

MLL202 Term Paper Report

On

Interface Mobility in case of Austenite-to-Ferrite Phase Transformation

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Submitted

To

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Abstract: -

This investigation looked at the kinetics of the Austenite-to-Ferrite γ/α phase transformation in steel grades characterized by minimal levels of substitutional and interstitial components, such as ultra low carbon and interstitial free steels. They concluded that these are known to be governed by interface reactions.

They investigated & analyzed these materials in depth & came to a conclusion that the long-range diffusion of components is believed to have negligible influence on this transformation kinetics. Experimental investigations including dilatometer tests, yielded time-dependent data related to the volume fraction of ferrite, from which they drew insights into the transformation process. For the particular steel grade under analysis in this term paper, they adopted realistic & simple assumptions. Two such assumptions are regarding the morphology of the ferrite phase & the notable planar & spherical growth.

Through numerical analysis, they observed that during the initial stages of transformation, planar growth was dominant. This observation contributed to the determination of effective mobility of the austenite-ferrite interface. Moreover, this interfacial mobility is a critical factor in understanding transformation kinetics. The study delved into estimating reasonable estimates for the intrinsic, thermally activated mobility by taking solute drag into account.

Such implications were helpful in broad understanding of phase transformations in steel, enlightening the factors governing kinetics in low carbon & interstitial materials.

1. Introduction :-

The kinetics of the γ/α phase transformation in steels can be influenced by diffusion processes [1] of components & interfacial reactions [2], either separately or in combination [3]. In certain cases, the mechanism of transformation may change during the process [4, 5]. Advanced sharp interface models have been developed to calculate transformation kinetics in binary [3], ternary, & higher-order systems with immobile substitutional components [6]. Models have been developed for iron alloys with only substitutional components [4]. Challenges arise when one considers both fast interstitial & slower substitutional diffusion. In recent years, attempts have been made to address this, such as in Fe-C-X alloys, where kinetics are determined solely by factors including interface mobility, carbon diffusion, & short-range X-diffusion [7].

However, determination of interface mobility remains a challenge, often requiring investigation under conditions where kinetics are solely controlled by interfacial reactions. In 1975, Hillert [8] estimated interface mobility from experiments on grain growth & recrystallization in pure Fe. In Fe-X alloys with minimal substitutional X, interface mobility controls kinetics, but experimental values have varied significantly [9-12] & are often much smaller than initially proposed by Hillert [8].

Sophisticated techniques like hot-stage transmission electron microscopy (TEM) can directly be employed to measure interface velocity, hence, allowing the determination of interface mobility if driving pressure is known [13]. However, these experiments are limited in scope. Traditional methods, like dilatometer

tests, provide data on the time-dependent volume fraction of ferrite, but do not offer insights into the evolution of the γ/α phase arrangement satisfactorily.

The primary aim of this term paper is to predict the effective interface mobility, M_{eff} in ultra-low carbon steel as a function of temperature. It is crucial for the calculations to demonstrate that assumptions about the shape of growing α -phase align with the empirical data. Despite advancements in this field, a comprehensive understanding of interface mobility & its effects on kinetics of phase transformations remains difficult to achieve / track down.

2. Theory :-

The experimental data from dilatometer tests conducted on continuously cooled ultra-low carbon steel [14] are examined, assuming that the ferrite nucleation occurs mainly at austenite grain boundaries & is completed at the start of the growth phase. Consequently, the experimental data primarily reflects the growth kinetics, neglecting the nucleation process. Additionally, the final ferrite sizes exceed those of austenite grains, & ferrite nuclei may grow either as spheres or coalesce into plates. For non-equilibrium processes close to equilibrium, a linear relationship between interface normal velocity, v & driving pressure, $\Delta\rho$ was established by Svoboda. This relationship suggests that interface mobility, M_{eff} can be expressed as

$$M_{\text{eff}} = \frac{v}{\Delta\rho} \quad \text{---(1)}$$

Various studies [7] have revealed that under particular conditions, such as low Mn

content & high undercooling, the formation of substitutional spikes in front of the advancing interface becomes unnatural. In such cases, substitutional diffusion may not significantly influence the kinetics as the material transforms entirely before substitutional spikes develop. The chemical driving pressure, $\Delta\rho_{\text{chem}}$ for the migration of the γ/α -interface is described mathematically, considering the mole fractions & chemical potentials of substitutional components.

