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ScienceDirect
Acta Materialia 59 (2011) 4387–4394
Acta MATERIALIA
www.elsevier.com/locate/actamat

# Experimental and numerical study on geometrically necessary dislocations and non-homogeneous mechanical properties of the ferrite phase in dual phase steels

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Received 21 January 2011; received in revised form 19 March 2011; accepted 22 March 2011
Available online 12 April 2011

**Abstract**

The microstructure of dual phase steels can be compared with a composite composed of a matrix of ferrite reinforced by small islands of martensite. This assumption has been used in several attempts to model the mechanical properties of dual phase steels. However, recent measurements show that the properties of the ferrite phase change with distance from the martensite grains. These measurements showed that the grains of the ferrite phase are harder in the vicinity of martensite grains. As a consequence of this local hardening effect, the ferrite phase has to be considered as an inhomogeneous matrix in modeling dual phase steels. This experiment inspired the idea that local hardening is caused by geometrically necessary dislocations. The idea is investigated experimentally and numerically in the present analysis, which for the first time leads to good agreement with experimental observations of the mechanical stress–strain behavior.


*Keywords:* Dual phase steels; Nano hardness test; Geometrically necessary dislocations; Local hardening; Micromechanical model

## 1. Introduction

### 1.1. Motivation for dual phase steels

Present day industrial applications of sheet metal forming require materials with high plastic deformation potential and high strength. This goal is not easy to achieve, because usually an increase in the mechanical characteristics of the sheet involves a reduction in its workability, in terms of ductility, drawability, and formability. Despite these considerations, dual phase steels have good formability with relatively high strength; in particular they have shown good ductility, continuous yielding followed by rapid work hardening, a low yield to tensile strain ratio and non-aging behavior at ambient temperature.

Dual phase steels are low carbon micro-alloyed steels, characterized by a ferritic multiphase structure in which martensite is dispersed. They have a purely ferrite matrix and about 5–30% martensite dispersed in patches as a second phase. They behave like composite materials in which the ferrite matrix ensures good cold formability, while the martensite is the strengthening element. The correct proportions of the two phases allows a low yielding stress, a high elongation value and a smooth flow–stress curve with a high strain hardening coefficient [1,2].

### 1.2. Tensile properties of dual phase steels

Tremendous efforts have been expended on exploring various aspects of dual phase steels. The effect of the volume fraction ($V_m$), for example, of the harder phase (martensite) has been investigated by different authors [3–7]. Increasing the volume fraction of the harder phase

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doi:10.1016/j.actamat.2011.03.062

was found to increase the yield and ultimate strengths of the aggregate. Shen et al. [8] have shown, using a scanning electron microscope equipped with a tensile straining stage, that the distribution of strain between the ferrite and martensite phases, as well as among the different grains of each phase, was observed to be inhomogeneous.

Various studies aimed at a better understanding of the excellent mechanical properties of dual phase steels [9–16]. There is broad consensus that the low elastic limit (defined as the first deviation from Hooke's law in the stress–strain curve), the continuous yielding and the high strain hardening rate are a consequence of the austenite–martensite transformation, which involves volume expansion. In our materials the volume expansion is approximately 2.9–4% at the martensite start temperature [9]. The strains produced by transformation result in residual stresses in the surrounding ferrite [9]. These internal stresses are assumed to facilitate plastic flow and, hence, reduce the elastic limit. Furthermore, the volume change induces plastic deformation of adjacent ferrite grains and, therefore, creates a high density of unpinned dislocations in the vicinity of martensite [10–12], as was qualitatively studied by transmission electron microscopy (TEM) [13–15]. These dislocations are assumed to be (at least partly) mobile during the early stages of deformation and contribute to work hardening. The heterogeneous distribution of dislocations is supposed to control continuous yielding in dual phase steels. It is assumed that the deformation starts in ferrite areas with low dislocation densities and spreads with increasing plastic strain into regions with higher dislocation densities [16].

At least some of the adjacent ferrite grains have to deform plastically owing to volume expansion during austenite–martensite transformation. During this deformation, geometrically necessary dislocations (GNDs) are required to maintain lattice continuity [17–19] and statistically stored dislocations (SSDs) evolve from random trapping processes [18]. After such transformation-induced deformation residual stresses remain due to inhomogenity of the plastic deformation throughout the grains. However, it is still not understood to what extent GNDs, SSDs, and the associated residual stresses contribute to the yielding behavior of dual phase steels. It is well known that GNDs cause local hardening of the microstructure. But, to the best of the author's knowledge, no experimental observations of this phenomenon have been reported in dual phase steels.

