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# STEEL – AB INITIO: QUANTUM MECHANICS GUIDED DESIGN OF NEW FE-BASED MATERIALS

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## Abstract

This contribution reports the results of the collaborative research unit SFB 761 "Steel - ab initio", a cooperative project between RWTH Aachen University and the Max-Planck-Institute for Iron Research in Düsseldorf (MPIE) financed by the German Research Foundation (DFG). For the first time, it is exploited how ab initio approaches may lead to a detailed understanding and thus to a specific improvement of material development. The challenge lies in the combination of abstract natural science theories with rather engineering-like established concepts. Aiming at the technological target of the development of a new type of structural materials based on Fe-Mn-C alloys, the combination of ab initio and engineering methods is new, but could be followed quite successfully. Three major topics are treated in this research unit: a) development of a new method for material- and process-development based on ab initio calculations; b) design of a new class of structural materials with extraordinary property combinations; c) acceleration of development time and reduction of experimental efforts and complexity for material- and process-development. In the present work, an overview of the results of the first five years as well as an outlook for the upcoming three-year period is given.

## Introduction

The design of new steels usually is based on three major principles: a) requests: the material has to meet specific requirements for the envisaged future application; b) tools: various experimental and numerical methods are applied for materials development; the best balance of effort and accuracy needs to be chosen for a specific materials design task; and c) constraints: steel, being an engineering material characteristically produced in large quantities, always needs to be processed according to the economic rules. Thus, the processes available today and in the future or the impacts of recycling and environment have to be considered already in the early stages of the material development.

Currently, a new class of steels with an austenitic matrix having Mn content of 15 to 35 wt.-% together with additional alloying elements like C, Si, Al is under investigation. The interest in these materials is due to the occurrence of different deformation mechanisms that can attribute to the extraordinary strain hardening and the resultant high formability and high strength. The deformation mechanisms are controlled by the stacking fault energy (SFE). This opens the stage for a new chapter of materials design as new modelling tools based on the numerical understanding of the electronic structure of metals can be used to identify the interaction of different alloy compositions. These ab initio or first principles methods are currently tested with respect to the accuracy of the property prediction. There is a good chance that this will lead to the first real physical based design of a new group of structural materials.

## Materials

High Mn steels (HMnS) composed of single phase austenite or multiphase matrix with a large volume fraction of austenite can be divided according to the characteristic phenomena occurring during the plastic deformation into Transformation Induced Plasticity (TRIP) and Twinning Induced Plasticity (TWIP) steels. Furthermore, by adding Al, the group of Microband Induced Plasticity (MBIP) steels have also been developed. Recently, specific interest grows for easily processed medium Mn steels with a combined ferritic/austenitic matrix. Common to all these steels is the fact that they develop a much better combination of strength and ductility compared to the current industrially used group of Advanced High Strength Steels (AHSS). This can easily be demonstrated by comparing the ECO-index, the product of ultimate tensile strength and uniform elongation that is usually limited to max 20 GPa% in AHSS and typically exceeds this value significantly in HMnS. The research centre “Steel – ab initio” currently concentrates on the TWIP steels and the transition between the TWIP and the TRIP effect. Some of the investigated alloys are indicated in **Table 1** with respect to chemical composition and in **Figure 1** with respect to Mn content and ECO-Index.

Table 1: Alloying content of exemplary HMnS, mass contents in %.

| | C | Mn | Si | P | S | Cr | Ni | Al |
|---|---|---|---|---|---|---|---|---|
| I | 0.315 | 22.8 | 0.07 | 0.0073 | 0.0012 | 0.016 | 0.037 | 0.0054 |
| II | 0.573 | 23.2 | 0.17 | 0.0090 | 0.0002 | 0.310 | 0.019 | 0.0049 |
| III | 0.282 | 28.0 | 0.10 | 0.0084 | 0.0010 | 0.016 | 0.037 | 0.0054 |
| IV | 0.594 | 18.4 | 0.05 | 0.0071 | 0.0091 | 0.015 | 0.039 | 0.0045 |
| VII | 0.714 | 23.5 | 0.06 | 0.0071 | 0.0071 | 0.016 | 0.039 | 0.0059 |