$$\Delta\rho_{\text{chem}} = \sum_{i=1}^n x_i^{\alpha} [[\mu_i]] \text{---(2)}$$

The substitutional components are labelled from 1 to n here. This was described by [15-17]. 1 denotes the main component iron. The mole fractions in ferrite & the chemical potentials are denoted by x_i^{α} & μ_i , respectively. In the context of immobile substitutional components, the ratios K_i , representing the mole fraction of iron, must remain constant throughout the transformation of both phases.

Mathematically, this condition is expressed as:

$$K_i = x_1 / x_i = \text{constant} \text{---(3)}$$

In the study, dilatometer test data on a specific steel grade microalloyed with Ti are analyzed. Due to the microalloying, virtually no interstitials remain in the solution. The exact composition of investigated steel grade is shown in Table 1 below. A binary Fe-Mn steel system is considered for calculating $\Delta\rho$. The mechanical part of the driving pressure, $\Delta\rho_{\text{mech}}$ is also calculated, but it's often negligible compared to the chemical driving pressure. Therefore, $\Delta\rho$ is approximated by $\Delta\rho_{\text{chem}}$.

Table 1

Chemical composition of the investigated steel grade

Mn	C	S	P	Ti	Si	Al	N	Nb
0.11	0.002	0.008	0.01	0.059	0.01	0.033	0.0041	0.009

Values are mass fractions in %

$$\Delta p_{mech} = \langle V_m \rangle \cdot dW / dV^\alpha \quad -(4)$$

The above mechanical part of driving pressure was obtained following [7, 17-19]. Here V_m denotes the average value of the molar volumes of both phases. The study considers the mechanical aspect of phase transformation, with the total mechanical work (W) calculated in [7]. The derivative of W with respect to volume $[dW / dV^\alpha]$ remains nearly constant during transformation. While [20] suggests that the mechanical driving pressure, or its retarding counterpart, is comparable in magnitude to the chemical driving pressure, in realistic scenarios, the mechanical driving pressure is relatively small, typically around 10 J mol^{-1} , compared to chemical driving pressures, which can reach around 100 J mol^{-1} or higher. Moreover, stress relaxation via diffusion processes at the temperatures of γ/α phase transformation in ultra-low carbon steels occurs rapidly, rendering the mechanical term negligible. In the papers [9-12], mechanical term is neglected too.

Now, in this work, simple assumptions are made regarding the morphology of evolving α -phase, with a motive to compute interface velocity. From the dilatometer tests, the time-dependent volume fraction of ferrite $\xi(t)$ is observed & analyzed & it can be described accurately by following analytical function,

$$\xi(t) = \frac{a}{1 + b e^{-ct}} \quad -(5)$$

Here, t denotes the transformation time, a , b & c denotes the fitting parameters. These fitting parameters a , b & c depend on the rate of cooling, dT/dt . The transformation rate, $d\xi/dt$ is given by,

$$\frac{d\xi}{dt} = abc e^{-ct} / [1 + b e^{-ct}]^2 \quad (6)$$

Regarding the γ/α phase arrangement, the study delineates three distinct choices, each illustrated in Figure 1 : (i) spherical growth, (ii) planar growth of a single plate, & (iii) planar growth of two merging plates. The incorporation of the last configuration is particularly notable as it provides a simplistic means to consider impingement effects.