Various homogenization techniques are used in predicting and quantifying the tensile mechanical properties and initial work hardening behavior of various materials of composite microstructure such as dual phase steels [20–23]. None of these models consider local hardening inside the microstructure.

### 1.3. Grain refinement in dual phase steel

In ultrafine single phase alloys it has been shown that the increase in yield stress is accompanied by a decrease in the work hardening rate, which is responsible for poor ductility. This effect has been shown for Al- and Ti-containing ultra-low carbon steel produced by accumulative roll bonding (ARB) [24], in pure titanium [25] and in low carbon steels [26] produced by equal channel angular pressing (ECAP), and in ferritic steels produced by ECAP or ARB [27].

Ultrafine grain (UFG) dual phase steels with a ferrite grain size of around 1 μm have been produced by applying a two-step processing route consisting of (1) a deformation treatment to produce UFG ferrite and finely dispersed cementite or pearlite and (2) a short intercritical annealing in the ferrite/austenite two-phase field followed by quenching to transform all austenite to martensite. Grain refinement in step (1) was achieved by ECAP [28], cold rolling [29] and cold swaging [21]. A single pass processing route based on deformation-induced ferrite transformation (DIFT) was proposed by Mukherjee et al. [30].

It was consistently found that yield strength and tensile strength increased on grain refinement, whereas uniform and total elongation were less affected. The strain hardening rate was found to increase with decreasing grain size [28], which is in contrast to the observation of a very restricted strain hardening rate in UFG low carbon ferrite/cementite steels [31,32]. As the number of investigations on this topic is very limited, a better understanding of the mechanical response of dual phase steels to ferrite grain sizes close to or below 1 μm is required.

In contrast to other methods to increase the strength of steels, grain refinement simultaneously improves the toughness of the material, i.e. its capability to absorb energy under impact conditions [33,34]. Also, The Hall–Petch coefficient of the yield strength is lower than in ferrite/cementite steels that are refined to 1 μm and below [33,34].

CG ferrite exhibits wavy and strongly intersecting slip bands without a preferred orientation, while UFG ferrite basically shows two sets of nearly planar slip bands which are oriented ~40° to the tensile direction [33,34].

In the case of CG steel the failure process is mainly brittle, which is documented by well-defined facets and cleavage steps on these facets, and only some small areas consist of dimples. The dominant fracture mode of FG steel is ductile, although smaller parts of the specimen have undergone brittle fracture. The UFG steel shows dimples throughout the specimens. This suggests a failure process of void nucleation and growth and, hence, entirely ductile fracture [33,34].

### 1.4. Present study

It has been mentioned that all the investigations on grain size effects in dual phase steels were on laboratory produced dual phase steel. The current work mainly focuses on commercial fine grain dual phase steel (2 μm grain size) produced by Thyssen-Krupp Steel AG. In this sense, the result may be interesting. The results of detailed investigations of this material are reported in this paper.

The analysis of tensile properties in the material began from observations of additional hardening in the microstructure when it is compared with the mixture of properties in constituent phases. It was observed that dislocation density pattern pile-up in grain boundaries causes local hardening in the phase boundary and hardening in the microstructure.

In this paper a review will first be carried out of experimental investigations which have been carried out to measure GNDs in the matrix near ferrite–martensite phase boundaries [35]. The measured data indicate that GNDs close to the ferrite–martensite phase boundaries are around one order of magnitude higher that GNDs inside the ferrite grains. Also, the hardness at different locations inside ferrite grains was measured. Finally, a finite element model is developed which considers hardness variation in the ferrite grains of the dual phase steels investigated. In the last part of paper the effects of hardness variation inside the ferrite grains on the macroscopic behavior of the tensile model will be investigated through simulation.

## 2. Experimental study of GND and local hardening in the ferrite phase

To investigate GND distribution inside the microstructure two-dimensional EBSD measurements were carried out on dual phase steel specimens. Electron backscattered diffraction (EBSD) maps were taken in a JEOL JSM 6500F electron microscope equipped with a field emission gun. The small beam diameter and its high brightness yield high contrast Kikuchi patterns so that information about small orientation deviations, even in areas with high dislocation densities like phase or grain boundaries, were obtained. A high speed DigiView CCD camera was used for pattern acquisition. Data were recorded at a 50 nm step size and analyzed using TSL software [35].