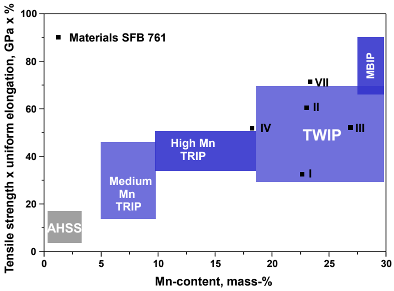


Figure 1: Characteristics of new steel concepts: schematic representation of Mn-content and the tensile properties [1].

## Deformation Mechanisms in Low SFE Regime

Any deviation from the normal sequence of stacking of the atomic planes (as defined by the crystal structure) is called a stacking fault. A stacking fault is a two-dimensional crystal defect. The SFE is defined as the difference in energy per unit fault area between the faulted and the perfect structures. The SFE determines the plastic deformation behaviour of an fcc alloy, **Figure 2**. The dominant deformation mechanism below the SFE value of 20 $mJ/m^2$ is TRIP while above 20 $mJ/m^2$ the TWIP mechanism dominates [2,3]. A further increase of the SFE leads to reduced twinning activity by increasing the critical resolved shear stress (CRSS) for twinning. The fact that a CRSS is needed indicates that twinning is crystal orientation dependent and even at low SFE unfavourably oriented grains will remain twin free even at high deformation degrees. Dislocation slip occurs at any SFE, but dominates at low deformation degree and/or high SFE.

There is no clearly defined limit in SFE above which TWIP ceases. The interaction between the microstructural components resulting from the low-SFE and other constituents like solute atoms, precipitates, etc. (Figure 2) defines the mechanical response of HMnS.

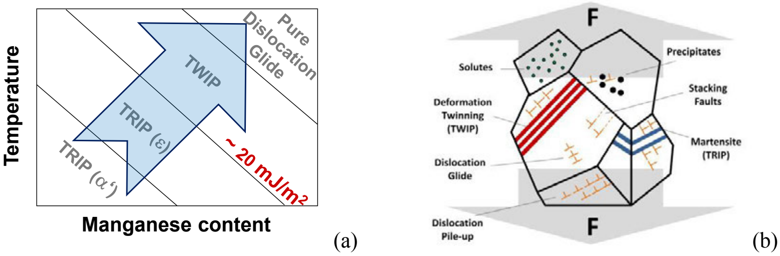


Figure 2: Deformation mechanisms in HMnS and the characteristic SFE for the TRIP/TWIP transition (a); strengthening mechanisms in this system (b) [1,4].

## Material Modeling and Simulation

The so-called deformation mechanism maps can be developed by means of a range of thermodynamic calculations in which the SFE value is correlated with other parameters like the free energy change during the austenite to martensite transformation, and the interface energy between austenite and martensite, **Figure 3** [5]. Since a stacking fault can be viewed as a two atomic layers slice of hcp (ε martensite) within the fcc crystal, the SFE should be related to the difference in Gibbs energy between the hcp and fcc phases. This idea has been applied successfully by Allain et al. [3] and Cotes et al. [6], using the following equation:

$$\gamma_{SFE} = 2\rho\Delta G^{\gamma\rightarrow\varepsilon} + 2\sigma \qquad (1)$$

