Multidomain modelling of the magneto-mechanical behaviour of dual-phase steels

F MBALLA-MBALLA 1,2, O HUBERT 1, S LAZREG 1, P MEILLAND 2

1 LMT-Cachan (ENS-Cachan/UMR CNRS 8535/UPMC/Pres Universud Paris) 61, avenue du président Wilson
94235 Cachan cedex, France
2 ArcelorMittal Maizières Research BP 30320 - Voie Romaine F-57283 Maizières-lès-Metz, France

Abstract
The microstructure and mechanical behaviour of dual-phase steels are highly sensitive to the variation of the process (temperature of austeno-ferritic heat treatment). Online control by magnetic method is relevant to detect any fluctuation of the microstructure. The dual-phase is a steel composed of ferrite and martensite phases. Each phase can be considered as a sphere embedded in a homogeneous equivalent medium. The magnetic model used for each phase is based on a magneto-mechanical coupled model. This is an explicit single crystalline model representative of the behaviour of the corresponding phase. Localization rules allow the simulation of the average medium. Experiments are carried out and compared to the modelling.

Keywords: magneto-mechanical behaviour, dual phases microstructure, localization.

1. Introduction

Last few years a growing interest of car industry for the use of high performance steels as dual phase (DP) steels has been observed. Steel production involves several processes: casting, rolling (hot /cold) and heat treatments. These complex processes lead to the production of steels with microstructure exhibiting two phases (fig. 1). The mechanical behaviour of these steels is particularly suited to the automobile sector (high strength, high ductility). The microstructure (fraction and composition of phases) and so mechanical behaviour is highly sensitive to the thermo-mechanical history of the material (heat treatments, rolling rate...) and especially sensitive to small variations in the process (e.g. temperature of ovens). ArcelorMittal plans to set up a non-destructive monitoring technique to evaluate the quality of their DP steels online. This testing uses the magnetic properties of the material: a change in the microstructure and stress would lead to a change in the magnetic behaviour measured by the system. Its implementation is a part of the DPS-MMOD project [1] supported by the French national agency for research.

![Figure 1. Dual phase steel microstructure: distribution of martensite in white, and ferrite in dark.](image-url)
The work presented in this paper was conducted as part of this project. It is a contribution to the modelling of the magneto-mechanical behaviour of dual phase steels (magnetic and magnetostrictive behaviours). The modelling approach consists in using the multidomain model developed at LMT-Cachan [2] applied to each phase. This model is based on the partition in magnetic domains of magnetic materials. This is a single crystalline model. In the context of the intended application, we shall take into account the nature of the two phases of DP steels leading to:
- heterogeneous magnetic field and associated demagnetizing effects
- heterogeneous mechanical field and associated residual stress effects.
This means to set up rules for magnetic and mechanical localization.

2. Dual phase steel metallurgy and magnetic behaviour

The morphology and the distribution of the martensite islands in the ferritic matrix are the keys of the dual phases steel behaviour. This microstructure is obtained by quenching of a low carbon steel (wt%C<0.3% typically) from austeno-ferritic domain of the phase diagram (fig. 2). At a given chemical composition \( C_0 \), the volume fraction of ferrite \( \alpha \) or austenite \( \gamma \) strongly depends on the temperature \( T_0 \). However we know that temperature of ovens on the production lines is subject to fluctuations. Equation (1) gives the change in the fraction of ferrite \( \Delta \%\alpha\gamma \) as function of the thermal variation \( \Delta T \) (fig. 2). This will lead to a change in martensite proportion after quenching.

\[
\Delta \%\alpha\gamma = -100 \, C_0 \frac{\Delta C_\gamma}{C_\gamma^2}
\]

with

\[
\Delta C_\gamma = -\frac{\Delta T}{245.5}
\]

and

\[
C_\gamma = -\frac{190 - 912}{245.5}
\]

The change in ferrite proportion leads on the other hand to a change in carbon content into the austenite (and martensite) (3).

Magnetic measurements presented herein are performed thanks to a magnetic measurement benchmark (fig. 3) where two coils are wounded around the sample. The primary coiling creates the external magnetic field to magnetize the sample. The secondary coiling is
measuring the electromotive force due to the change in the magnetic flux density. A simple time integration of the signal allows to reach the magnetization. Magnetization vs. magnetic field gives the magnetic behaviour of the sample. Two shielded strain gauges (longitudinal and transverse directions) are stuck on both faces to carry out the magnetostrictive behaviour after averaging. This information is not required for NDE: it allows us to evaluate the quality of the modelling. Two ferrimagnetic yokes are put in contact with the sample to close the magnetic circuit and reduce the macroscopic demagnetising field. Cyclic (hysteretic) and anhysteretic measurements are performed with this equipment.