The kernel average misorientation (KAM) method was then used to calculate the GND densities from EBSD data. As a first order approach KAM, which is retrieved directly from the EBSD data, was chosen as a measure of the local misorientations. KAM quantifies the average misorientation around a measurement point with respect to a defined set of nearest or nearest plus second nearest neighbor points. It has been shown elsewhere [35] that this method is appropriate for the calculation of GND densities. Fig. 1 shows GND densities in a microstructural sample. It can be observed that the GND densities are one order higher close to the ferrite–martensite interface than away from the interface.

To investigate the effect of GND densities on hardening of the material, nanohardness testing was carried out on the same microstructure. The nanohardness value ($H$) is defined as the applied load divided by the projected area of contact between the indenter and the sample. $H$ (GPa) is calculated in terms of $P$ (nN) and $A$ (nm$^2$). Fig. 2 shows the results of this test. Local hardening in the ferrite phase near the ferrite–martensite interface can be observed. The extent and rate of hardening are different in different grains, but the general trend is the same within ferrite grains. In all cases near interface hardening can be observed.

To micromechanically model the impact of GND on macroscopic mechanical behavior the size and mechanical properties of the interface region have to be specified. For this purpose a more detailed test was carried out on a typical sample area from the experiments in order to specify the size and mechanical properties of the interface region. The nanohardness test was carried out at 60 different points on a commercial dual phase steel microstructure. The results can be seen in Fig. 3. From the results of this test the size of the interface region (in which the hardness varies) can be assumed to typically be of a thickness of 1.5 μm and the mechanical properties were specified relative to the basic ferrite phase.

## 3. Modeling of the microstructure

Within the framework of the unit cell approach, the behavior of materials with complex microstructures is

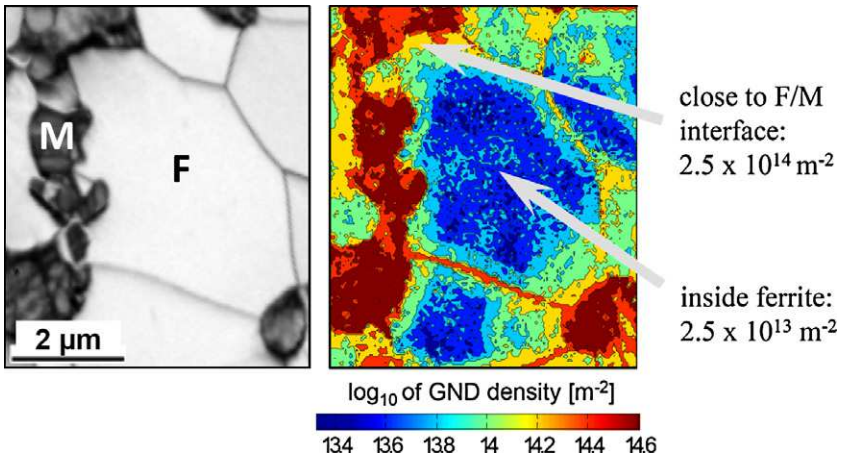


Fig. 1. GND in the microstructure [24].

