Effect of Cooling Rate on Transformation Plasticity of 0.45% Carbon Steel

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This study aims at investigating the effect of cooling rate on transformation plastic strain in 0.45 mass% carbon steel. It has been revealed that slow cooling rate increases the magnitude of transformation plastic strain especially at the cooling rate less than 10°C/s. Based on Greenwood-Johnson mechanism (strain accommodation mechanism), transformation plasticity modelling is made using crystal plasticity fast Fourier transform numerical method. It is shown that there are three inter-related mechanisms that control the amount of transformation plasticity as a function of cooling rate: the dependence of yield stress of weaker phase with temperature, the dependence of volume change to cooling rate (higher volume change at higher cooling rate) and the influence of viscoplasticity behaviour that enhances creep strain at high temperature. The model predicts the transformation plastic strain relatively close to those of experimental ones at high cooling rates (typically 10°C/s and above) where phase transformation happens at low temperatures, while it under estimates the transformation plastic strain at slow cooling rates where phase transformation happens at high temperatures. These results show that other mechanisms like creep/viscoplasticity should be considered by the model to predict influence of cooling rate on transformation induced plasticity.

KEY WORDS: transformation plasticity; carbon steel; crystal plasticity; FFT.

1. Introduction

During phase transformation, external stress, even though it is smaller than the yield stress, leads to a large strain development called transformation plastic strain.^{1,2)} Transformation plastic strain plays an important role during quenching of carbon steels as it can affect the shape and residual stress distribution.³⁾ This is the reason why many attempts have been made to measure the transformation plastic strain for number of steel grades^{4–12)} under certain heat treatment conditions. These results were applied to the finite-element simulations to estimate accurately the residual stress of quenched steels.^{13–15)}

The mechanism of transformation plasticity is a great controversy. Greenwood and Johnson¹⁶⁾ claimed that the main mechanism of the transformation plasticity for diffusive phase transformation is the strain accommodation caused by transformation volume difference between two phases. This reasoning was put forward by Leblond *et al.*¹⁷⁾ and theoretical modelling was made.^{18,19)} The mechanism has been further approached numerically using Finite Element Method (FEM)^{20–22)} and the crystal plasticity fast Fourier transform (CPFFT).^{23,24)} In contrast to the strain accommodation effect, diffusion controlled mechanism is also suggested by Han *et al.*²⁵⁾ In contrast, for displacive phase

transformation, transformation plasticity is controlled by a certain variant selection which is favourable for the applied stress called Magee mechanism.²⁶⁾ However, Greenwood-Johnson mechanism has been found to be a non-negligible agent for displacive phase transformation as well.⁹⁾

According to the analytical model for diffusive phase transformation proposed by Greenwood and Johnson¹⁶⁾ or Leblond,¹⁸⁾ the transformation plastic strain is proportional to the volume change (or transformation strain – Leblond's model) and inverse proportion to the yield stress of the weaker phase. More recently, the Leblond's model has been extended to consider plasticity of all phases during cooling under phase transformation.²⁷⁾ However, all these models cannot consider the cooling rate dependency because on the one hand they consider perfectly plastic or elasto-plastic behaviour of the materials (*e.g.* plasticity independent on time). On the other hand, one cannot assert the effect of cooling rate with these models because of the opposite effect between the transformation volume change which is larger at higher cooling rate as the transformation temperature lowers (producing higher transformation plastic strain) and the yield stress of weaker phase which is harder at higher cooling rate (producing smaller transformation plastic strain). Thus, it is not clear how the cooling rate affects the transformation plastic strain.

Hence, the aim of this study is defined to determine the effect of cooling rate on transformation plasticity during diffusive phase transformation (austenite to ferrite/pearlite

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transformation) of 0.45% carbon steel. The transformation plastic strain of 0.45% carbon steel is measured experimentally under several different cooling rates. In addition, the experimental results will be assessed using crystal plasticity fast Fourier transform (CPFPT) numerical scheme incorporating the transformation effect. A comparison of numerical and experimental results will be made followed by discussion on Greenwood-Johnson mechanism.

2. Experiment

2.1. Experimental Equipment

The transformation plastic strain is measured by using Instron 8802 hydraulic fatigue machine equipped with an extensometer and heat treating devises (heating by induction heating and cooling by He gas or Ar gas depending on the required cooling rate). The machine appearance is shown in **Fig. 1** and the specimen geometry is in **Fig. 2** (unit is mm). The gauge length is 12.5 mm. Before starting a test sequence, atmosphere air in the chamber is replaced by Ar gas in order to prevent oxidation at high temperature.

