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Stacking fault energies in austenitic stainless steels

Jun Lu [a], Lars Hultman [a], Erik Holmström [b, *], Karin H. Antonsson [c], Mikael Grehk [c], Wei Li [d], Levente Vitos [d], Ardeshir Golpayegani [c]

[a] Thin Film Physics Division, Dept. of Physics, Chemistry and Biology (IFM), Linköping University, Linköping SE-581 83, Sweden
[b] Sandvik Coromant R&D, Stockholm SE-126 80, Sweden
[c] R&D Center, Sandvik Materials Technology, Sandviken SE-81181, Sweden
[d] Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-100 44, Sweden

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ABSTRACT

We measure the stacking fault energy of a set of 20 at% Cr-austenitic stainless steels by means of transmission electron microscopy using the weak beam dark field imaging technique and the isolated dislocations method. The measurements are analyzed together with first principles calculations. The results show that experiment and theory agree very well for the investigated concentration range of Mn (0–8%) and Ni (11–30%). The calculations show that simultaneous relaxation of atomic and spin degrees of freedom is important in order to find the global energy minimum for these materials. Our results clearly show the great potential of the weak beam dark field technique to obtain accurate measurements of the stacking fault energy of austenitic steels and that the reliable predictability of first principles calculations can be used to design new steels with optimized mechanical properties.

1. Introduction

The stacking-fault energy (SFE) is a composition and temperature-dependent characteristic of crystalline materials and plays an important role for the austenitic steel deformation [1,2]. The response to plastic deformation can in the case of austenitic stainless steels give rise to the microstructural changes: slip, twinning, or/and phase transformations. The SFE is a measure of the distance between the shockley partial dislocations and thus the tendency for forming local stacking faults. High SFE values result in microstructural response where dislocation glide of perfect and partial dislocation can accumulate into slip band. Independent on the size of the SFE dislocation glides along the slip planes to accommodate the plastic deformation, and there is a complex interaction between the different types of microstructural responses. The interesting thing is that it is possible to identify specific regions where three characteristic microstructural changes mentioned above are pronounced. Low SFE (<20 mJ/m^2) favors the phase transformation from austenitic phase to martensitic phase (ε- or α'-martensitic transformations) and leads to phase transformation induced plasticity (TRIP); Middle SFE (20–45 mJ/m^2) yields deformation through twinning mechanisms, leading to twinning induced plasticity (TWIP). The primary influence of twins seems to be that they enhance the work-hardening rate by subdividing the grains into twinned and untwinned regions and thereby delaying local necking [3]. In the high SFE case (>45 mJ/m^2), dislocations are rarely dissociated, thus, the deformation process is controlled mainly by dislocation glide [4].

By adjusting the SFE to a proper value, a suitable austenitic stainless steel with desired mechanical properties can be designed and produced. The SFE of stainless steel is strongly dependent on its composition. To achieve TRIP or TWIP, a low value of the SFE is desired and possible to achieve by tuning the chemical composition of the designed stainless steel. However, the details of the composition influence from alloying elements on the SFE are complex and need to be investigated closely in each case in order to be fully understood. For instance, Ni and Cr raise the SFE in Fe-Mn alloys but have the inverse effect for carbon steels [5]. The correlation between the SFE and composition can be experimentally investigated by X-ray diffraction [6] or transmission electron microscopy (TEM) [7–9], or estimated by empirical relationships [10]. The outcome from the experimental methods relies on the resolution, sample preparation, and assumptions made in the evaluation process. Other factors are the micro-structural properties of

* Corresponding author.
E-mail address: erik.holmstrom@sandvik.com (E. Holmström).

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the alloy under investigation in terms of grain size, number of inclusions, residual stresses, purity, and in particular, the concentration levels of interstitial atoms such as N and C. The latter property depends on quality of melting and casting and the following thermomechanical treatment of the alloy. Without proper control of how the samples are manufactured, the results from experiments have a potential of high levels of error and sometimes result in contradictory data compared to similar studies. The drawback of empirical methods is its application limitation due to the limited available data. Furthermore, the complicated interactions of different elements is difficult to represent by a simple empirical formula.

To explore the influence of different elements on the SFE and the mutual correlations between the elements, theoretical calculations is an effective method. Computational thermodynamics has recently been used [11–15] and several groups have investigated SFE via quantum mechanical first-principles calculations for steels [16,17]. The advantage with such calculations is the ease by which the theory provides fundamental understanding of the effects that the complex relationships between the different elements have on the SFE. The calculations can also span a whole concentration space to provide insights on general trends. In order to perform calculations over large concentration spaces it is necessary to make balanced approximations so that the computational effort is minimized. To verify the approximations that are used in the calculations, SFE values from selected reference alloys should be measured experimentally.

SFE for steels has been obtained experimentally previously by TEM [7–9,14,18,19]. However, a quantitative comparison between calculations and measured SFE has traditionally been hampered by the large uncertainties in both the measured values and in the approximations used in the calculations. The aim of this work is to measure the SFE of a set of high-purity stainless steels on the most quantitative level possible via TEM and subsequently compare the experimental data with state-of-the-art theoretical first principles simulations.