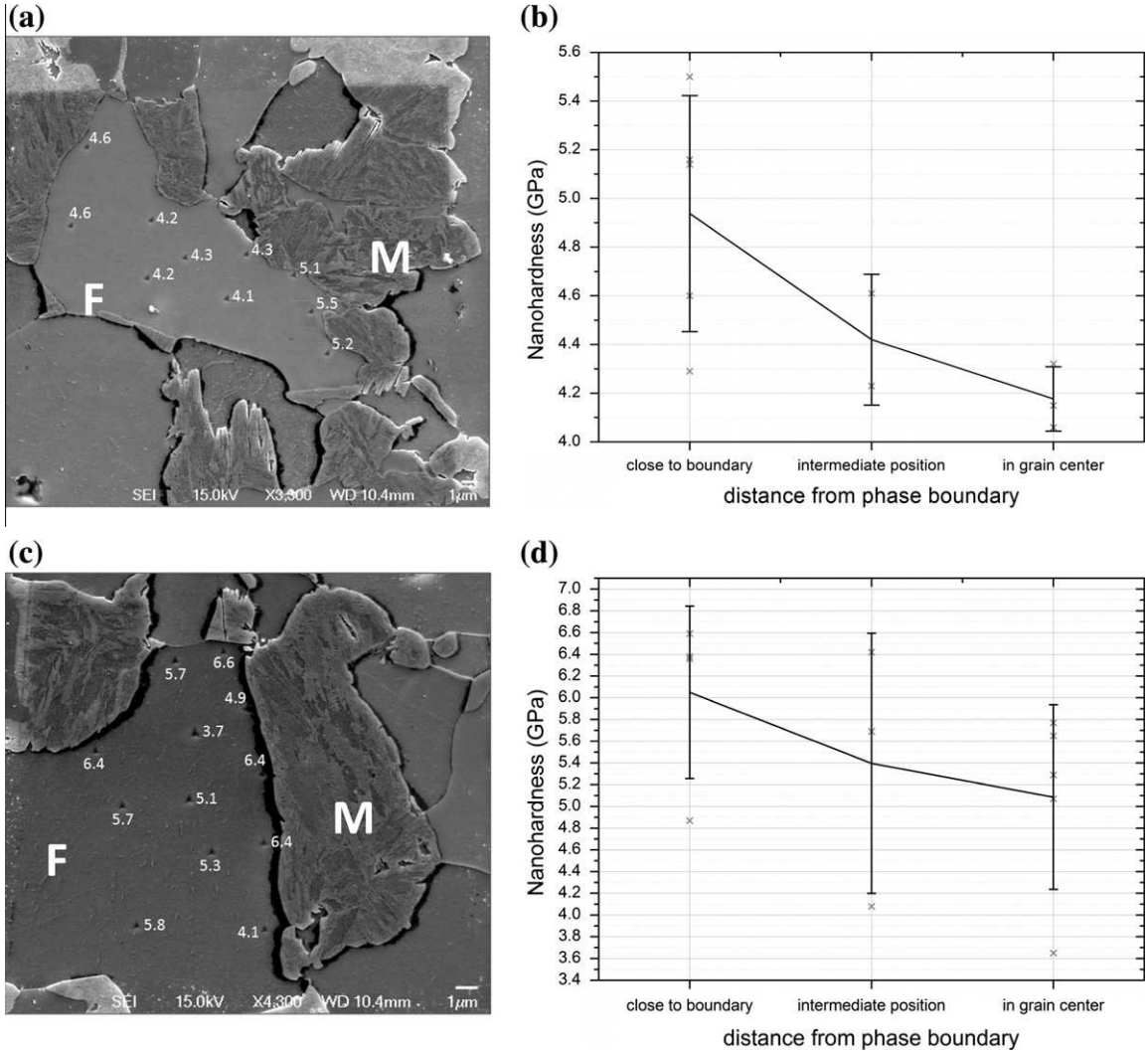


Fig. 2. Nanohardness tests on the microstructure of dual phase steel. (a and c) The nanohardness value at different locations in the microstructure; (b) the nanohardness value according to distance from the grain boundary in case (a); (d) the nanohardness value according to distance from the grain boundary in case (c).

studied by carrying out numerical or analytical studies of the behavior of some part of the microstructure. The main assumption, which must be justified, is that the microstructure of the material can be considered as a periodic repeat of the area under study, and that the sample is therefore representative of the microstructure of the material.

A computer unit cell model for dual phase steel was set up in which the region between ferrite and martensite is considered to be a phase boundary layer. The thickness of this layer, derived from detailed experimental tests, is given in Fig. 3. An elasto-plastic material model was used for both the ferrite and martensite phases, based on the experimental data presented in Fig. 6. The flow curves of bulk ferrite and martensite were determined by uniaxial tensile testing of the individual phases, performed in the laboratories of Thyssen-Krupp Steel AG. For this purpose test specimens of pure ferrite and pure martensite were prepared. Due to the fact that in the heterogeneous dual phase steel martensite has a much higher carbon content than in the artificially produced pure martensite steel, a special martensite melt was prepared having nearly the same carbon content as the dual phase steel. For the boundary layer material data were assigned with respect to the ferrite matrix according to Fig. 3. It can be observed in Fig. 3 that the ferrite matrix gradually hardens as it comes nearer to the martensite. The gradual hardening was approximated by different layers in the model. Fig. 4 gives the model and mesh for two layer and ten layer models. Elasto-plastic material behavior is considered for the ferrite and martensite phases and the interphase layers. An isotropic hardening law is assigned for the plastic state. The yield stress is given as a tabular function of plastic strain from the experimental results.