2.2. Experimental Condition and Calculation of Transformation Plasticity

The employed steel grade is 0.45% carbon steel whose chemical composition is shown in **Table 1**. The objective of this experiment is to identify the magnitude of transformation plastic strain during austenite to ferrite/pearlite phase transformation and reveal the effect of cooling rate on transformation plasticity. Thus the specimens are heated up to 900°C at 10°C/s heating rate followed by isothermal

holding with duration of 2 min for fully austenisation. Right after the isothermal holding, constant stress (0, 10, 30 and 50 MPa) are loaded and subsequent cooling at several cooling rates (0.1, 1, 10 and 20°C/s) are applied. In the course of the sequence, temperature, strain and stress are measured. The schematic of these sequences are depicted in **Fig. 3**.

By followings, the details will be explained of how the transformation plasticity coefficient can be related to the experimental results. The transformation plasticity coefficient K is defined as:¹³⁾

Table 1. Chemical composition of S45C carbon steel (mass%).

C	Si	Mn	P	S	Cu	Ni	Cr
0.43	0.20	0.70	0.010	0.0044	0.005	0.008	0.11

Fig. 3. Schematic of temperature and stress during heat treatment process.

Fig. 1. Uniaxial tensile (fatigue) machine.

Fig. 2. Geometry of a sample (typical thickness = 1.5 mm).

$$\dot{\varepsilon}^p = 3K(1-z)\dot{z}s, \dots\dots\dots (1)$$

where ε^p is the transformation plastic strain, z is the volume fraction of daughter phase and s is the deviatoric stress. In the present experiment, the applied stress is uniaxial and thus the integral of Eq. (1) from transformation start point to the end point gives the total transformation plastic strain, such that:

$$\varepsilon^p = K\sigma. \dots\dots\dots (2)$$

According to the Eq. (2), the transformation plasticity coefficient K can be deduced from the relation between transformation plastic strain and applied stress, which can be measured by experiments.

An alternative semi-analytic approach to calculate transformation plasticity coefficient has been suggested by Greenwood and Johnson.¹⁶⁾ The main mechanism of transformation plasticity is the plastic strain in the weaker phase (mother phase in this case) accommodating the transformation strain induced in the daughter phase. In this case, the transformation plastic strain can be expressed using volume change by phase transformation $\Delta V/V$ and the yield stress of the weaker phase σ_1^y , such that:

$$\dot{\varepsilon}^p = \frac{5}{6\sigma_1^y} \frac{\Delta \dot{V}}{V} \sigma. \dots\dots\dots (3)$$

Equation (3) is in a uniaxial form and needs to be extended to a multi axial form. After Greenwood-Johnson mechanism, Leblond¹⁸⁾ has analytically solved the elastoplastic deformation of mother phase which surrounds daughter phase and obtained following transformation plastic strain rate:

$$\dot{\varepsilon}^p = \begin{cases} 0 & \text{if } z \leq 0.03 \\ \left(\frac{-2\beta}{\sigma_1^y} \right) \ln(z) \dot{z} \frac{3}{2} s & \text{if } z > 0.03 \end{cases}, \dots\dots\dots (4)$$

where β is the transformation strain ($\cong \Delta V/3V$) and z is the volume fraction of daughter phase.

In this case, the transformation plasticity coefficient can also be defined by taking time integration of Eq. (4), such that:

$$K \cong \frac{2\beta}{\sigma_1^y}. \dots\dots\dots (5)$$

According to Eq. (5), the yield stress of mother phase is necessary to the calculated transformation plasticity coefficient. In addition to that, for full-field numerical analyses which will be discussed in the later section, the constitutive relations of daughter phase are imperative as well. Hence, stress-strain curves of both mother and daughter phase are measured.

2.3. Experimental Results

2.3.1. Temperature-strain Curves under Free of Stress

Cooling rate dependent strains versus temperature under free stress condition are shown in **Fig. 4**. Obviously, the transformation temperature lowers as cooling rate accelerates. The final strains after phase transformation coincide each other independent of the cooling rate; it indicates that the transformation strain is getting large in accordance with

Fig. 4. Comparison of cooling curves under stress free condition.

Table 2. Cooling rate dependence of transformation strain.

Cooling rate (°C/s)	Transformation start temperature (°C)	Transformation finish temperature (°C)	Transformation strain β
0.1	690	640	2.63×10^{-3}
1	670	615	2.93×10^{-3}
10	640	585	3.21×10^{-3}
20	590	540	3.77×10^{-3}

the acceleration of cooling rate because coefficient of linear thermal expansion in austenite phase is larger than that of ferrite/pearlite phase.