where ρ is the number of moles of atoms per $m^2$ in one atomic layer, $\Delta G^{\gamma\rightarrow\varepsilon}$ is the difference in Gibbs energy between the hcp and fcc phases, and σ is the related interface energy. There is no independent way to determine the interface energy σ. This parameter has been estimated to be in the range of 5 to 15 $mJ/m^2$ [3,6,7] based on the measured SFE values, the observation of ε-martensite formation, and the activation of deformation mechanisms. The major contribution to the composition and temperature dependency of the SFE comes from $\Delta G^{\gamma\rightarrow\varepsilon}$. The Gibbs free energy of the fcc and hcp phases for pure elements can be taken from Calphad evaluations of the appropriate systems; $\Delta G^{\gamma\rightarrow\varepsilon}$ is then calculated by taking the difference. However, it should be noted that the hcp phase is not a stable phase in the Fe–Mn–C (or other steel systems) and its properties cannot be directly measured. Instead, the hcp phase can be transformed as ε-martensite from the fcc phase in the range 15 to 30 wt-% Mn. Data from this transformation are used to model the Gibbs energy of the hcp phase. The Gibbs energies of the hcp and fcc phases are equal at the so called $T_0$ line, which must be located between the $M_s$ and $A_s$ temperatures. Thus, the $\Delta G^{\gamma\rightarrow\varepsilon}$ from Calphad evaluations is closely related to the formation of ε-martensite, which is the kind of martensite formed via TRIP mechanism. Below 15% Mn, α-martensite forms instead of ε-martensite and above 30% Mn a magnetic transition in the fcc phase increases the stability of the fcc phase so that the ε-martensite formation is suppressed.

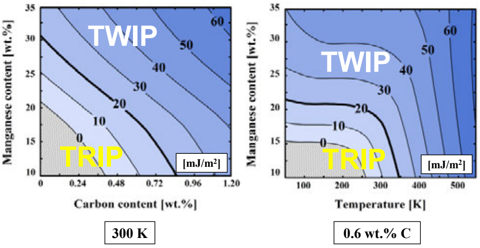


Figure 3: Mechanism maps indicating the relationship between deformation mechanisms, chemical composition, temperature and SFE [5,8,9].

Ab initio methods describe the properties of crystals without using any fitting parameter by the explicit description of the electrostatic interactions between the atomic cores and electrons based on the equations of Schrödinger and Dirac. The input data required for ab initio calculations is given by the atomic structure and the chemical type of the involved atoms. The density functional theory (DFT) is one of the most established ab initio methods providing an efficient way to calculate the electronic properties and the total energy of a material system. This scheme, however, describes the system in its ground state (at T = 0 K) and in practice relies on an approximated description of a small but crucial energy contribution which is due to quantum interaction effects between the constituent particles (the so-called exchange-correlation energy). In order to overcome the limitations of T = 0 K, the DFT calculations are combined with concepts of thermodynamics or with molecular dynamics (MD) simulations.

In steels, usually a random distribution of C atoms in the octahedral voids of the lattice is assumed. In HMnS, the question arises whether short-range atomic ordering might exist that contributes to a void selection according to the number of Fe and Mn atoms that forms the specific octahedral void. Ten different octahedral voids from pure Fe to pure Mn neighbour situation have been considered in one super cell of 16 Fe and 16 Mn atoms, thus representing an alloy with 50% Mn, **Figure 4** [10]. By ab initio modelling the whole structure of the super cell has been calculated including one C atom that is positioned within different voids. The reaction enthalpy has been calculated as a function of the coordination number of the Fe atoms forming the void. It becomes obvious that the smaller the coordination number the more stable is the compound, indicating the strong interaction of Mn and C. This coincides with the fact that stoichiometric manganese carbides are more stable than iron carbides indicating that the Mn-C bond is more attractive than the Fe-C bond.

The mechanical properties of HMnS are characterized by their pronounced strain hardening that is significantly different from the strain hardening behavior of bcc steels. Specifically, mechanically induced twinning leads to an adaptive and continuous refinement of the microstructure during the mechanical testing. Adaptive means, the strain hardening is dependent on the local amount of strain. The measured flow curves sometimes show characteristic turning points that lead to the local minima in the 1st derivative over strain which is the strain hardening curves. The microstructural observations show that during forming individual grains exist without twins together with grains with one or more active twin systems. Thus, the crystallographic nature of twinning has to be considered by means of Crystal Plasticity Finite Element Modeling (CPFEM) [11]. As the SFE and by this the selection of deformation mechanisms is strongly dependent on temperature, it is essential that a suitable model has to consider temperature and strain rate effects. Furthermore, the CPFEM model used distinguishes between the dislocation densities in the cell center and in the cell walls as well as the twin density [12,13].

