SIMULATION OF PRECIPITATION IN V-CONTAINING HSLA STEEL FOR THE STRENGTHENING ENHANCEMENT

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Abstract. *The precipitation of the microalloying elements in high strength low alloyed (HSLA) steel controls the strength of the steel greatly through grain refinement and particle hardening mechanisms. The current work simulates the precipitation of vanadium a hot rolling process for the optimized strengthening effect in a microalloyed steel. Taking into account the effect of deformation, cause of the drastic increase in the dislocation density, namely higher nucleation site density, it can be clearly seen that the precipitation of all species at dislocations, dominate the precipitation kinetics. The diffuse interface effect on the interfacial energy as well as a volumetric misfit of AlN at dislocations is also taken into account. The latter is because of its significant difference in the lattice parameter from the matrix. The presence of AlN at dislocations does not override that of V(C,N) as found in other cases with low density of dislocation. Slow cooling rate in the process ensures the consumption of the microalloying elements which in turn strengthen the product and minimise the production cost. The experimental verifications for the precipitates are performed by scanning transmission electron microscopy (STEM) as well as X-ray absorption spectroscopy (XAS) from synchrotron radiation.*

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1 INTRODUCTION

This work focuses on the application of physically-based simulation approaches for a thermomechanical process of high strength low alloyed (HSLA) steel. The approaches are based on the classical nucleation and thermodynamic extremal principal or SFFK model for the growth and coarsening of precipitates, with thermodynamic and diffusion databases calculated by CALPHAD method.

To study the optimisation of the hot rolling process of V-microalloyed steel according to the precipitation hardening by vanadium, the effect of deformation and cooling rate before the coiling process in hot strip mill were studied by thermokinetics approach of precipitationcontained in the software MatCalc. It enables the possibilities to simulate the precipitation kinetics as a result of different processing parameters, i.e, thermomechanical cycles as well as the microstructure parameters such as grain size and equilibrium dislocation density. All changes in the thermomechanical cycle are able to be compiled in separated steps in the software.

Precipitates nucleate both at dislocations and grain boundaries. The increase in the dislocation density by deformation provokes much larger number of nuclei and the diffusion is immensely accelerated through pipe diffusion at the dislocation core. Long interpass times were allowed in the experiments to ensure high degree of recrystallisation of austenite after each rolling pass to allow repeated recrystallisation and consequently austenite grain refinement. The density of dislocations is updated along the simulated process.

Large retained strain together with slow cooling rate is expected to facilitate the precipitation of fine V(C,N) in ferrite and lead to higher strength by the advantage of particle hardening, which is strictly called dispersion hardening [1-2]. They impede the movement of dislocations by the well-known Orowan-Ashby looping mechanism.

2 THE RELATIONSHIP OF PLASTIC DEFORMATION AND DISLOCATION DENSITY

2.1 Balance of generation and annihilation of dislocations

The increase in the dislocation density under deformation can be described by the so-called one parameter model [3] as

$$\frac{d\rho}{dt} = \left(\frac{M\dot{\varepsilon}}{bL} \right),$$
(1)

where M is the Taylor factor, which is 3.06 for FCC crystals [4], $\dot{\varepsilon}$ is the strain rate and b is Buger's vector. The travelling distance L is limited by the average spacing between dislocations as shown in

$$L = \frac{A}{\sqrt{\rho}},$$
(2)

where A is a materials constant in a range of 50 to 100.

The opposing dislocations with antiparallel Burger's vectors annihilate the formed dislocation and can be calculated by

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$$\frac{d\rho}{dt} = -B \cdot 2\frac{d_{ann}}{b}\rho M\dot{\varepsilon},\qquad(3)$$

where B is a constant related to the number of activated slip planes. The term d_{ann} represents the critical distance, controlled by shear modulus of the matrix, Poisson's ratio, vacancy formation energy. Also, dislocation density is reduced by thermally activated dislocation climb [5], which is controlled by self-diffusion coefficient along dislocations or the so-called pipe-diffusion, D_d, [6] as represented in Eq.4.

$$\frac{d\rho}{dt} = -C \cdot 2 \cdot D_d \frac{Gb^3}{k_B T}\left(\rho^2 - \rho_{eq}^2\right),\qquad(4)$$

where k_B is the Bolzmann constant, T is temperature in Kevin, ρ_{eq} is the equilibrium dislocation density and C is a constant, related to the solute trapping effect.