As mentioned above, the γ phase has a greater coefficient of thermal expansion than that of α phase, namely $\alpha_\gamma = 2.2 \times 10^{-5}$ and $\alpha_\alpha = 1.8 \times 10^{-5}$. This means that the transformation strain during γ/α phase transformation becomes larger as transformation temperature decreases (with faster cooling rate). Transformation strains depending on the cooling rate are deduced from **Fig. 4** and are summarised in **Table 2**: the higher the cooling rate is the higher the volume change is.

2.3.2. Temperature-strain Curves under Stress

In addition to the stress free condition (0 MPa), the temperature-strain curves under stress (10, 30, 50 MPa) will be demonstrated in this section. The stress is applied just before phase transformation takes place and the stress is kept constant during phase transformation. In this way, the transformation plastic strain can be measured under constant applied stress. The obtained temperature-strain curves are shown in **Fig. 5**. For the 0.1°C/s cooling rate and 50 MPa applied stress case, the strain curve was not stabilised because of the creep strain. In this case, it is difficult to separate the transformation plastic strain from creep strain.⁷⁾ Therefore, the data will not be used in the following analyses.

Large strain development around 550–600°C with the application of external stress can be observed from **Fig. 5**. This phenomenon is called transformation plasticity and the obtained additive strain is transformation plastic strain. The transformation plastic strain shown on **Fig. 5** can be calculated from removing the transformation strain (the strain of stress free condition) from the total strain under stress. This procedure provides the transformation plastic strain depending on the applied stress magnitude, which is

Fig. 5. Temperature-strain curves under applied stresses.

exhibited in Fig. 6.

It is clear from Fig. 6 the magnitude of transformation plastic strain increases with the applied stress. A slight non-linearity between the transformation plastic strain and the applied stress can be found in when applied stress is relatively large,²³⁾ but this is considered to be negligible small for taking the approximate slopes (transformation plasticity coefficient) of each result.

2.3.3. Stress-strain Curves

Tensile tests with strain rate of 0.5 s^{-1} are conducted at

Fig. 6. Transformation plastic strain versus applied stress deduced from experiment.

Fig. 7. Stress-strain curves for austenite and pearlite phase by experiment at a strain rate of 0.5 s^{-1} .

Table 3. 0.2% proof stress and average temperature during tensile tests.

Cooling rate (°C/s)	Average testing temperature (°C)		0.2% proof stress (MPa)	
	Austenite	Pearlite	Austenite	Pearlite
0.1	695	613	95.8	183.9
1	672	587	102.8	223.4
10	648	533	105.5	349.9
20	617	483	111.2	402.8

temperatures just before initiation of phase transformation and as well as just after finishing of phase transformation (same specimen geometry is employed). The obtained

results are shown in **Fig. 7**. The mean temperature at which each tensile test was conducted as well as the measured 0.2% proof stress are listed in **Table 3**. In this research, the measured 0.2% proof stress will be used as a yield stress. The testing temperature lowers as increase the cooling rate, reflecting the phase transformation dependent on cooling rate.

Making use of the transformation strain (Table 2) and the yield stress (Table 3) the transformation plasticity coefficient can be estimated according to Eq. (5). The calculated transformation plasticity coefficient results are shown in **Table 4**. The experimental results are generally larger than those by Leblond's analytical model (Eq. (5)) and this tendency is

Table 4. Transformation plasticity coefficient – a comparison between values by experiment and Leblond model.

Cooling rate (°C/s)	K by experiment (MPa ⁻¹)	K by Leblond model (MPa ⁻¹)
0.1	23.7×10^{-5}	5.49×10^{-5}
1	18.0×10^{-5}	5.70×10^{-5}
10	10.9×10^{-5}	6.08×10^{-5}
20	7.82×10^{-5}	6.78×10^{-5}

Fig. 8. Microstructure by optical microscope for each heat treatment condition (left value = cooling rate, right value = applied constant stress).

more pronounced for the case of slow cooling rate, *i.e.* high phase transformation temperature. This phenomenon will be further more investigated in the later section.

2.3.4. Microstructure

The microstructures for each heat treating condition are demonstrated in **Fig. 8**. The specimens were cut at their centre and etched in nital solution to reveal microstructure after heat treatment.

The application of stress seems little effect on the microstructure, while the cooling rate effect is more pronounced. As being faster the cooling rate, less ferrite formation is observed at the prior austenite grain boundaries and more pearlite fraction is obtained. This microstructure strengthens the material but degradation in elongation is observed.

2.3.5. Pearlite Structure

In this section, pearlite microstructure formed under each cooling rate will be investigated. The lamellar spacing is known to be an inverse proportion to cooling rate; narrow lamellar spacing with high cooling rate.

