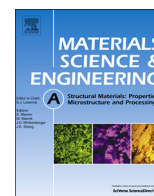




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## Materials Science &amp; Engineering A

journal homepage: [www.elsevier.com/locate/msea](http://www.elsevier.com/locate/msea)

## Impact of short-range ordering on yield strength of high manganese austenitic steels

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## ARTICLE INFO

## Article history:

Received 7 June 2014

Received in revised form

7 July 2014

Accepted 8 July 2014

Available online 15 July 2014

## Keywords:

Steels

Austenite

Mechanical characterisation

Yield strength

Short-range ordering

## ABSTRACT

A model is suggested to quantitatively predict the compositional and temperature effects on the yield strength of high manganese austenitic steels. In the model, short-range ordering is considered to be an effective obstacle against the dislocation glide at the yield point, and the required stress to destroy the short-range ordering was calculated by employing the reported cell model as well as ab initio calculations. The obtained stress depends on both composition and temperature and is systematically related to the yield strength. The model is successfully validated with a number of experimental results and can be employed to tailor the yield strength of the high Mn austenitic steels.

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## 1. Introduction

During the last decade, high Mn austenitic steels have been intensively investigated thanks to their excellent mechanical properties [1]. One of the fundamental mechanical properties of a metal is its yield strength, which is the stress where transition from elastic to plastic deformation takes place [2]. Hence, the yield strength of austenitic steels has been studied to identify a grain size effect [3] as well as a compositional effect [4].

According to Cuevas et al., 0.2% proof stress of a 22 Mn–0.6 C (wt%) austenitic steel at room temperature shows the Hall–Petch relationship, where the slope of the relationship is 11.3 MPa mm<sup>1/2</sup> [3]. Such dependency is reasonable based on other high Mn steels [5,6], and it is comparable with the polygonal ferritic steels case, where the slope is 15–18 MPa mm<sup>1/2</sup> [7]. However, the influence of an alloy composition on the yield strength is very different between ferrite and austenite due to their crystal structure. In ferrite, carbon, which is an interstitial element, generates a tetragonal distortion in the body-centred cubic structure, resulting in a strong strengthening effect despite its low solubility. In austenite, on the other hand, the interstitial atom creates an isotropic strain field, which is not very effective for solid solution hardening [8].

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Considering the relatively low strengthening ability of interstitial atoms in austenite, it is surprising that the reported empirical relationship shows a large difference between the strengthening effect of C and Mn as

$$\sigma_y \text{ (MPa)} = 228 + 187 \text{ (wt\%C)} - 2 \text{ (wt\%Mn)}, \quad (1)$$

where  $\sigma_y$  is the yield strength of a high Mn austenitic steel, (wt%C) and (wt%Mn) are the weight percents of C and Mn [4,9]. Moreover, it is interesting that Mn shows a negative effect on the yield strength in the equation; Bouaziz et al. suggested that such an effect is attributed to the complex interaction among C, Mn, and dislocations. Besides, C can also influence the yield strength via static strain ageing as in austenitic stainless steels owing to the Cottrell atmosphere formation and the Suzuki effect [10,11]. In this case, strengthening due to strain ageing would be superposed to  $\sigma_y$  in Eq. (1). In addition to the C effects on the yield strength, interstitial atoms in austenitic steels may affect strain hardening by affecting the number of dislocation pile-ups at the twin boundary. Accordingly, work hardening rate can be enhanced with C content in the alloy [12].

The complex interaction among Mn, C, and dislocations causing the negative contribution of Mn to yield strength suggested by Bouaziz et al. [4] may be well explained in terms of short-range ordering (SRO) which is generated in the high Mn austenite. SRO is defined to be a local order occurring when the number of the unlike atom pairs is larger than that in a random solution [13,14].

A previous ab initio study has shown that Mn enrichment adjacent to C is energetically favourable, which suggests the existence of the SRO in a Fe–Mn–C system [15]. Due to such attraction between Mn and C atoms, the SRO can act as an obstacle to dislocation glide [13,16]. Accordingly, a number of studies have attributed the SRO to the special mechanical properties of high Mn austenitic steels; e.g. improved strain hardening behaviour [17], planar slip [18,19], serrated flow [19–21], and strain aging [22].

At the yield point of a metal, plastic deformation begins as a multitude of dislocations starts to glide. It is plausible that the passage of only one or two dislocations may be enough to locally destroy the SRO in the system [23]. Hence, a certain amount of stress needs to be introduced at the yield point so that dislocations can overcome the SRO. In this study, such stress required to destroy SRO is calculated by employing McLellan’s cell model [24] and ab initio calculation results [15]. Then, the calculated stress is related to the yield strength and experimentally validated. Based on the suggested model, the empirical relation suggested by Bouaziz et al. [4,9] (Eq. (1)) is explained. Furthermore, the composition and temperature dependencies of the yield strength of high Mn austenitic steels are studied.