The unit cell was then put under tensile loading and the results were homogenized for comparison with the experimental data. The homogenization scheme can be described as follows. Macroscopic stress is defined as integration:

$$\sum_{ij} = \frac{\int_{\forall} \sigma_{ij} d\forall}{\forall} \tag{1}$$

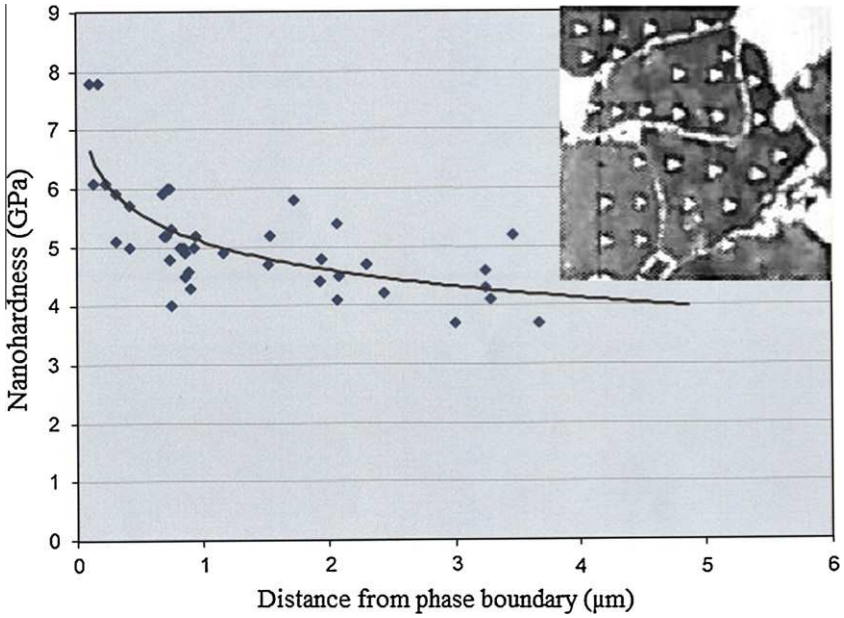


Fig. 3. Detailed nanohardness tests on dual phase steel microstructure.

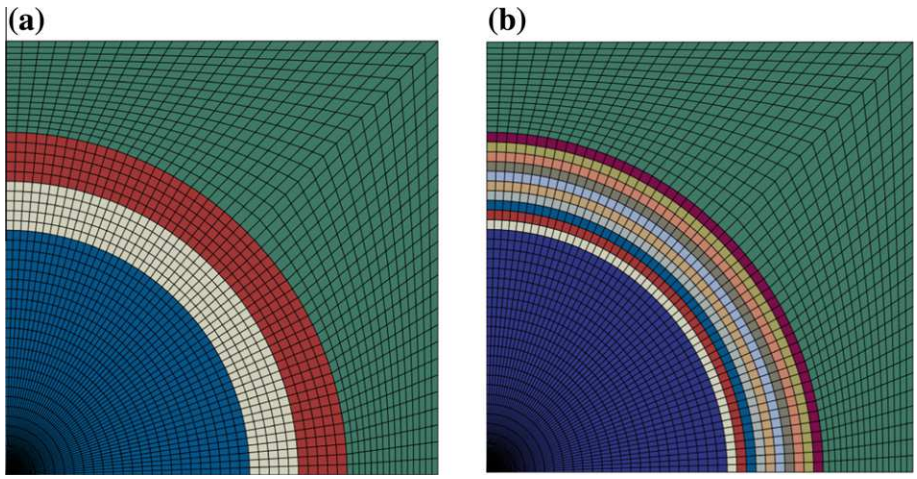


Fig. 4. Modeling of dual phase steel using (a) two layer and (b) 10 layer phase boundary models.

For a discrete field emission volume the above equation can be rewritten as:

$$\sum_{ij} = \frac{\sum_1^n \sigma_{ij} \forall_n}{\forall} \tag{2}$$

where $n$ is the number of finite elements and $\forall_n$ is the volume of the nth element. Analogously, the strains are calculated as:

$$E_{ij} = \frac{\sum_1^n \varepsilon_{ij} \forall_n}{\forall} \tag{3}$$

The plot is for equivalent stress on the basis of equivalent strain. The equivalent stress is calculated as:

$$\sum_{\text{eqv}} = \sqrt{\frac{3}{2} \sum_{ij}^{'} \sum_{ij}^{'}} \tag{4}$$

in which:

$$\sum_{ij}^{'} = \sum_{ij} - \left(\frac{1}{3}\right) \sum_{kk} \tag{5}$$

The equivalent strain can also be calculated as:

$$E_{\text{eqv}} = \sqrt{\frac{2}{3} E_{ij} E_{ij}} \tag{6}$$

in which:

$$E_{ij} = E_{ij} - \left(\frac{1}{3}\right) E_{kk} \tag{7}$$

## 4. Simulation results and discussions

Using these results a unit cell model was built in which the phase boundary was considered according to the exper-