The typical pearlite lamellar structures observed by the scanning electron microscope are shown in **Fig. 9** and measured lamellar spacing is in **Table 5**. From these results, the applied stress magnitude effect is little on the pearlite structure and the lamellar spacing. It is obvious that the relation between cooling rate and tensile strength originates from the pearlite lamellar spacing depending on the cooling rate.

It must be noted that the strong dependency of yield stress to cooling rate observed on **Fig. 7** is not due to a strain rate effect (as all tensile tests are carried out with the same 0.5 s^{-1} strain rate) but is mainly due to the dependency of pearlite interlamellae spacing with cooling rate as reported

Fig. 9. Pearlite lamellar structure by scanning electron microscope (left value = cooling rate, right value = applied constant stress).

Table 5. Relation between cooling rate and measured pearlite lamellar spacing (μm).

Stress (MPa)	Cooling rate (°C/s)			
	0.1	1	10	20
0	0.208	0.179	0.195	0.112
10	0.202	–	–	–
50	–	0.166	0.130	0.108

in Table 5: the higher the cooling rate is, the lower the inter-lamellae spacing is, making the material strengthen.

3. Numerical Simulation

3.1. FFT Modelling of Elastoplasticity in a Heterogeneous Medium

The homogenisation technique using FFT has been firstly introduced by Moulinec *et al.*^{28,29} This method uses Green's function to solve differential equation of elastoplastic problems of the heterogeneous materials under periodic boundary condition.

In the case of a periodic boundary problem, the local displacement in position $\mathbf{x}$ can be divided into fluctuation and average terms such that:

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}'(\mathbf{x}) + \bar{\boldsymbol{\varepsilon}} \mathbf{x}, \quad (6)$$

where, $\mathbf{u}'(\mathbf{x})$ is the periodic displacement and $\bar{\boldsymbol{\varepsilon}}$ is the macroscopic strain, which is constant in the local region. The strain field reads:

$$\boldsymbol{\varepsilon}(\mathbf{u}(\mathbf{x})) = \boldsymbol{\varepsilon}(\mathbf{u}'(\mathbf{x})) + \bar{\boldsymbol{\varepsilon}}, \quad (7)$$

with $\langle \boldsymbol{\varepsilon}(\mathbf{u}'(\mathbf{x})) \rangle = 0$.

For a heterogeneous elasto-plastic material, the constitutive relation reads:

$$\begin{aligned} \dot{\boldsymbol{\sigma}}(\mathbf{x}) &= \mathbf{C}(\mathbf{x}) : \dot{\boldsymbol{\varepsilon}}^e(\mathbf{x}) \\ &= \mathbf{C}(\mathbf{x}) : (\dot{\boldsymbol{\varepsilon}}(\mathbf{x}) - \dot{\boldsymbol{\varepsilon}}^p(\mathbf{x}) - \dot{\boldsymbol{\varepsilon}}^{th}(\mathbf{x}) - \dot{\boldsymbol{\varepsilon}}^m(\mathbf{x})), \quad \dots (8) \end{aligned}$$

where $\mathbf{C}(\mathbf{x})$ is the elastic tensor at local position $\mathbf{x}$ and $\boldsymbol{\varepsilon}^e$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^p$, $\boldsymbol{\varepsilon}^{th}$ and $\boldsymbol{\varepsilon}^m$ are elastic, total, plastic, thermal and transformation strain tensor respectively. Equivalently, the constitutive law can be rewritten:

$$\dot{\boldsymbol{\sigma}}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}) + \dot{\boldsymbol{\tau}}^p(\mathbf{x}) + \dot{\boldsymbol{\tau}}^{thm}(\mathbf{x}), \quad (9)$$

where

$$\begin{aligned} \dot{\boldsymbol{\tau}}^p(\mathbf{x}) &\equiv -\mathbf{C}(\mathbf{x}) : \dot{\boldsymbol{\varepsilon}}^p(\mathbf{x}) \text{ and} \\ \dot{\boldsymbol{\tau}}^{thm}(\mathbf{x}) &\equiv -\mathbf{C}(\mathbf{x}) : (\dot{\boldsymbol{\varepsilon}}^{th}(\mathbf{x}) + \dot{\boldsymbol{\varepsilon}}^m(\mathbf{x})). \quad \dots (10) \end{aligned}$$

