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Impact of nanodiffusion on the stacking fault energy in high-strength steels

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Abstract

A key requirement of modern steels – the combination of high strength and high deformability – can best be achieved by enabling a local adaptation of the microstructure during deformation. A local hardening is most efficiently obtained by a modification of the stacking sequence of atomic layers, resulting in the formation of twins or martensite. Combining ab initio calculations with in situ transmission electron microscopy, we show that the ability of a material to incorporate such stacking faults depends on its overall chemical composition and, importantly, the local composition near the defect, which is controlled by nanodiffusion. Specifically, the role of carbon for the stacking fault energy in high-Mn steels is investigated. Consequences for the long-term mechanical properties and the characterisation of these materials are discussed.

Keywords: Stacking fault energy; Iron; Carbon; In situ TEM; DFT

1. Introduction

In order to combine high strength and high ductility in steels, adaptive microstructures are required, which allow the material to react only locally to potential failure mechanisms caused by high stress levels. This adaptation can occur by diffusionless (martensitic) transformations to another well-defined crystal structure – the so-called transformation induced plasticity (TRIP) mechanism; alternatively, materials showing twinning-induced plasticity (TWIP) make use of twin boundary formation, accommodating strain and creating obstacles for dislocation motion.

Both deformation processes can be realised by locally modifying the sequence of atomic layers in the affected region [1]. However, this is only possible if the energy to create the change in stacking sequence – the stacking fault energy (SFE) – is sufficiently low. Therefore, the SFE serves as an indicator for the occurrence of either of the aforementioned deformation mechanisms. The observation that adjusting the SFE influences the adaptation of the microstructure allows new routes in designing damage-tolerant, high-strength steels with tailored mechanical properties [2].

Changing the chemical composition of a material is the most suitable strategy for such an adjustment. Austenitic steels, for example, in which the face-centred cubic (fcc) crystal structure is stabilized by a high Ni or Mn content (above 20 wt.%) and a C content of the order of 1 wt.% form an important class of adaptive structural materials. It is generally accepted that the SFE in high-Mn steels is of the order of 20 mJ m^{-2} and that a reduction by about 5 mJ m^{-2} changes the dominant deformation mechanism from TWIP to TRIP [1]. However, compiling experimental results for the dependence of the SFE on the C content in steels reveals strikingly inconsistent trends: some sets of

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experiments show only a slight change [3], whereas others report a steep increase in the SFE with C content [4] (see Fig. 1(a)). The discrepancies between the various experiments deviate more than an order of magnitude from the desired accuracy of 5 mJ m^{-2}. Consequently, the reliability of determined values of the SFE (Fig. 1) is debated in the literature [3,5].

Here, we demonstrate that knowing the defect-mediated local chemical composition is critical for understanding and interpreting the origin of the conflicting experimental data. This finding goes beyond the above cited studies, which assume a homogeneous atomic compositions of the steel samples. Instead, we bring experimental observations into context with the Suzuki [6] effect. The thermodynamics of segregation of solute atoms to stacking faults was first introduced several decades ago [7,8]. The energetics involved in such a process can be interpreted as the chemical driving force for local diffusion, but also as a way to reduce the SFE as a function of temperature [9]. These concepts are predominantly reported for substitutional elements that are attracted by the stacking fault (SF). In contrast to this, the C atoms behind the discussion in this paper are interstitials that are repelled from the SF. While the absolute changes in the local concentrations might be smaller in such a case, the jumps happen on a different timescale and potential energy surface than vacancy-mediated bulk diffusion. In addition, we were able to prove by ab initio calculations that just a few atomic jumps of interstitial carbon out of the SF are sufficient to substantially lower its energy. In this respect, C probably behaves similarly to, for example, nitrogen in high-N steels, for which an increase in the SFE has also been revealed by ab initio [10]. Based on the insights obtained in this work, we provide experimental evidence for such a Suzuki effect and its relevance for macroscopic deformation in high-Mn steels.