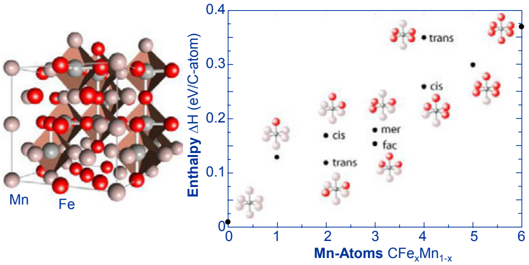


Figure 4: Supercell of 16 Fe (red) and 16 Mn (white) atoms with 10 different types of octahedral voids; enthalpy change by adding 1 C atom to the different voids [10].

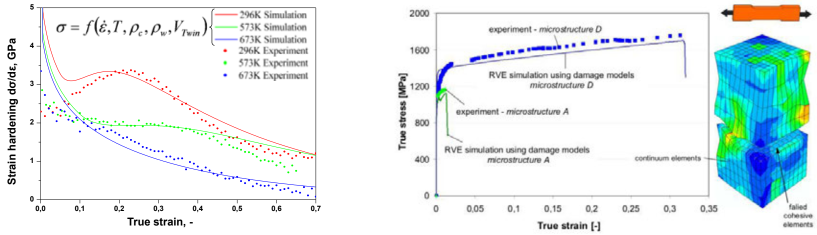
From this, a modified free mean path $\lambda$ is calculated that is a combination of the mean free path of a dislocation $\lambda_{dis}$ and the distance between twins $\lambda_{twin}$:

$$1/\lambda = 1/\lambda_{dis} + 1/\lambda_{twin} \qquad (2)$$

$\lambda_{twin}$ is calculated according to the equation

$$\lambda_{twin} = s\,(1-V_{twin})/V_{twin} \qquad (3)$$

with s medium thickness and $V_{twin}$ volume fraction of twins. The results in **Figure 5a** indicate that by choosing a proper parameter set the temperature dependency can be properly derived. The main governing fit parameter is the twin density that needs to be determined accurately. This results in the demand for a proper quantitative identification method of twins in these steels.



(a) (b)

Figure 5: a) Stress-strain-curves and strain-hardening curves as the function of temperature for alloy I; comparison of experimental results and CPFEM calculations.[11] b) failure modeling of dual phase steels based on CZM using model parameters as function of microstructure in terms of martensite fraction.[16]

Besides the description of strain hardening, an evaluation procedure for the prediction of microcracks as a result of applied mechanical loading is required. The concept of representative volume elements (RVE) is used to describe microstructures with their characteristic phases and defects within the framework of continuum mechanics. The RVE is generated as a submodel of macroscopic models and simplifies the complex microstructures by homogenization. The deformation tensor computed from the macromodel is transferred to the RVE as boundary conditions [14,15]. The RVE is arranged according to the volume fraction and morphologies derived from the real microstructure, **Figure 5b**. In TWIP steels, the interaction of different twin systems might result in an additional damage source especially when the overall strain hardening capacity is exhausted. In any case, the morphology of the phases, their spatial distribution, and the crystallographic constraints have to be considered. The experimental and numerical flow curves (derived from RVE calculation with periodic boundary conditions) have been precisely modeled for two microstructures: A = martensitic, D = dual phase ferrite + martensite. The failure mechanisms are accurately described as a competition between ductile failure due to a void mechanism according to the Gurson-Tveergard-Needleman (GTN) approach and a cohesive zone model (CZM) for the interface ferrite/martensite.

## Conclusions

The high manganese steels show an excellent balance of strength and ductility due to continuous adaptive grain refinement during straining. The full exploitation of these properties request for a basic understanding of the physical phenomena involved.  New numerical tools are applied and in some cases needed to be developed to predict the properties and parameters but also for improved understanding of involved mechanisms. Especially ab initio techniques help to elucidate the specific effects of these high alloy systems with the occurrence of short range ordering and deformation twinning. The crystallographic nature of the different deformation mechanisms requires crystal plasticity and new continuous damage mechanics modeling.

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