By introducing homogeneous reference media with elasticity $\mathbf{C}^0$, Eq. (9) can be rewritten as:

$$\begin{aligned} \dot{\boldsymbol{\sigma}}(\mathbf{x}) &= \mathbf{C}^0 : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}) + (\mathbf{C}(\mathbf{x}) - \mathbf{C}^0) : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}) + \dot{\boldsymbol{\tau}}^p(\mathbf{x}) + \dot{\boldsymbol{\tau}}^{thm}(\mathbf{x}) \\ &= \mathbf{C}^0 : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}) + \dot{\boldsymbol{\tau}}(\mathbf{x}) + \dot{\boldsymbol{\tau}}^p(\mathbf{x}) + \dot{\boldsymbol{\tau}}^{thm}(\mathbf{x}) \\ &= \mathbf{C}^0 : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}) + \dot{\boldsymbol{\tau}}'(\mathbf{x}) \end{aligned}$$

$$\forall \mathbf{x} \in V, \partial \dot{\boldsymbol{\sigma}} / \partial \mathbf{x} = 0 \quad \forall \mathbf{x} \in V,$$

$$\dot{\mathbf{u}} : xyz\text{-periodic}, \dot{\boldsymbol{\sigma}} \cdot \mathbf{n} : xyz\text{-periodic}, \quad \dots (11)$$

where $\dot{\boldsymbol{\tau}}'(\mathbf{x})$ is a polarisation tensor which comprises the contributions from the elastic heterogeneity, the plastic strain and eigenstrains. Equations (11) in Fourier space are written as follows:

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) = i\mathbf{C}^0 : (\hat{\mathbf{u}}'(\boldsymbol{\xi}) \otimes \boldsymbol{\xi}) + \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}), i\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) \cdot \boldsymbol{\xi} = 0, \dots (12)$$

where, $\boldsymbol{\xi}$ is frequency, and the non-italic character i represents imaginary number. By eliminating $\hat{\boldsymbol{\sigma}}$ from Eq. (12), we obtain

$$\hat{\mathbf{u}}'(\boldsymbol{\xi}) = \frac{i}{2} (\mathbf{N}^0 \otimes \boldsymbol{\xi} + \boldsymbol{\xi} \otimes \mathbf{N}^0) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}), \dots (13)$$

where,

$$\mathbf{N}^0(\boldsymbol{\xi}) = \mathbf{K}^0(\boldsymbol{\xi})^{-1}, \mathbf{K}^0(\boldsymbol{\xi}) = \mathbf{C}^0 : (\boldsymbol{\xi} \otimes \boldsymbol{\xi}), \dots (14)$$

$$\hat{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = \frac{i}{2} (\boldsymbol{\xi} \otimes \hat{\mathbf{u}}'(\boldsymbol{\xi}) + \hat{\mathbf{u}}'(\boldsymbol{\xi}) \otimes \boldsymbol{\xi}) = -\hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}), \dots (15)$$

$$\hat{\Gamma}^0(\boldsymbol{\xi}) = \frac{1}{4} (\mathbf{N}_{li}^0 \boldsymbol{\xi}_j \boldsymbol{\xi}_k + \mathbf{N}_{ki}^0 \boldsymbol{\xi}_j \boldsymbol{\xi}_l + \mathbf{N}_{ij}^0 \boldsymbol{\xi}_i \boldsymbol{\xi}_k + \mathbf{N}_{kj}^0 \boldsymbol{\xi}_i \boldsymbol{\xi}_l). \dots (16)$$

$\hat{\Gamma}^0$ is a periodic Green's operator. Inverse Fourier transformation of Eq. (15) gives the strain field within the heterogeneous medium.

The iterative algorithm to solve this problem is described below.

Iterative algorithm:

Initialisation: $\dot{\boldsymbol{\varepsilon}}^0 = \dot{\boldsymbol{\varepsilon}}^n(\mathbf{x})$, $\forall \mathbf{x} \in V$

Iteration: $(n + 1)$: $\dot{\boldsymbol{\varepsilon}}^n(\mathbf{x})$ and $\dot{\boldsymbol{\sigma}}^n(\mathbf{x})$ are known