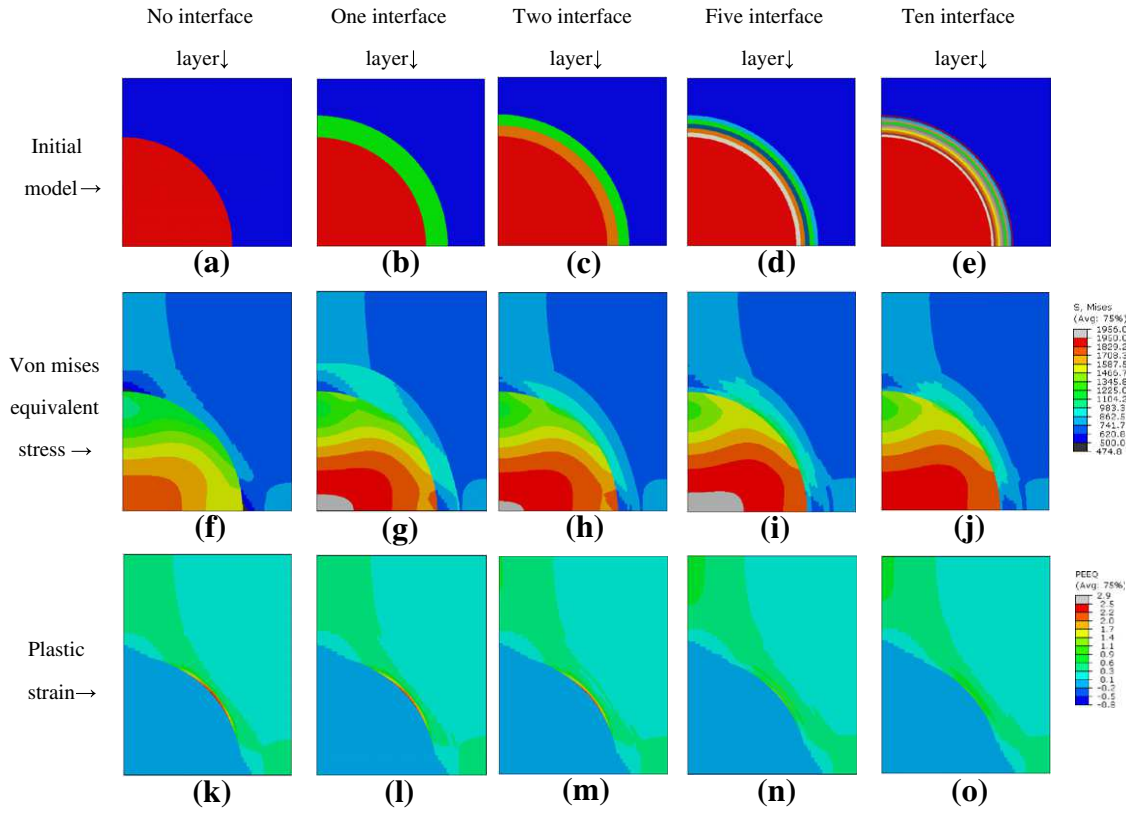


Fig. 5. Results of the simulation for the layered model. (a–e) Initial model with different numbers of interface layers; (f–j) von Mises stress for tensile loading; (k–o) equivalent plastic strain for tensile loading.