3   SIMULATION SETUP

The precipitation simulation was performed in MatCalc version 5.60. The chemical composition of the investigated steel is shown in Table 1. The content of titanium did not involve the simulation calculation but some amount of nitrogen was calculated according to mass balance of the formation of TiN, which usually forms during the solidification of steel melt and is generally not dissolved during the reheating. The thermomechanical cycle simulating a hot strip rolling is represented in Figure 1. It can be seen that the varying parameters in this work are the degree of deformation in the last rolling pass, ε_4, and the final cooling rate before the coiling process, $\dot{T}_{coil}$. They are taken into account in the simulation. The high strain rate helps produce a large number of dislocations. The experimental work is described in details earlier [7].

Material	C	S	M	P	S	C	Mo	Al	T	V	N
V- HSLA	0.	0.	0.	0.0	0.0	0	0.0	0.0	0.	0	0.0

Table 1: The chemical composition of the simulated steel, in mass%.
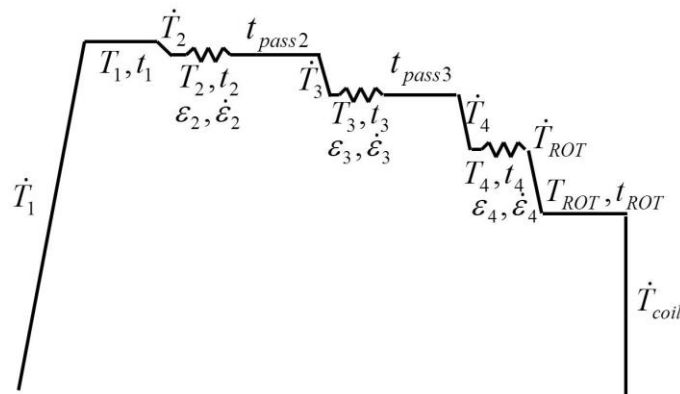
Figure 1: The thermomechanical cycles adopted in the simulation to simulate the precipitation.

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$\dot{T}_1, T_1, t_1$	200 °C/minute, 1250 °C, 15 minute
$\dot{T}_2, T_2, t_2$	5 °C/s, 1200 °C, 3 s
$\varepsilon_2, \dot{\varepsilon}_2, t_{pass2}$	0.2, 12 s^{-1}, 10 s
$\dot{T}_3, T_3, t_3$	60 °C/s, 1150 °C, 3 s
$\varepsilon_3, \dot{\varepsilon}_3, t_{pass3}$	0.4, 12 s^{-1}, 10 s
$\dot{T}_4, T_4, t_4$	60 °C/s, 900 °C, 3 s
$\varepsilon_4, \dot{\varepsilon}_4, t_{pass4}$	<u>0.0/0.3/0.6</u>, 12 s^{-1}, 0 s
$\dot{T}_{ROT}, T_{ROT}, t_{ROT}$	60 °C/s, 680 °C, 6 s
$\dot{T}_{coil}$	<u>0.1/ 1/ 5/ 10/ 60</u> °C/s

Table 2: The parameters in the thermomechanical cycle in Figure 1.

Only sharp transformation temperature can be set up in the calculation. Hence, the simulated temperature of Run Out Table (ROT), T_{ROT}, of 680 °C was chosen for the transformation from austenite into ferrite, as ferrite was only little to observed before reaching this isothermal period. The precipitation of AlN and V(C,N) is both at grain boundaries and dislocations in both austenite and ferrite parent phases, while that of cementite is at dislocations only. The grain sizes of 100 μm and 10 μm were selected for austenite and ferrite, respectively. The equilibrium dislocation density in austenite was assigned as 10^{11} m^{-2} while that in ferrite as 10^{12} m^{-2}. The grain refinement in austenite due to recrystallisation during the hot rolling process was not considered. But the generation and annihilation of dislocation were considered by choosing one parameter model from Sherstnev and Kozesnik with the parameter A in Eq.2 of 50, B in Eq.3 of 2 and C in Eq.4 of 1×10^{-4}. The volumetric misfit of only AlN at dislocations was considered, which is 0.27. As the critical temperature is recommended to take into account for the calculation of interfacial energy due to the diffuse interface, a critical temperature of 1727 °C was selected for V(C,N) as an estimation from those reported for VC and VN in both austenite and ferrite [8].

4 MATERIALS CHARACTERISATION

Samples under different process parameters were measured for the amount of vanadium in different states by means of synchrotron X-ray Absorption Spectroscopy (XAS), combined with Linear Combination Fitting (LCF) as published earlier in [9]. Also, selected sample were investigated for different morphology and size of precipitates by Scanning Transmission Electron Microscopy (STEM).