A DP600 from ArcelorMittal has been considered for the study in order to underline the effect of the thermo-mechanical history on the magnetic behaviour of these steels. Six samples have been cut out regularly from the same cast steel (1000m length) submitted to thermal variations.

The chemical composition of the six samples is the same. We observe nevertheless a significant fluctuation of the magnetic and magnetostrictive behaviours (fig. 4) from one sample to another. These changes indicate a variation of the microstructure (volume fraction, carbon content of phases, morphology...) that is the direct consequence of thermal variations.
fluctuations during the process. Table 1 indicates the typical mechanical behaviour (yield stress $\sigma_y$ and ultimate stress $\sigma_{\text{max}}$) of the material where the six samples have been cut out. A correlation between magnetic behaviour and mechanical behaviour is expected.

The magnetic measurement appears as an interesting way to evaluate the change of microstructure and mechanical behaviour of DP steels. To be efficient this evaluation should be based on a numerical reversible model, strong enough to describe the magnetic behaviour of complex microstructures, and fast enough to be implemented on the production line of these steels.


The multidomain modelling is a two-scale reversible modelling allowing the prediction of the magneto-mechanical behaviour of isotropic polycrystals under magnetic or mechanical loading. It comes from a simplification of the so-called multiscale modelling [3]. This modelling is inspired by the partition in domains of magnetic materials. A six magnetic domains configuration is considered associated to the six easy axes of cubic symmetry for materials that exhibit a positive magneto-crystalline constant such as steels (fig. 5a). Each domain family $\alpha$ is defined by a magnetization vector $\vec{M}_\alpha$ so that $|\vec{M}_\alpha| = M_s$, and by a magnetostriction tensor $\epsilon^\mu_\alpha$ (5). $y_i$ parameters figure the direction cosines of magnetization; $\lambda^{100}$ and $\lambda^{111}$ are the two magnetostrictive constants. This single crystal is considered as submitted to a magnetic field $\vec{H}$ or to an external stress $\sigma$.

Uniform strain and field hypotheses are used over the crystal and domain walls contribution to the total energy is neglected [3]. The energy of a magnetic domain $W_\alpha$ is the sum of the magnetostatic energy $W^H_\alpha$ (6), the magneto-crystalline energy $W^K_\alpha$ (7) and of the magneto-elastic energy $W^\sigma_\alpha$ (8) ($\mu_0$ the vacuum permeability = $4\pi.10^{-7}$ $H.m^{-1}$; $K_1$ is the magneto-crystalline constant of the material). The stress tensor is supposed uniaxial; magnetic field and stress are applied along a same direction $\vec{n}_e$ defined by angles $\phi_e$ and $\theta_e$ of the spherical frame (fig. 5c). This direction is restricted to the standard triangle defined by crystallographic directions $<100>$, $<110>$ and $<111>$: cubic symmetry means that at any loading direction is corresponding a direction in this triangle. The resolution of the problem (i.e calculation of the mean magnetization and deformation) requires an evaluation of the direction of magnetization and the volume fraction of each domain family $\alpha$.

$$\vec{M}_\alpha = M_s y_i \vec{e}_i = M_s \left( \cos \phi^\alpha \sin \theta^\alpha \quad \sin \theta^\alpha \sin \phi^\alpha \quad \cos \theta^\alpha \right)^T \quad (4)$$

$$\epsilon^\mu_\alpha = \frac{3}{2} \begin{pmatrix} \lambda_{100}(y_1^2 - \frac{1}{3}) & \lambda_{111}(y_1 y_2) & \lambda_{111}(y_1 y_3) \\ \lambda_{100}(y_2^2 - \frac{1}{3}) & \lambda_{100}(y_2 y_3) & \lambda_{111}(y_2 y_3) \\ \lambda_{100}(y_3^2 - \frac{1}{3}) & \lambda_{100}(y_3 y_1) & \lambda_{111}(y_3 y_1) \end{pmatrix} \quad (5)$$

$$W^H_\alpha = -\mu_0 \vec{H}.\vec{M}_\alpha \quad (6)$$

$$W^K_\alpha = K_1 \left( y_1^2 y_2^2 + y_2^2 y_3^2 + y_3^2 y_1^2 \right) \quad (7)$$

$$W^\sigma_\alpha = -\sigma : \epsilon^\mu_\alpha \quad (8)$$
\[ \vec{n}_c = (\cos\phi_c \sin \theta_c \ sin \phi_c \sin \theta_c \ cos \theta_c) \]  