2. Experiment

2.1. Experimental measurement of SFE by TEM

Transmission electron microscopy (TEM) can be used to determine SFE in different ways; 1) high-resolution TEM (HRTEM) where the width of a stacking fault is observed directly in cross-section [20]; 2) the extended dislocation node method [7]; and 3) the isolated dislocation approach [21–23]. In general, the HRTEM method is the most direct since it measures a visible quantity, but it has drawbacks. It needs a very thin sample region, which means a very limited area is available for this kind of characterization. Because of the very thin specimen, the surface effect on the SFE cannot be eliminated. It should be noted that the HRTEM method may be the sole way for some materials with very high SFE because of the high point resolution [20]. The extended node method to measure SFE by TEM was first suggested by Whelan [24]. This technique does not have resolution problems to measure the radius of curvature (R) of extended nodes. However, it is difficult to determine R as nodes are rarely symmetrical or uniform in size. In addition, there are no simple relationships between the geometrical parameters of the node and the corresponding SFE, resulting in a large scatter of measured SFE values [7]. The third method, the isolated dislocation method is a promising technique since SFE of high accuracy (16 ± 2 mJ/m^2) has been shown possible to measure for Fe-Mn-Al-Si austenitic twinning-induced plasticity steels [7]. Due to the demonstrated accuracy of the isolated dislocation technique, this approach was chosen in the present study.

2.1.1. Isolated dislocation method

According to Heidenreich & Shockley's suggestion, a perfect dislocation in a face-centered cubic lattice can dissociate into two partial dislocations [25]. The two partial dislocations repel each other and leave a stacking fault between them. The distance d (dissociation width) between the two partial dislocations is determined by the attractive force exerted by the stacking fault and the repulsive interaction between the partial-dislocation strain fields. Thus, SFE, here denoted γ can be calculated based on anisotropic elasticity theory. The equation below is in the general case an approximation to anisotropic elasticity theory that is based on isotropic theory. In our case of {111} glide planes and dislocations along [110], the equation is exact [26] and

$$\gamma = \frac{\mu b_p^2}{8\pi d}\left(\frac{2-\nu}{1-\nu}\right)\left(1-\frac{2\nu\cos 2\alpha}{2-\nu}\right) \tag{1}$$

where μ is the effective shear modulus in the (111) fault plane, ν is the effective Poisson ratio and α is the angle between the total Burgers vector and the dislocation line. b_p is the magnitude of the partial Burgers vector, which is approximately 0.148 nm for the lattice parameters of the materials in this study and d is the separation of the partials, which is to be measured. The effective shear modulus μ and Poisson ratio ν were calculated for each sample according to the following equations:

$$\mu = \left(C_{44}\frac{(C_{11}-C_{12})}{2}\right)^{0.5} \tag{2}$$

$$\frac{1}{1-\nu} = \frac{1}{3\mu}(C+C_{12})\left[\frac{C_{44}(C-C_{12})}{C_{11}(C+C_{12}+2C_{44})}\right]^{0.5}\left(1+2\frac{C_{11}}{C}\right) \tag{3}$$

where

$$C = \left[\frac{1}{2}C_{11}(C_{11}+C_{12}+2C_{44})\right]^{0.5}. \tag{4}$$

We used experimental elastic stiffness constants from Ref. [27] where alloys with very similar concentrations were measured. In the cases where the exact alloy concentrations could not be found, we used data from the closest available alloy. Since the values of the elastic constants do not change much when the alloy concentrations are altered by a few percent this error is well within the measurement uncertainty of the elastic constant themselves. In the case of the samples that contain Mn we have not been able to obtain elastic constants so we have used the same values as for the samples without Mn.

Since the value of d is in the nanometer range, the weak beam image technique is available to determine the separated partials at the condition of the effective excitation error $s > 0.2$ nm^{-1} [22].

The relationships between the perfect dislocations, the relative partial dislocations and the corresponding reflections are demonstrated by the Thompson tetrahedron [28] as shown in Fig. 1. It can be seen that a perfect dislocation can be dissociated into two partial dislocations

$$\frac{a}{2}\left[\bar{1}10\right] \leftrightarrow \frac{a}{6}\left[\bar{1}2\bar{1}\right] + \frac{a}{6}\left[\bar{2}11\right]. \tag{5}$$

Moreover, the Burgers vectors $[1\bar{1}0]$, $[1\bar{2}1]$ and $[2\bar{1}\bar{1}]$ are in the (111) plane. In addition, in the same plane, there are another two perfect dislocations $[10\bar{1}]$ and $[0\bar{1}1]$, which can be dissociated into $[11\bar{2}]$, $[2\bar{1}\bar{1}]$ and $[1\bar{2}1]$, $[\bar{1}\bar{1}2]$, respectively. To determine the SFE, the separation of two partial dislocations (d) and the angle between the total Burgers vector and the perfect dislocation line α have to be