Regardless of the geometric assumptions made, the transformation rate, denoted as $d\xi/dt$ is derived from experimental data utilizing the fitting function described by the above equation (in yellow), while the driving pressure $\Delta\rho$ is computed using equation, $\Delta\rho_{\text{chem}} = \sum_{i=1}^n x_i^{\alpha} [[\mu_i]]$.

Consequently, this methodology enables the calculation of effective mobility, M_{eff} , for the three different configurations of the growing ferrite phase. Each configuration holds significance in understanding the dynamics of phase transformation & its implications on material properties.

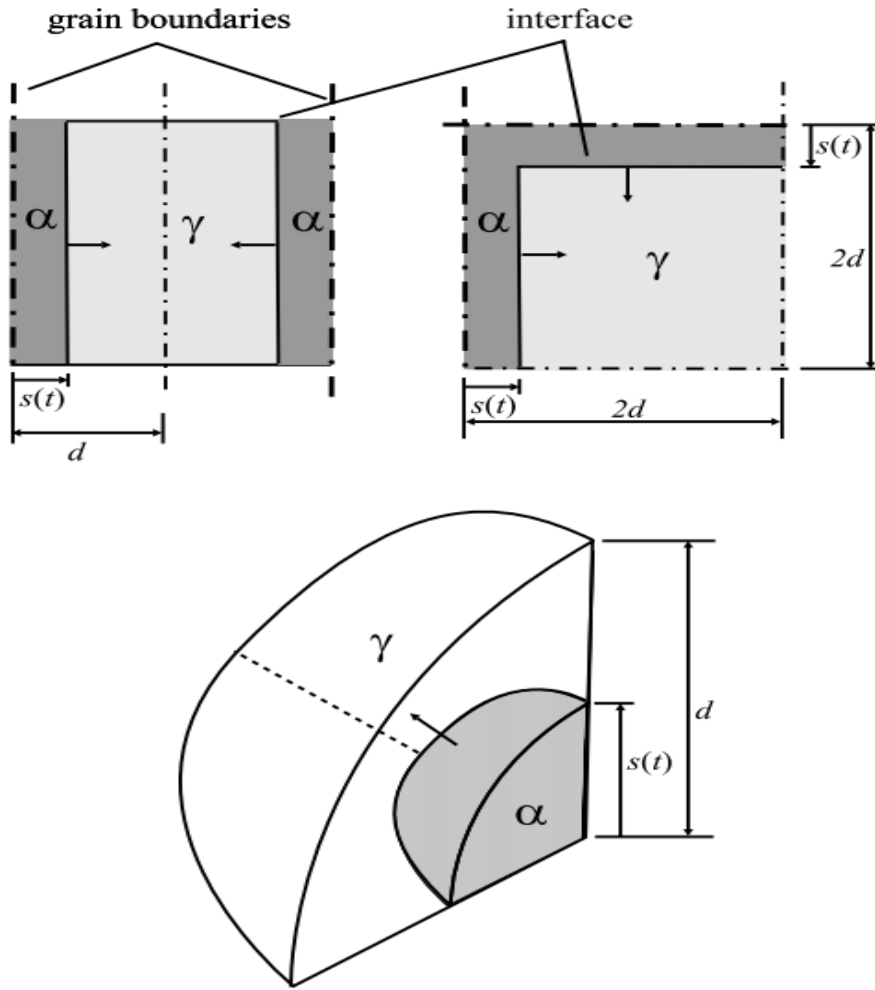


Figure 1 : Independent planar growth, planar growth of two coalescing plates & spherical growth of ferrite

For planar growth. The study expressed the volume fraction of ferrite in terms of actual interface position $s(t)$ as $\xi = s(t)/d$, with d being the half grain size.