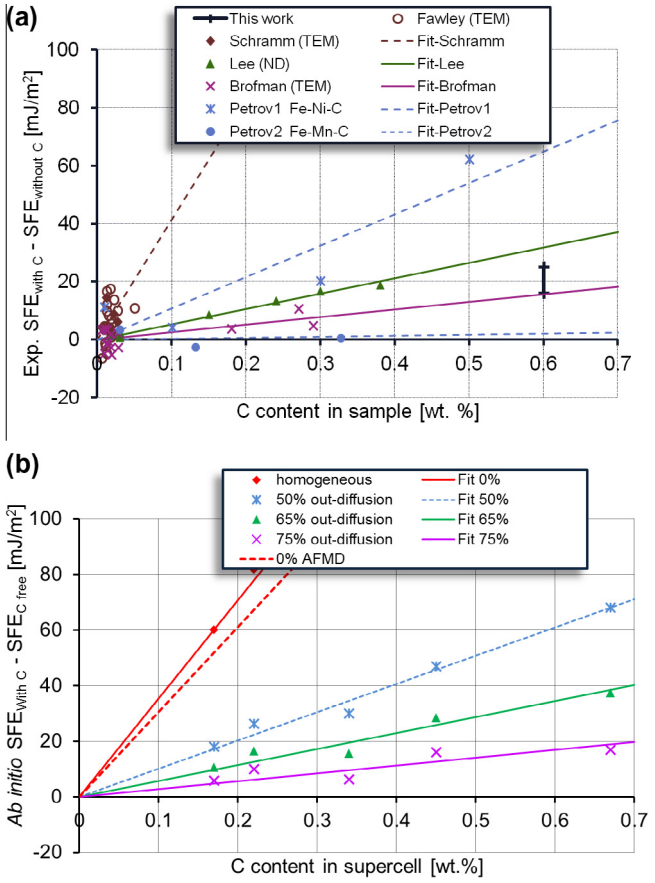

Fig. 1. Dependence of the stacking fault energy (SFE) in Fe–C based austenitic alloys on the C concentration. (a) Experimental data [3,4,11–13] using different techniques (X-ray diffraction, neutron diffraction and transmission electron microscopy) yield conflicting trends for the SFE. Dashed lines indicate less reliable extrapolations due to the sparseness of experimental data. The black bar indicates our experimental result (see Section 5) for the absolute changes for the SFE within the same sample due to nano-diffusion. (b) Ab initio calculations for the SFE in Fe–C assuming different distributions of C atoms. The red symbols correspond to a completely homogeneous C distribution. The impact of the Suzuki effect, where a certain percentage of the C atoms (see legend) diffuses out of the atomic layers that form the stacking fault is shown by blue, green and purple symbols. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2. Ab initio methodology

To resolve the controversy about the role that C plays for the SFE, we have first used density functional theory (DFT), which allows us to focus on the influence of C without being simultaneously confronted with the full complexity of multicomponent and magnetic steels. The DFT calculations were carried out with the Vienna ab initio simulation package (VASP) [14] using the projector-augmented wave basis set [15] and the PBE exchange–correlation functional. Explicit calculations of intrinsic stacking faults as well as calculations using the axial next-nearest-neighbour Ising (ANNNI) [16] approach have been performed. A numerical convergence of the stacking fault energy values, in the sense that an interaction of ISFs with their periodic images becomes negligible (<1 mJ m^{-2}), was obtained for supercells with a minimum of six atomic layers. The independence of the SFE on the particular set-up is ensured by a comparison with recently published results [17]. For the non-magnetic results in Fig. 1(b), one carbon atom in supercells starting from 32 up to 128 Fe atoms has been used and the independence of the atomic configuration has been ensured [18]. Atomic relaxation of the internal atomic positions perpendicular to the stacking fault have been included. Furthermore, a comparison of the non-magnetic approach (solid lines in Fig. 1(b)), with a complete antiferromagnetic double-layer (AFMD) calculation (red dashed line in Fig. 1(b)), has been performed to ensure the independence of the C trend with respect to magnetism. Other numerical parameters were chosen such that a precision of energies within 10^{-5} eV $atom^{-1}$ (corresponding to errors in the SFE below 10 mJ m^{-2}) was achieved. Specifically, an energy cut-off of 400 eV and a k-point mesh of $8 \times 8 \times 8$ for a $2 \times 2 \times 2$ fcc cell as well as $6 \times 12 \times 7$ for a $4 \times 2 \times 2$ hexagonal close-packed