(a) $\hat{\boldsymbol{\sigma}}^n = FFT(\dot{\boldsymbol{\sigma}}^n)$

(b) Check convergence

$$e^n = \left| \sqrt{\langle \|\text{div}(\dot{\boldsymbol{\sigma}}^n)\|^2 \rangle} - \sqrt{\langle \|\text{div}(\dot{\boldsymbol{\sigma}}^{n-1})\|^2 \rangle} \right| =$$

$$\left| \sqrt{\langle \|\boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^n(\boldsymbol{\xi})\|^2 \rangle} - \sqrt{\langle \|\boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^{n-1}(\boldsymbol{\xi})\|^2 \rangle} \right| < \epsilon$$

and

$$e^n = \sqrt{\langle \|\text{div}(\dot{\boldsymbol{\sigma}}^n)\|^2 \rangle} = \sqrt{\langle \|\boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^n(\boldsymbol{\xi})\|^2 \rangle} < \epsilon \text{ if no macroscopic stress is imposed}$$

$$e^n = \frac{\sqrt{\langle \|\text{div}(\dot{\boldsymbol{\sigma}}^n)\|^2 \rangle}}{\|\dot{\boldsymbol{\sigma}}^n(0)\|} = \frac{\sqrt{\langle \|\boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^n(\boldsymbol{\xi})\|^2 \rangle}}{\|\hat{\boldsymbol{\sigma}}^n(0)\|} < \epsilon \text{ otherwise}$$

(c) $\hat{\boldsymbol{\varepsilon}}^{n+1}(\boldsymbol{\xi}) = \hat{\boldsymbol{\varepsilon}}^n(\boldsymbol{\xi}) - \hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^n(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq 0$ and $\hat{\boldsymbol{\varepsilon}}^{n+1}(0) = \hat{\boldsymbol{\varepsilon}}^n(0)$

(d) $\dot{\boldsymbol{\varepsilon}}^{n+1} = FFT^{-1}(\hat{\boldsymbol{\varepsilon}}^{n+1})$

(e) $\dot{\boldsymbol{\sigma}}^{n+1}(\mathbf{x}) = g(\dot{\boldsymbol{\varepsilon}}^{n+1}(\mathbf{x})) \quad \forall \mathbf{x} \in V$

where, g is a constitutive equation which relates strain and stress (Eq. (8), in the present case).

3.2. Constitutive Behaviour, Microstructure and Phase Transformation

Plastic strain is the result of dislocation glide. The slip occurs along certain directions on certain planes. Such combinations of directions and planes are called slip systems. Let $\dot{\gamma}^\alpha$ be the slip rate on the α slip system, the plastic strain rate can be determined by the summation of the slip rates on all slip systems:

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_{\alpha} \mathbf{p}^\alpha \dot{\gamma}^\alpha, \quad (17)$$

where $\mathbf{p}^\alpha$ is the Schmid tensor of α slip system,

$$\mathbf{p}^\alpha = \frac{1}{2} (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha + \mathbf{m}^\alpha \otimes \mathbf{s}^\alpha). \quad (18)$$

$\mathbf{s}^\alpha$ and $\mathbf{m}^\alpha$ are respectively the slip direction and slip plane normal of the α slip system. According to the Schmid law, the slip system becomes active when the resolved shear

stress τ^α becomes equal to the Critical Resolved Shear Stress (CRSS) g^α :

$$|\tau^\alpha| = |\mathbf{p}^\alpha : \boldsymbol{\sigma}| = g^\alpha. \quad (19)$$

During elasto-plastic deformation, the Eq. (19) is satisfied. In other words, stress increases according to the hardening of each slip system.

For such a rate-independent problem, Hutchinson³⁰⁾ proposed the following solution for determining the slip rate of each slip system by using the consistence condition:

$$\dot{\tau}^\alpha = \text{sgn}(\tau^\alpha) \dot{g}^\alpha. \quad (20)$$

For the small deformation problems, Eq. (20) can be rewritten as:

$$\dot{\boldsymbol{\sigma}} : \mathbf{p}^\alpha = \sum_{\beta} h^{\alpha\beta} \dot{\gamma}^\beta, \quad (21)$$

and the general form of the hardening law is:

$$\dot{g}^\alpha = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^\beta|, \quad (22)$$

with $h^{\alpha\beta}$ the hardening coefficients. They can be expressed phenomenologically with an additional evolution law. We adopt the following form:³¹⁾

$$h^{\alpha\alpha} = h = H_0 \text{sech}^2 \left[\frac{H_0 \sum_{\beta} \gamma^\beta}{\tau_s - \tau_0} \right], \quad (23)$$

$$h^{\alpha\beta} = qh + (1-q)h\delta_{\alpha\beta}, \quad (24)$$

where H_0 is a coefficient parameter, τ_0 is the initial yield stress value and τ_s is the saturated stress value. The parameter q , which describes latent hardening, takes values from 1.0 to 1.4 depending on the material.³²⁾ $\delta_{\alpha\beta}$ is Kronecker delta so equals 1 when $\alpha=\beta$ and otherwise takes 0.