## 2. Methods

### 2.1. Short-range ordering

A short-range ordering (SRO) in a Fe–Mn–Al–C system is assessed by employing the octahedral cell model suggested by McLellan [24]. In this model, a face-centred cubic (FCC) structure is composed of octahedral cells, at whose centre lies an octahedral interstitial site and whose six corners are substitutional atomic sites occupied by Fe, Mn, or Al. The cells without C can be classified as *kl*-type by the number of Mn (*k*) and Al (*l*) atoms in each cell. If C is placed at the centre, the cell is designated to be *Ckl*-type. Firstly, random distribution of substitutional atoms is assumed and the number of *kl*-type cells ( $n_{kl}$ ) can be calculated as

$$n_{kl} = \frac{6!N}{(6-k-l)!k!l!} \theta_{Fe}^{(6-k-l)} \theta_{Mn}^k \theta_{Al}^l \quad (2)$$

where *N* is the total number of Fe, Mn, and Al atoms in the system and  $\theta_i$  is the atomic fraction of element *i* in respect with *N*. Note that  $\theta_i$  is different from the general atomic fraction, since *N* excludes the number of interstitial atoms. Then, the sites for C among the cells are determined considering the energy state of *Ckl*-type cells according to the Fermi-Dirac distribution. When the system is dilute in the interstitial solute atoms, i.e. the number of *Ckl*-type cells ( $n_{Ckl}$ ) is sufficiently smaller than  $n_{kl}$ , the distribution

can be approximated to the Maxwell–Boltzmann distribution. Therefore,  $n_{Ckl}$  for each cell can be obtained with

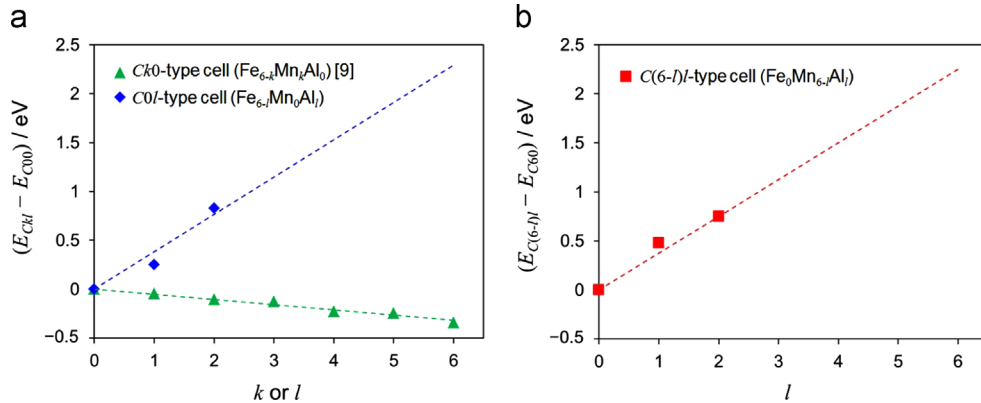
$$n_{Ckl} = \frac{\theta_C}{Q} n_{kl} \exp\left(-\frac{E_{Ckl}}{k_B T}\right), \quad (3)$$

where  $E_{Ckl}$  is the energy level of the *Ckl*-type cell,  $k_B$  is the Boltzmann constant, and *T* is the temperature in K. *Q* in the denominator is a cell partition function, which is defined as

$$Q = \sum_{k=0}^6 \sum_{l=0}^6 \left\{ n_{kl} \exp\left(-\frac{E_{Ckl}}{k_B T}\right) \right\}. \quad (4)$$

Accordingly, a C distribution can be assessed for a certain composition ( $\theta_{Fe}, \theta_{Mn}, \theta_{Al}, \theta_C$ ) and temperature once  $E_{Ckl}$  is known.

In this study,  $E_{Ckl}$  is adopted from ab initio calculation results for single-layered antiferromagnetic FCC systems of Fe–Mn–C, Fe–Al–C, and Mn–Al–C. Model cells of composition  $M_{106}Al_2C$  (*M*=Fe/Mn,  $3 \times 3 \times 3$  FCC supercells) have been structurally optimised with density-functional theory based program VASP [25–28] using plan waves and projector augmented waves (PAW;  $E_{cut}=500$  eV) [29,30]. Contributions from electronic exchange and correlation were considered by the generalised gradient approximation (GGA) functionals of Perdew et al. [31]. The Brillouin zone integration was performed by using the scheme of Monkhorst and Pack [32]. Energy differences were calculated as a function of carbon’s different octahedral voids position using a fixed metal lattice  $M_{106}Al_2$ . The latter was constructed so that the carbon can be coordinated by 0, 1, and 2 Al atoms in the octahedron. Higher Al-coordinated C was not taken into account due to typical small Al contents (< 8 wt%) and can subsequently be excluded by the calculated course of energies (Fig. 1). For Fe–Mn–C, however, smaller energy differences made any coordination possible. The extensive investigation of this phase and more computational details can be found in [15]. Taking octahedral sites of six Fe atoms containing a C atom at their centre (C 00-type) as a reference state, the energy change brought by incorporating *k* Mn atoms or *l* Al atoms is shown in Fig. 1a. These results suggest that incorporation energy of Mn and Al varies nearly proportional to *k* and *l*. Therefore, the proportional coefficients for Mn and Al ( $\Delta E_{Mn}, \Delta E_{Al}$ ) are determined from the slope of each curve as –0.0528 eV/Mn atom and 0.382 eV/Al atom, respectively.  $\Delta E_{Mn}$  is negative implying an attractive force between Mn and C atoms, while  $\Delta E_{Al}$  is positive showing the repulsive interaction between Al and C. In addition, the energy necessary to include *l* Al atoms in a cell with initially six Mn atoms (C 60-type) is shown in Fig. 1b; in this case the proportional coefficient is 0.375 eV/Al atom, which is similar to the energy change by incorporating Al into a C 00-type cell (0.382 eV/Al atom). Therefore, the energy increase due to the



**Fig. 1.** (a) Energy change as a function of the number of Mn (green, *k*) and Al atoms (blue, *l*) surrounding carbon in a FCC Fe–Mn–Al octahedron. The reference state of a carbon in a pure Fe octahedron (C 00-type) is set to zero. (b) Same as in (a) but for Al substituting Mn atoms. The reference state here is the pure Mn octahedron (C 60-type). (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this paper.)

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