(9)

Considering the loading direction \( \vec{n}_c \) defined by two angles \( \phi_c \) and \( \theta_c \) (fig. 5c), the restriction to standard triangle allows an analytical minimization of the total energy (10), so that a constitutive law for the angles of each domain is obtained as function of magnetic field, stress, and loading direction parameters.

\[
\frac{dW_\alpha}{d\phi_\alpha}(H, \sigma, \phi_c, \theta_c, \phi_\alpha, \theta_\alpha) = 0 \quad \text{and} \quad \frac{dW_\alpha}{d\theta_\alpha}(H, \sigma, \phi_c, \theta_c, \phi_\alpha, \theta_\alpha) = 0
\]

(10)

For example for the domain \( \alpha = 1 \), the magnetization direction given by the two angles \( \phi_1 \) and \( \theta_1 \) is:

\[
\phi_1(H, \sigma, \vec{n}_c) = \frac{\mu_0 M_s H \phi_c + \arctan \left( \frac{3}{2} \lambda_{111} \sigma \sin(2\phi_c) \right)}{\mu_0 M_s H + 2K_1 + 3\lambda_{100} \sigma \cos(2\phi_c)}
\]

(11)

\[
\theta_1(H, \sigma, \vec{n}_c) = \frac{\pi}{2} - \frac{\mu_0 M_s H (\frac{\pi}{2} - \theta_c) + \arctan \left( \frac{3}{2} \lambda_{111} \sigma \sin(2(\frac{\pi}{2} - \theta_c)) \right)}{\mu_0 M_s H + 2K_1 + 3\lambda_{100} \sigma \cos(2(\frac{\pi}{2} - \theta_c))}
\]

(12)

Where \( \vec{H} = H \vec{n}_c \) and \( \vec{\sigma} = \sigma \vec{n}_c \) are stress and the magnetic field vectors along the loading direction. The volume fraction of each domain \( f^\alpha \) is calculated thanks to statistical Boltzmann formula:

\[
f^\alpha = \frac{\exp(-A_s W^\alpha)}{\sum_{\alpha} \exp(-A_s W^\alpha)}
\]

(13)

\( A_s \) is an adjusting parameter proportional to the initial susceptibility \( \chi_0 \) of the magnetization curve:

\[
A_s = \frac{3\chi_0}{\mu_0 M_s^2 (\cos \phi_c \sin \theta_c)^2}
\]
necessary given by a loading along a specific direction inside the triangle. Since the
behaviours are not linear, this direction is not the average direction and is theoretically
changing with stress or magnetic field level. We consequently make the assumption that this
change is small enough to be neglected. The only parameters to be identified are finally \( \varphi_c, \theta_c \)
and \( A_s \) that requires few experimental data.

\[
\vec{M} = \sum f_\alpha \vec{M}_\alpha \quad \epsilon^\mu = \sum f_\alpha \epsilon^\mu_\alpha \quad M = \vec{M} \cdot \hat{n}_c \quad \epsilon^\mu = \hat{n}_c \epsilon^\mu \cdot \hat{n}_c
\]

(14)

### 4. Dual phase steel modelling, magnetic and stress localization

The presence of two different phases creates a local perturbation called demagnetizing field in
magnetism and residual stress in mechanics. The local fields are not generally the same as the
mean fields. Their calculation requires a mathematical operation called localization. We
consider a two phases medium composed of ferrite \( (f) \) and martensite \( (m) \). We call ‘\( i \)’ the
inclusion that could be alternately \( f \) or \( m \). The local magnetic field \( \vec{H}_i \) applied to the phase ‘\( i \)’
is a complex function of macroscopic field \( \vec{H} \) and the properties of the mean medium. In the
case of spheroidal inclusion [3], the field is demonstrated as homogeneous on each phase.
Considering on the other hand a linear behaviour (susceptibility), local magnetic field acting
on the phase ‘\( i \)’ is:

\[
\vec{H}_i = \vec{H} + \frac{1}{3 + 2\chi_0} \left( \vec{M}_i - \vec{M}_c \right) = \vec{H} + \vec{H}_{d_i}
\]

(15)

Where \( \chi_0 \) and \( \vec{M}_c \) are the mean medium susceptibility and magnetization, \( \vec{M}_i \) is the local
magnetization. \( \vec{H}_{d_i} \) is the so called demagnetizing field. The extension to nonlinear behaviour
involves to use the sequent susceptibility for the definition of \( \chi_0 \).