Hence, the interface velocity $v(t)$ is related to the rate of transformation $d\xi/dt$ by

$$d\xi/dt = v(t)/d$$

The interface velocity can be substituted as per equation (1) as :

$$M_{\text{eff}} = \frac{d}{\Delta\rho} \cdot \frac{d\xi}{dt} \quad (7)$$

Experiments yield that the spherical growth, $\xi = s^3/d^3$, with d being the radius of final ferrite sphere. From the transformation rate, $\frac{d\xi}{dt} = 3s^2v(t)/d^3$, the interface mobility is obtained as :

$$M_{\text{eff}} = [d^3 / 3s^2 \Delta\rho] \frac{d\xi}{dt} \quad (8)$$

The volume fraction of ferrite in case of two coalescing plates is $\xi = (4sd - s^2)/4d^2$, & once again from the rate of transformation $\frac{d\xi}{dt}$, the interface mobility can be obtained as:

$$M_{\text{eff}} = [2d^2 / (2d - s)\Delta\rho] \frac{d\xi}{dt} \quad (9)$$

3. Discussion & Evaluation of experimental data :-

In this section of the term paper, evaluated experimental data obtained from dilatometer tests conducted on an ultra low carbon steel. These reports are reported in [14]. The dilatometric studies involve measuring displacement versus temperature, and the volume fraction versus time is calculated using the lever rule. The data are collected for four different cooling conditions, corresponding to nominal cooling rates of 1 K/s, 10 K/s, 55 K/s, and 195 K/s.

Table 2

Fit-parameters a , b and c at different nominal cooling rates

Cooling rate/ K s^{-1}	a	b	c
1	1.07	90.6	0.16
10	1.02	94.5	0.89
55	0.97	65.0	3.02
195	1.10	40.0	9.72

The experimental data are analyzed by fitting them to a specific function (Eq. (5)), and the fit parameters are presented in Table 2. Additionally, the time-temperature data pairs collected during the dilatometer tests are fitted by polynomial curves to eliminate noise associated with temperature measurement.

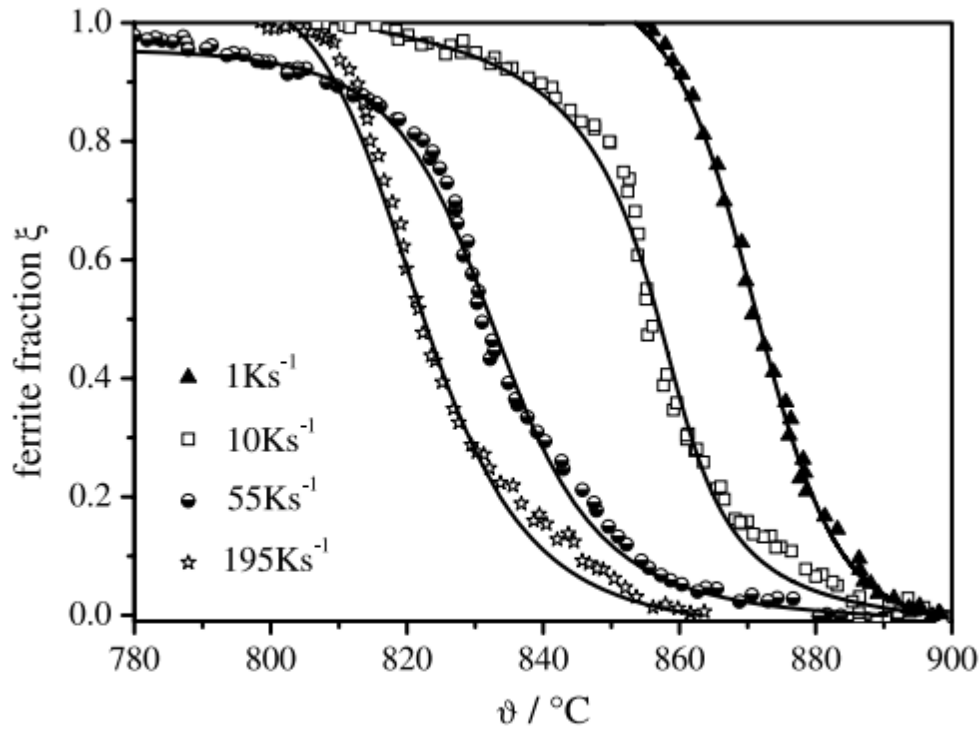


Fig. 2. Volume fraction of ferrite versus temperature at different cooling rates, symbols indicate experimental data

Figure 2 displays the experimental volume fraction as a function of temperature, with solid curves obtained using both the derivative of the fit function (Eq. (6)) and the time-temperature function.

