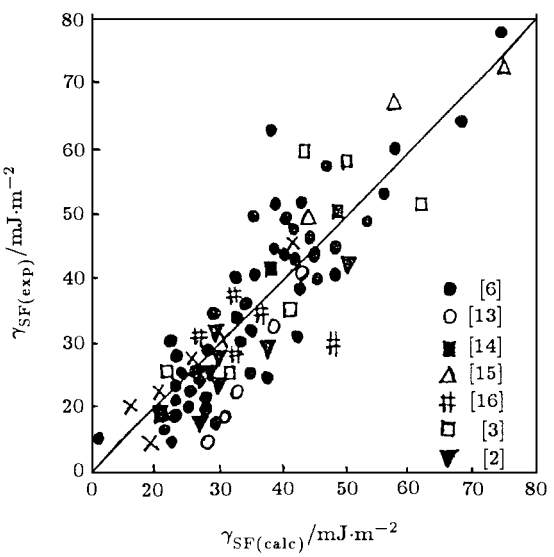


Fig.1. Relational curve of measured and calculated results of γ_{SF}.

3.2. The effect of temperature on the SFE

The SFE (γ_{SF}) of the strain energy and the boundary energy is caused by abnormally stacked atoms. Extraneous factors such as temperature and pressure may change inter-atomic spacing, and thus changes in atomic diameter and lattice constant will also take place. The following equation is the relation between the SFE and the width of a stacking fault:[8]

$$\gamma_{SF} = \frac{\mu b^2}{8\pi d}\frac{2-\nu}{1-\nu}\left(1-\frac{2\nu\cos 2\beta}{2-\nu}\right). \qquad (3)$$

In Eq.(3), μ is the shearing modulus, $\boldsymbol{b}$ is the Burgers vector of a perfect dislocation, d is the width of a single stacking fault, and ν is Poisson's ratio. From the above expression, the reason why γ_{SF} changes with temperature is that it is mainly related to μ and b. Because μ increases linearly but b decreases as temperature decreases, the width of a single stacking fault may also change with the temperature. Gong[3] determined the SFE of Ni–Cr alloyed austenitic by experiments, and held that γ_{SF} increases as temperature rises. But at least the changes of parameters such as μ and b have not been taken into account. For the present subject, the data directly obtained from experiments are open to question. Hence further research is necessary in order to find inherent laws of γ_{SF} changing with temperature.

4. Analysis and discussion

From Eq.(2), it can be seen that the effects of the alloying element on γ_{SF} are very complicated. In addition to the effects of alloying elements themselves, the interactions among alloying elements should not be ignored. The interactions are sometimes considerable and mainly exist among carbide-forming elements, such as Cr, Mn, and C, N, or among Ni and Cr, Mn. The interactions lead to γ_{SF} rising, which accounts for the disagreements in many works. Figure 2(a) shows the combined effect of C and N on $\Delta\gamma_{SF}$ with different amounts of (Cr+Ni). With a decreasing amount of C and N in steel, γ_{SF} decreases, and vice versa. Figure 2(b) illustrates the effect of Cr on $\Delta\gamma_{SF}$ with different amounts of C and N; γ_{SF} decreases with an increasing content of Cr. Of course, when the amount of (C+1.2N) is over 0.2%, $\Delta\gamma_{SF}$ becomes greater than zero, which can be considered as the contribution of the ordinary content of Cr to γ_{SF}. The role of Mn is to raise γ_{SF} (Fig.2(c)). Only if the contents of C and N are very little, does γ_{SF} decrease and reach its limit point at about 12%. The element Si makes the SFE decrease. As the amount of Ni rises, γ_{SF} increases almost linearly (Fig.2(d)). All these analytical results are in agreement with the calculated results or the experimental data obtained by Matsumura,[17] Ishida and Nishizawa,[18] Holden *et al*[19] and Zhang *et al.*[20]

Although the measurement of γ_{SF} varies with different conditions, methods, and even measuring errors according to the researchers, Eq.(2), obtained on the basis of a large amount of experimental data processed by a computer, can show the combined effect of alloying elements on γ_{SF} in an all-round way. Both the calculated and measured results are proven to be satisfactory (Fig.1). It is very important to comprehensively understand the affecting laws of alloying elements and their interactions for γ_{SF}, and this will be a great help in the study of phase transformation, deformation characters and optimum composition design of cryogenic austenitic steels.