\[
\chi_0 = ||\vec{M}| / ||\vec{H}||
\]

(16)

This approach is applied to a dual phase microstructure \( (f, m) \).

\[
\vec{H}_f = \vec{H} + \frac{1}{3 + 2\chi_0} \left( \vec{M}_f - \vec{M}_f \right) \quad \vec{H}_m = \vec{H} + \frac{1}{3 + 2\chi_0} \left( \vec{M}_m - \vec{M}_m \right)
\]

(17)

with:

\[
f_f \vec{H}_f + f_m \vec{H}_m \quad \vec{M} = f_f \vec{M}_f + f_m \vec{M}_m
\]

(18)

\( f_f \) and \( f_m \) are the volume fraction of \( f \) and \( m \) phases. \( \vec{H}_f \) and \( \vec{H}_m \) are introduce as loadings in the
multidomain modelling so that the modelling gives the magnetization of each phase. An
averaging operation allows to compute the macroscopic magnetization. A new estimation of
local magnetic fields is calculated and compared to the previous loading. The process is
iterated until convergence (minimization of quadratic error).

The solution of Eshelby's problem is the basis of the modelling of heterogeneous media's
behaviour in mechanics [4]. Its formulation has been extended by Hill considering a
deformable matrix [5]. Equation (19) gives the stress field within the inclusion ‘\( i \)’ submitted
to a macroscopic stress $\sigma$ in the case of homogeneous behaviour (same elastic properties of both phases). $\epsilon^I_i$ is the magnetostriction strain of the inclusion considered as free to deform (output of the multidomain modelling). $\epsilon^\mu$ is the average magnetostriction strain over the volume.

$$\sigma_i = \sigma + C(\mathbb{I} - S^E) : (\epsilon^\mu - \epsilon_i^I) = \sigma + \sigma_{res,i}$$ \hspace{1cm} (19)

$C$ is the media stiffness tensor, $S^E$ is the Eshelby's tensor depending only on the stiffness constants of the material and on the shape of the inclusion. $\sigma_{res,i}$ is the so called residual stress tensor.

This approach is applied to a dual phases microstructure $(f, m)$:

$$\sigma_f = \sigma + C(\mathbb{I} - S^E) : (\epsilon^\mu - \epsilon_f^I) \hspace{1cm} \sigma_m = \sigma + C(\mathbb{I} - S^E) : (\epsilon^\mu - \epsilon_m^I)$$ \hspace{1cm} (20)

leading to macroscopic quantities:

$$\sigma = f_f \sigma_f + f_m \sigma_m \hspace{1cm} \epsilon^\mu = f_f \epsilon_f^\mu + f_m \epsilon_m^\mu$$ \hspace{1cm} (21)

The local fields $\sigma_f$ and $\sigma_m$ are introduced as loadings into the two multidomain computations as well as the local magnetic fields. After convergence these computations give the strain and the magnetization of each phase, and the average quantities. The numerical convergence is reached easily since the mechanical behaviour is linear.

5. Experimental and modelling results

5.1 Materials considered

The magneto-mechanical behaviour of a dual phase steel is deeply linked to its microstructure and especially to the behaviour of its constituents. An accurate modelling of the mean medium supposes consequently to have an accurate modelling of each phase separately. The behaviour of ferrite is supposed very close to the behaviour of pure iron, that was the subject of many works. The measurements presented hereafter have been carried out using an Armco pure iron sample.

The behaviour of martensitic phase is still unknown. Tab. 2 gives the chemical composition of the DP steel used for the study. The carbon content is close to 0.15wt%. Figure 1 gives the typical microstructure observed for the material as quenched. The volume fraction of martensite has been evaluated to 40±2%. Assuming that carbon content of ferrite is about 0.02wt%, the carbon content in the martensite phase can be so evaluated to 0.4wt%.

Table 2. Chemical composition of the DP steel used for the study.

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>S</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>1461</td>
<td>18852</td>
<td>14</td>
</tr>
</tbody>
</table>
This information is crucial since the behaviour of martensite is probably correlated to its carbon content (change in lattice parameters). Indeed, a steel exhibiting the same average carbon content and submitted to an appropriate thermal treatment (leading to the same microstructure: martensite, dislocations, residual stress...) could be representative of the martensitic phase of the dual phase.