5 SIMULATION RESULTS AND DISCUSSION

The multipass rolling thermomechanical cycles result in high dislocation density as shown in Figure 2. The first two peaks of dislocation density gradually drop after long interpass time, which allows the recovery during the long interpass time. One can see that without the retained strain in the last deformation step the dislocation density is annihilated to 3.79×10^{12} m^{-2}. With the logarithm strain of 0.3 and 0.6, the dislocation density reaches 3.62×10^{14} m^{-2} and 4.59×10^{14} m^{-2} respectively,

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interpreting that the retained strain therefore increases the dislocation density with 2 order of magnitude.

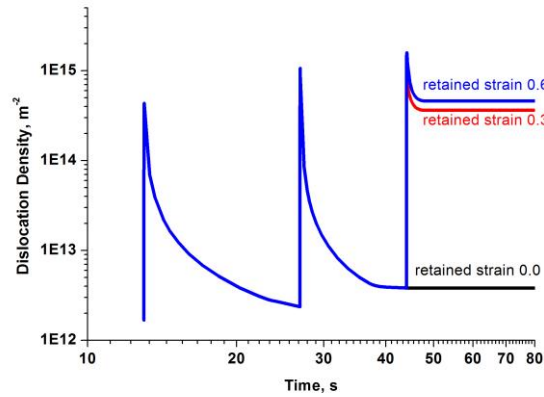Figure 2: The change in dislocation density as a result of generation and annihilation after deformation.
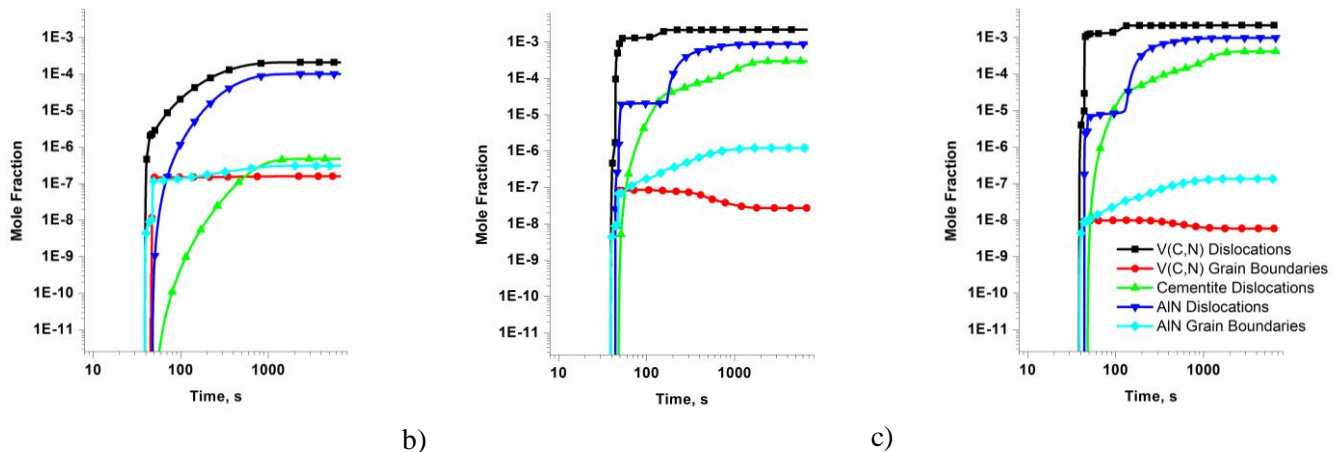

a)   b)   c)

Figure 3: The mole fraction of different precipitates, both at dislocations and grain boundaries under a slow cooling rate of 0.1 °C/s with a retained strain of a) 0.0 b) 0.3 and c) 0.6.

Figure 3 sums and compares different precipitate phase fractions under different degree of deformation at a slow cooling rate of 0.1 °C/s. The high density of dislocations, main nucleation site, results in up to 3 order of magnitude higher fraction of the precipitates at this site. Also, higher dislocations by retained strain in the last deformation step results in the consumption of V(C,N) at the grain boundaries. This is difference from what that found by Radis et al. [10], whose case shows that the predominant site of AlN is only grain boundaries and the precipitation of AlN at dislocations overrides that of V(C,N). The first short period showing constant fraction of V(C,N) and AlN at dislocations was the precipitation in austenite matrix, before transformed into ferrite. It can be clearly seen that the higher diffusivity in ferrite allows abrupt increase in the precipitation fraction.