By using the constitutive laws, one obtains.

$$\begin{aligned} \dot{\boldsymbol{\sigma}} : \mathbf{p}^\alpha &= \mathbf{C} : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^p - \dot{\boldsymbol{\varepsilon}}^{th} - \dot{\boldsymbol{\varepsilon}}^m) : \mathbf{p}^\alpha \\ &= \mathbf{C} : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{th} - \dot{\boldsymbol{\varepsilon}}^m) : \mathbf{p}^\alpha - \sum_{\beta} \mathbf{p}^\alpha : \mathbf{C} : \mathbf{p}^\beta \dot{\gamma}^\beta = \sum_{\beta} h^{\alpha\beta} \dot{\gamma}^\beta, \quad \dots (25) \end{aligned}$$

and the slip rates are expressible as:

$$\dot{\gamma}^\alpha = \mathbf{f}^\alpha : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{th} - \dot{\boldsymbol{\varepsilon}}^m), \quad \text{with} \quad \mathbf{f}^\alpha = \sum_{\beta} Y^{\alpha\beta} \mathbf{C} : \mathbf{p}^\beta, \quad \dots (26)$$

with

(a) initial state

(b) 7 volume % transformed

Fig. 10. Microstructures of an initial state and 7% transformed.

$$Y^{\alpha\beta} = (X^{\alpha\beta})^{-1} \quad \text{and} \quad X^{\alpha\beta} = h^{\alpha\beta} + \mathbf{p}^\alpha : \mathbf{C} : \mathbf{p}^\beta. \quad (27)$$

The matrix $X^{\alpha\beta}$ has to be non-singular. For that reason, the maximum number of active slip systems, *i.e.* rank of the matrix $X^{\alpha\beta}$, is limited to 5. From Eq. (26), we can find the value of the shear strain rates, which in turn depends on the prescribed strain rate or stress rate.

(a) cooling rate = 0.1 °C/s (695°C)

(b) cooling rate = 1 °C/s (672°C)

(c) cooling rate = 10 °C/s (648°C)

(d) cooling rate = 20 °C/s (617°C)

Fig. 11. S-S curve reproduction by FFT numerical model at a strain rate of 0.5 s^{-1} .

For the elasto-plastic transition problem, initial values of τ^α and g^α are generally different. The incremental form of Eq. (20) during a finite time increment can be written as follows:

$$\tau^\alpha + \Delta\tau^\alpha = \text{sgn}(\tau^\alpha)(g^\alpha + \Delta g^\alpha). \quad (28)$$

Note that τ^α and g^α are the values evaluated at the previous step. Δ represents one increment during one time step.

Consequently, Eq. (21) takes the form:

$$(\sigma + \Delta\sigma) : p^\alpha = \text{sgn}(\tau^\alpha)g^\alpha + \sum_\beta h^{\alpha\beta} \Delta\gamma^\beta. \quad (29)$$

Following the previous discussion, the plastic slip increments can be expressed as:

$$\Delta\gamma^\alpha = \sum_\beta Y^{\alpha\beta} (\sigma : p^\beta + p^\beta : C : (\Delta\varepsilon - \Delta\varepsilon^{th} - \Delta\varepsilon^m) - \text{sgn}(\tau^\beta)g^\beta). \quad (30)$$

3.3. Incorporation of Phase Transformation Effect

Polycrystalline aggregates, which counts 2 000 grains, in a representative volume element (RVE) with periodic microstructure are made by Voronoi tessellation technique. In the FFT numerical framework, the displacement in three dimensions as well as the strain and the stress are periodic. For the transformation plasticity analyses, predefined value of uniaxial macroscopic stress is applied (hereinafter the average value in the RVE is called “macroscopic” and the values defined at each local point is called “microscopic”). Daughter phase grain nuclei, which counts also 2 000, are randomly distributed inside the RVE and start growing after the stress is applied. The daughter phase has different density from initial phase and causes obviously strain accommodation according to the transformation strain β . This may cause the local plastic deformation. A sample view of initial polycrystal and 7% transformed (daughter phase in red colour) is depicted in Fig. 10.

3.4. Identification of Material Parameters

Parameters appear in the above constitutive equations require identifying elastic parameters (for example Lamé's constants) and plastic constants, namely H_0 , τ_s , τ_0 and q . This study considers transformation from fcc phase to bcc phase

Table 6. Parameter sets for each cooling rate and phase.