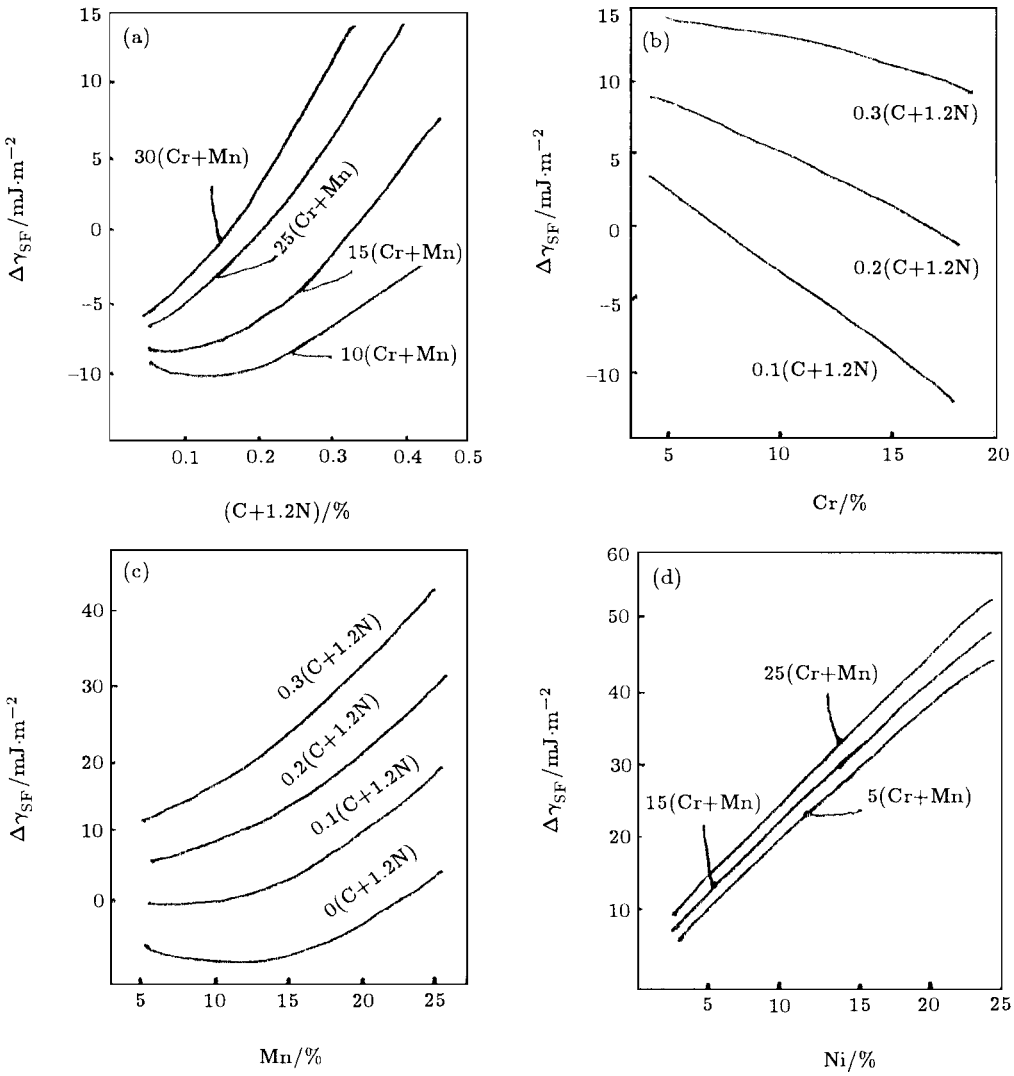


Fig.2. (a) Effect of (C+1.2N) on $\Delta\gamma_{SF}$; (b) effect of Cr on $\Delta\gamma_{SF}$; (c) effect of Mn on $\Delta\gamma_{SF}$; (d) effect of Ni on $\Delta\gamma_{SF}$.

5. Conclusion

The SFE is defined as the sum of the train energy and the boundary energy caused by the formation of a stacking fault. The stacking fault nucleation energy is the variation of the system energy, by which a stacking fault actually acts as the nucleus for phase transformation.

Alloying elements have a direct effect on the SFE. The expression for the room temperature SFE obtained from a large amount of data is

$$\begin{aligned}&\gamma_{SF}^{300}(\mathrm{mJ\cdot m^{-2}})\\ =&\gamma_{SF}^{0}+1.59\mathrm{Ni}-1.34\mathrm{Mn}+0.06\mathrm{Mn}^2\\ &-1.75\mathrm{Cr}+0.01\mathrm{Cr}^2+15.21\mathrm{Mo}-5.59\mathrm{Si}\\ &-60.69(\mathrm{C}+1.2\mathrm{N})^{1/2}+26.27(\mathrm{C}+1.2\mathrm{N})\\ &\times(\mathrm{Cr}+\mathrm{Mn}+\mathrm{Mo})^{1/2}+0.61[\mathrm{Ni}\cdot(\mathrm{Cr}+\mathrm{Mn})]^{1/2}.\end{aligned}$$

The effect of interactions among alloying elements on the SFE is remarkable and should not be ignored.

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