The authors calculate the effective mobility (M_{eff}) for each cooling curve considering three different phase arrangements (γ/α phase arrangements) and varying cooling rates. The initial γ -grain size before phase transformation is 40 μm . They observe that the grain sizes of the final α -grains decrease with increasing cooling rate.

The authors rule out the growth of spherical shells from austenite grain boundaries to the center for modeling the transformation kinetics, as the ferrite grain sizes are larger than the initial austenite grains. They suggest that plate-like or spherical nuclei grow until the microstructure consists of α -grains with an average grain size of $2d$. See [14].

Finally, the effective mobility is plotted versus temperature for different cooling rates in the case of growing α -spheres and plate-like growth in Figs. 3 and 4, respectively (shown below). The authors discuss the dependence of M_{eff} values on cooling rate and suggest that spherical growth of ferrite appears to be unrealistic / unnatural in this case, as it may occur only in the early stages of transformation at small volume fractions of ferrite, with subsequent growth primarily by thickening of plates along grain boundaries.

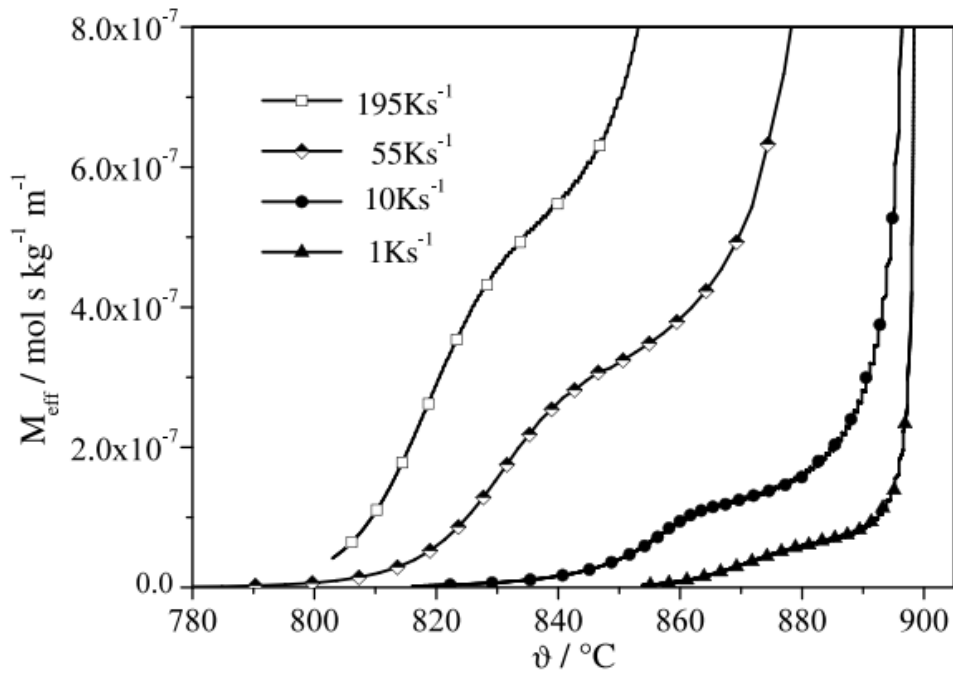


Fig. 3. Calculation of the effective mobility in case of growing α -spheres for different cooling rates.