A C38 carbon steel has been considered for this step (wt%C=0.38%). It has been submitted to various heat treatment (quenching) in order to transform the initial microstructure (fig. 6a) into a microstructure close to the microstructure of the second phase of the dual phase steel. Hardness measurements are used as indicator of the quality of the new microstructure. Figure 6b shows the microstructure obtained after the heat treatment that has been selected. As expected we have a quite homogeneous microstructure, composed of martensite needles, strained ferrite and bainite.

Figure 6. Micrographies of C38 steel: raw material (a), quenched material (b).

5.2 Identification of the parameters of the multidomain modelling

Magneto-mechanical experiments have been performed on a pure iron sample and on the C38 sample quenched following the selected heat treatment. Figure 7 shows the experimental results obtained (magnetic and magnetostrictive anhysteretic behaviours are plotted [6]).

The table below lists the parameters used for the modelling of each phase. Physical parameters for pure iron are well known (magnetocrystalline and magnetostrictive constants, saturation magnetization). The loading angles are the result of a global optimization. The physical parameters of the martensite are poorly documented. An isotropic behaviour has been supposed for the second phase that reduces the magnetostrictive parameters to one. \( M_s \) and \( \lambda^{100} \) levels have been chosen so that the modelling fits properly the experimental result for magnetostriction. Next, the value of angles \( \theta_c, \phi_c \) and \( K_1 \) parameters is the result of a global least square optimization.

<table>
<thead>
<tr>
<th></th>
<th>( \theta_c ) (°)</th>
<th>( \phi_c )</th>
<th>( \lambda^{100} )</th>
<th>( \lambda^{111} )</th>
<th>( K_1 ) (J.m(^{-3}))</th>
<th>( M_s ) (A.m(^{-1}))</th>
<th>( A_s ) (m(^{-3}).J(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>ferrite</td>
<td>88; 41</td>
<td>21.10(^{-6})</td>
<td>-21.10(^{-6})</td>
<td>4.8.10(^{4})</td>
<td>1.71.10(^{6})</td>
<td>3.5.10(^{-3})</td>
<td></td>
</tr>
<tr>
<td>martensite</td>
<td>90; 36</td>
<td>3.10(^{6})</td>
<td>3.10(^{-6})</td>
<td>10.10(^{4})</td>
<td>1.05.10(^{6})</td>
<td>4.10(^{-4})</td>
<td></td>
</tr>
</tbody>
</table>
Figure 7. Model vs experimental results for magnetic (a,b) and magnetostrictive (c,d) behaviours of pure iron (a,c) and pure martensite (b,d).

5.3 Modelling of DP steels

Once the best parameters describing the ferrite and martensite behaviour are found, a dual phase medium can be modelled. A sample exhibiting a volume fraction of martensite estimated to 42% is chosen (sample #6 – Cf figure 1 and table 1). The localization procedure is applied for magnetic field. Homogeneous stress condition is considered as a first step. The figure 8 allows us to observe the convergence of magnetic field values within the two phases. After few iteration the magnetic field becomes stable: Its value is higher inside the martensite (magnetically hard material) than in the ferrite (magnetically soft material). Figure 9 shows that magnetic behaviour is well described by the model. But over 6000 A.m\(^{-1}\) the localization process have no more effect on the magnetization. The effect of localization is relatively weak in this situation. Figure 9 allows to compare experimental and modelled results. Effect of localization is weak too. We observe that the magnetostriction strain is overestimated at high magnetization. Implementation of stress localization would help us to reach a better approximation of such behaviour.

Figure 8. Magnetic field localization \((f_m=42\%)\) (a) convergence of local fields at \(H=1.25 \times 10^7\) A.m\(^{-1}\)
Figure 9. Modelling ($f_m = 42\%$) vs experimental results for the magnetic (a) (b) and magnetostrictive (c) behaviour of a dual phase (DP #6).

6. Conclusions

The modelling strategy that has been proposed allows a fast estimation of the magneto-mechanic behaviour of a dual phase microstructure. This estimation requires the knowledge of the behaviour and the volume fraction of the both phases. Experimental results and modelling are quite in good agreement. The magnetostrictive behaviour is nevertheless overestimated. Implementation of the stress localization would probably improve this result. The effect of magnetic localization is weak because the microstructure is considered as a mix between two isotropic phases whereas the real microstructure corresponds to a mix between anisotropic single crystals.

Next step consists in making an inverse identification of volume fraction of phases thanks to a magnetic measurement. The sensitivity of the magnetic and magnetostrictive behaviours to the volume fraction of phases has been estimated. It becomes possible to discriminate between two microstructures exhibiting a difference in phase fraction less than 2%.

References

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