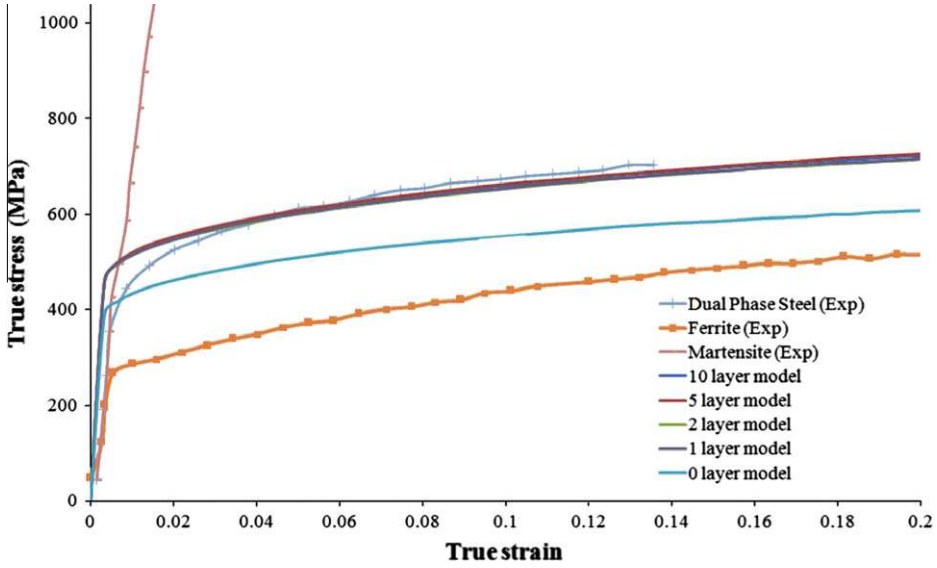


Fig. 6. Simulation vs. experimental results of tensile tests for dual phase steel.

imental data (Fig. 5). For the phase boundary different numbers of layers are considered in order to examine the accuracy of the model with respect to the macroscopic mechanical stress–strain behavior. The results are then compared with the experimental data (Fig. 6). The results show good agreement and it seems that the assumptions in this model are realistic. It is also apparent that by accurate parameter selection a one layer model provides good accuracy using this material model. Therefore, the one layer model will be used in this study for grain size influence investigations.

In the next step, the grain size effect was modeled. Grain size refers to the average size of the ferrite and martensite grains in the microstructure. The effect of grain size was

considered in the following way: as the grain size decreases the grain boundary layer occupies a greater volume fraction of the material. On the other hand, the strength of the grain boundary is unknown. The effect of GND on material hardening will be simulated in this part. Three different grain sizes were considered and different volume fractions of the

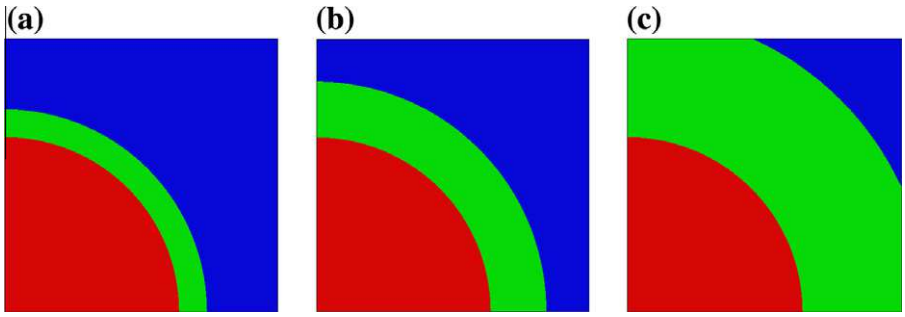


Fig. 7. Model for dual phase steels of different grain size (the average size of the ferrite and martensite phases is taken as the grain size). Grain size: (a) 10 μm; (b) 5 μm; (c) 2 μm.