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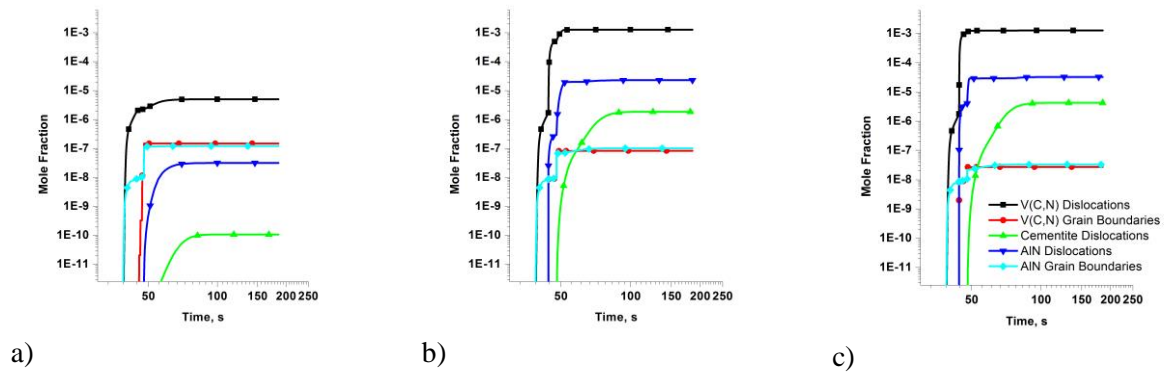

Figure 4: The mole fraction of different precipitates, both at dislocations and grain boundaries under a moderate cooling rate of 5 °C/s with a retained strain of a) 0.0 b) 0.3 and c) 0.6.

When the cooling rate is faster such as 5 °C/s as shown in Figure 4, the pronounced precipitation due to deformation is more obvious, up to 4 orders of magnitude for cementite. Due to shorter precipitation time at higher cooling rates, deformation obviously has a vital role in accelerating the precipitation. Comparing V(C,N) at dislocations between the two cooling rates, under a fixed retained strain of 0.3, its fraction shows double amount at slower cooling rate, i.e., 0.00219, compared with 0.00128.

To illustrate the consumption of the microalloying elements in from the matrix into the precipitates, their concentrations are plotted in Figure 5. It is quite clear that higher cooling rate does not complete the available amount of vanadium and aluminium. Therefore, significant amount of these elements is still dissolved in ferrite matrix at the end. This implies ineffective process control of microalloyed steel.
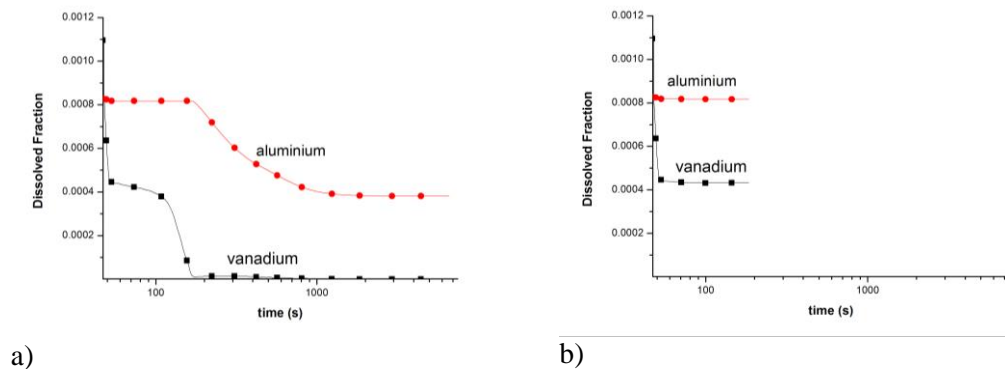

Figure 5: Decrease in the microalloying elements dissolved in ferrite matrix in case of a retained strain of 0.3 and a) a cooling rate of 0.1 °C/s and b) 5 °C /s. The plot starts from just before ferrite has formed at 680 °C in the simulation.

However, small inaccuracy might exist in these simulations due to the fact that only sharp transformation temperature from austenite to ferrite is able to assign. However, the trend of the influence of deformation and cooling rate from the simulation are in good agreement with the results from XAS as published in [9].

6   CONCLUSIONS

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The density of dislocation is immensely multiplied by deformation to several orders of magnitude. This results in the increase in the number of nuclei of V(C,N) and AlN that their precipitation at dislocations dominates the kinetics. Slower cooling rate allows enough time for the growth of precipitation and consumption of the available elements. This is beneficial for the coiling process as the cooling rate is very slow. This work is an example of how a physically based simulation of precipitation can help the optimisation of thermomechanical process parameters, which is advantage for the strength improvement of the products.

7   ACKNOWLEDGEMENTS

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