Cooling rate (°C/s)	0.1		1		10		20	
Phase	γ	α	γ	α	γ	α	γ	α
Bulk modulus (GPa)	136	150	136	150	136	150	136	150
Shear modulus (GPa)	63	69	63	69	63	69	63	69
H_0 (MPa)	5 000	3 000	20 000	2 500	395	100 000	410	200 000
τ_0 (MPa)	20	72	25	58	39	75	41	67
τ_s (MPa)	45	100	45	110	80	180	180	220

(both ferrite and pearlite phase are treated as α phase and thus no distinction is made between ferrite and pearlite in the numerical model) and thus the slip systems are selected according to the phase. Stress-strain curves are reproduced by the CPFFT model, which are shown in Fig. 11 and the identified parameters for each condition are in Table 6.

(a) cooling rate = 0.1 °C/s (613°C)

(b) cooling rate = 1 °C/s (587°C)

(c) cooling rate = 10 °C/s (533°C)

(d) cooling rate = 20 °C/s (483°C)

Fig. 12. Evolution of transformation plastic strain during phase transformation.

3.5. Numerical Estimation of Transformation Plastic Strain

The transformation calculations are conducted under applied uniaxial stresses of 0, 10, 30 and 50 MPa conditions for each cooling speed and the eventual macroscopic strains (transformation plastic strains) are retrieved from the results. These initial stresses invoke only elastic strain before phase transformation, while an additional plastic strain occurs dur-

ing phase transformation even though the constant stress is applied which in turn the transformation plastic strain. **Figure 12** shows the evolution of transformation plastic strain as a function of volume fraction of daughter phase under the cooling rates ranging from 0.1 to 20 °C/s. The figures show an apparent strain increase with applied stress: a qualitative reproduction of transformation plastic strain is confirmed.

4. Discussion

The relationship between applied stress and transformation plastic strain by calculation is demonstrated and compared with that of experiment in **Fig. 13**. Transformation plasticity coefficients are calculated taking the approximated slope of linear relation between transformation plastic strain (at the end of phase transformation) and applied stress and are summarised in **Fig. 14**. It is obvious that the calculation results, although small discrepancies, relatively match with those of experiment when cooling rate is high. However, under mild cooling rate, the calculation underestimates transformation plasticity. The calculated results give better accordance with the experimental ones than those by Leblond's model (Table 4), but still deviation is significant at slow cooling rates. According to Eqs. (4) and (5) (Leblond's model¹⁸), transformation plasticity coefficient is proportional to the transformation strain and inverse proportional to the yield stress of mother phase (weaker phase). When transformation temperature is low, both transformation strain and yield stress increase and thus no significant change in transformation plasticity coefficients are found by numerical simulation as demonstrated in **Fig.**

Fig. 13. Effect of applied stress on transformation plastic strain.

Fig. 14. Comparison of transformation plasticity by experiments and simulations.

Table 7. Transformation plasticity coefficient – a comparison between values by experiment and numerical simulation.

Cooling rate (°C/s)	K by experiment (MPa ⁻¹)	K by simulation, (MPa) Original Leblond's model	K by simulation (MPa) FFT model
0.1	23.7×10^{-5}	5.49×10^{-5}	11.2×10^{-5}
1	18.0×10^{-5}	5.70×10^{-5}	9.90×10^{-5}
10	10.9×10^{-5}	6.08×10^{-5}	8.00×10^{-5}
20	7.82×10^{-5}	6.78×10^{-5}	11.0×10^{-5}

14. However, the experimental results show a significant increase in transformation plasticity coefficients under slow cooling rate (high transformation temperature). This implies some other mechanisms, other than transformation strain and strain accommodation in mother phase, should be invoked by high temperature transformation plasticity. One of this mechanism might be viscoplastic or creep behaviour that is enhanced at high temperature transformation, e.g. at low cooling rate. Note also that low cooling rates produce a longer times during phase transformation at higher temperature so more ability of transformation viscoplastic strain to develop in the material: if we consider that the temperature range of phase transformation is approximately 75°C whatever the cooling rate (Fig. 4), the time during phase transformation for the different cooling rates 0.1, 1.0, 10.0 and 20.0°C/s is respectively 750, 75, 7.5 and 3.75 s. which enhances viscoplasticity at low cooling rates.

5. Conclusion

The experiments on 0.45% carbon steel revealed the transformation plasticity behaviour and their dependence on cooling rate. The transformation plastic strain increases as decrease of cooling rate. Numerical approach using CPFFT has also attempted to reproduce the effect of cooling rate on transformation plasticity. The simulation results are found to be relatively in good agreement with experimental ones when cooling rate is high (20°C/s.) where viscoplastic and creep effects are negligible. However, when cooling rate is low, the numerical simulation, as well as Leblond's analytical model, underestimates the transformation plastic strain. This implies that not only Greenwood-Johnson mechanism but some other mechanisms as viscoplasticity or creep invoking transformation plasticity involve the phenomena at high temperature phase transformation.

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