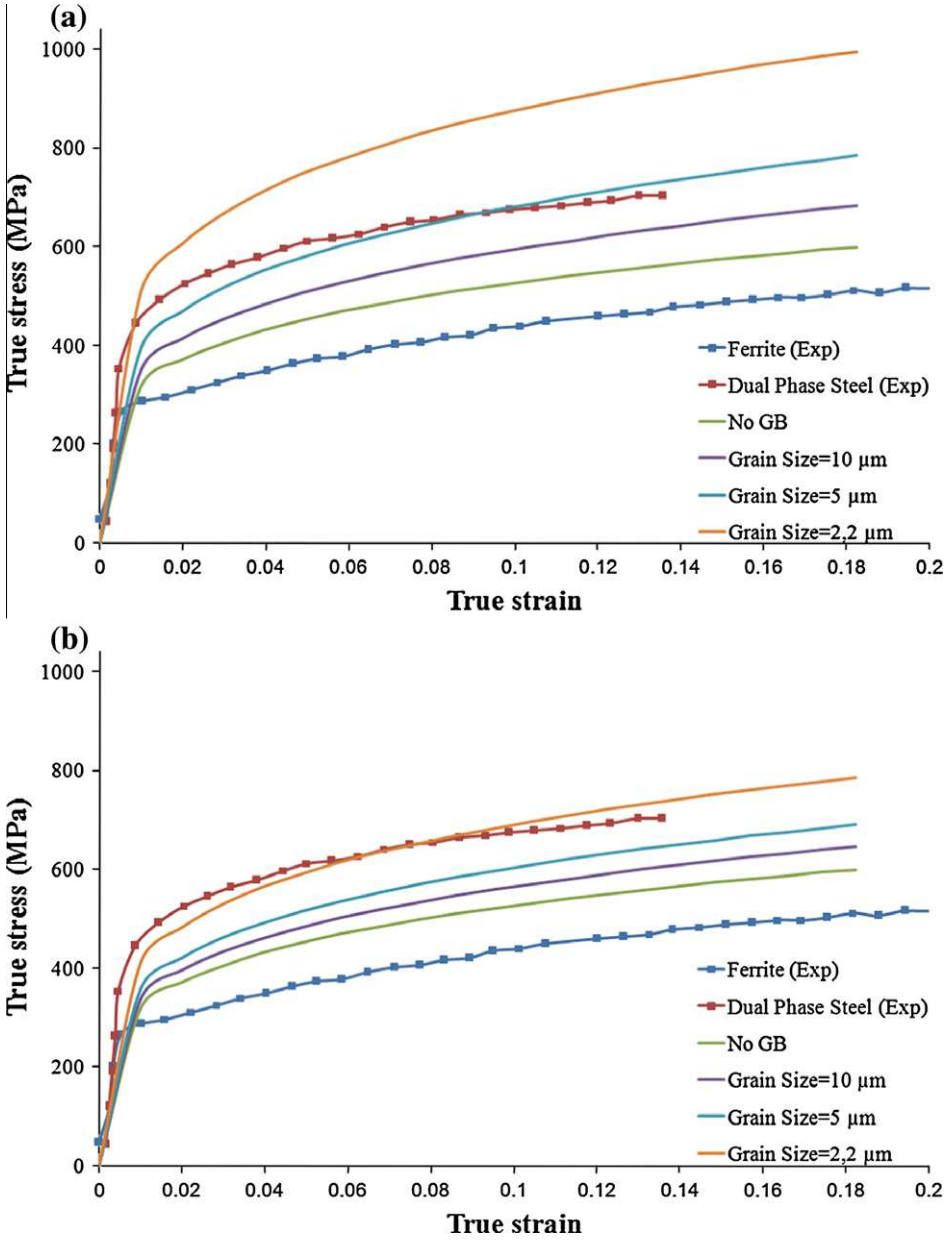


Fig. 8. Simulation vs. experimental results for different grain sizes for $\sigma_y$(GB): (a) 1.75 × $\sigma_y$(ferrite); (b) 1.35 × $\sigma_y$(ferrite).

phase boundary were assigned for each grain size (Fig. 7). It was assumed that the thickness of the boundary phase is constant and, therefore, the volume fraction will increase as a result of grain size reduction. The macroscopic behavior of the material is derived by homogenization of the behavior in the microscopic model. The results are plotted for two different strengths of phase boundary layers in Fig. 8. The strength of the boundary layer is the study parameter. According to Fig. 3 it seems that the strength of the boundary phase is 75% higher than that of the ferrite matrix. Therefore, $\sigma_y(\mathrm{GB}) = 1.75 \times \sigma_y(\mathrm{ferrite})$ was considered in the first simulation. The macroscopic behavior does not match the experimental results perfectly, because the grain size of the specimen was reported to be 2 μm and the simulation value is much higher than the experimental value for a 2 μm grain size. At this time no experimental database for the strength of the grain boundary layer for different grain sizes is available. In this study, in order to simulate the macroscopic behavior observed, for an average grain size reported to be 2 μm, the strength of the grain boundary layer is considered to be 35% higher than for the ferrite matrix. The macroscopic tensile behavior, which is reported in Fig. 8b, matches the experiments well.

According to the simulation results and previous observations [33] the deformation pattern in fine grained dual phase steel can be explained as follows. Grain refinement causes an increase in yield strength and the strain hardening rate of the ferrite matrix. It results in rapid stress transfer to martensite grains. Therefore, the macroscopic behavior increases.

## 5. Conclusions

Previous experimental investigations measuring GND dislocations at the ferrite–martensite boundary have been reviewed. The hardness at different locations inside ferrite grains was also measured. Finally, a finite element model was developed which considers the hardness variation in ferrite grains of dual phase steels. The effects of hardness variation inside ferrite grains on the macroscopic behavior of the dual phase material were investigated. Changing the grain size causes macroscopic hardening of dual phase steels. In this study the effect of GND and hardening due to GND in the material have been considered and the mechanism of hardening analyzed.

## Acknowledgements

We gratefully acknowledge financial support for J.K. by the Deutscher Akademischer Austauschdienst (German Academic Exchange Service, www.daad.org).

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