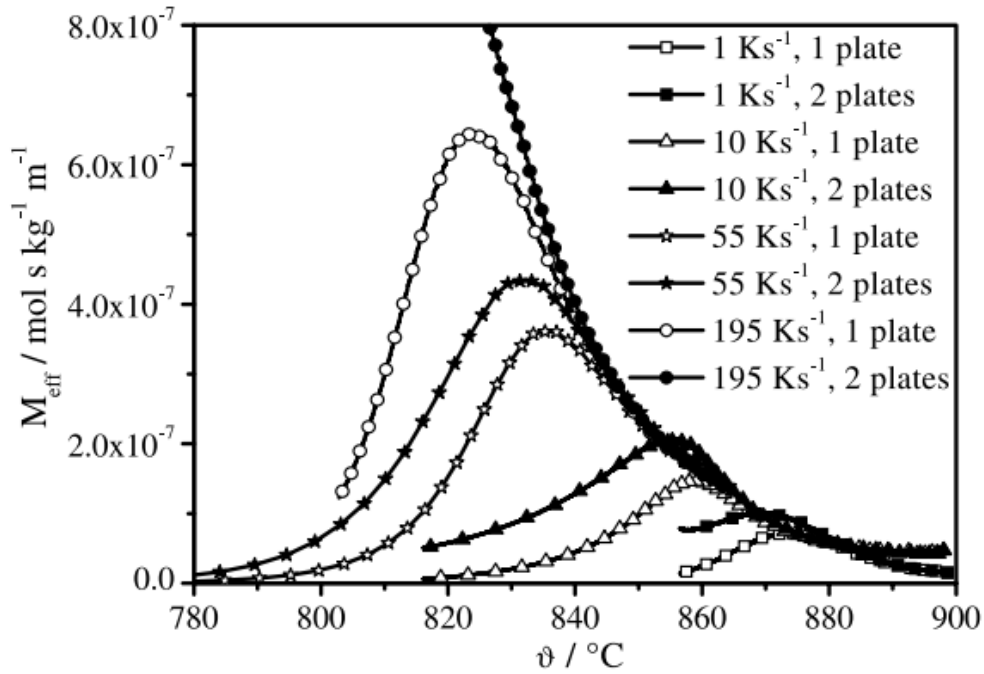


Fig. 4. Calculation of the effective mobility in case of growing α -plates for different cooling rates.

They further discuss the quantity $v_{n,\gamma}$, which relates to Mn-bulk diffusion in austenite, and $v_{n,int}$, which relates to Mn-diffusion across the interface [10]. They provide equations (10) and (11) to express these quantities, taking into account various parameters such as the Mn diffusion coefficient in austenite (D_{Mn}^γ), the diffusion coefficient across the interface (D_{int}), the half-thickness of the interface (d), and the distance between nearest neighboring atoms (a).

$$v_{n,\gamma} = va / D_{Mn}^\gamma \quad -(10)$$

$$v_{n,int} = v\delta / D_{int} \quad -(11)$$

In the temperature range of 830 to 880°C, the authors (see [21]) note the variation in D_{Mn}^γ and how it affects the velocity values. They observe a decrease in $v_{n,\gamma}$ from 2000 to 14, indicating that diffusion processes are slow compared to interface movement, particularly at lower temperatures. The authors argue that the diffusion of an Mn-spike in front of the interface is unlikely to influence interface motion significantly, as the half-thickness of such a spike would be comparable to the interface thickness itself.

Based on these observations, the authors conclude that substitutional diffusion in the Mn-bulk material is too slow to significantly impact the kinetics of the transformation process. Consequently, they suggest assuming immobile substitutional components in the γ -bulk as a reasonable approximation.

This discussion provides insight into the underlying physics of the transformation kinetics, particularly regarding the role of diffusion and interface movement in the process. It also highlights the importance of considering normalized velocities and

diffusion coefficients when analyzing such phenomena.

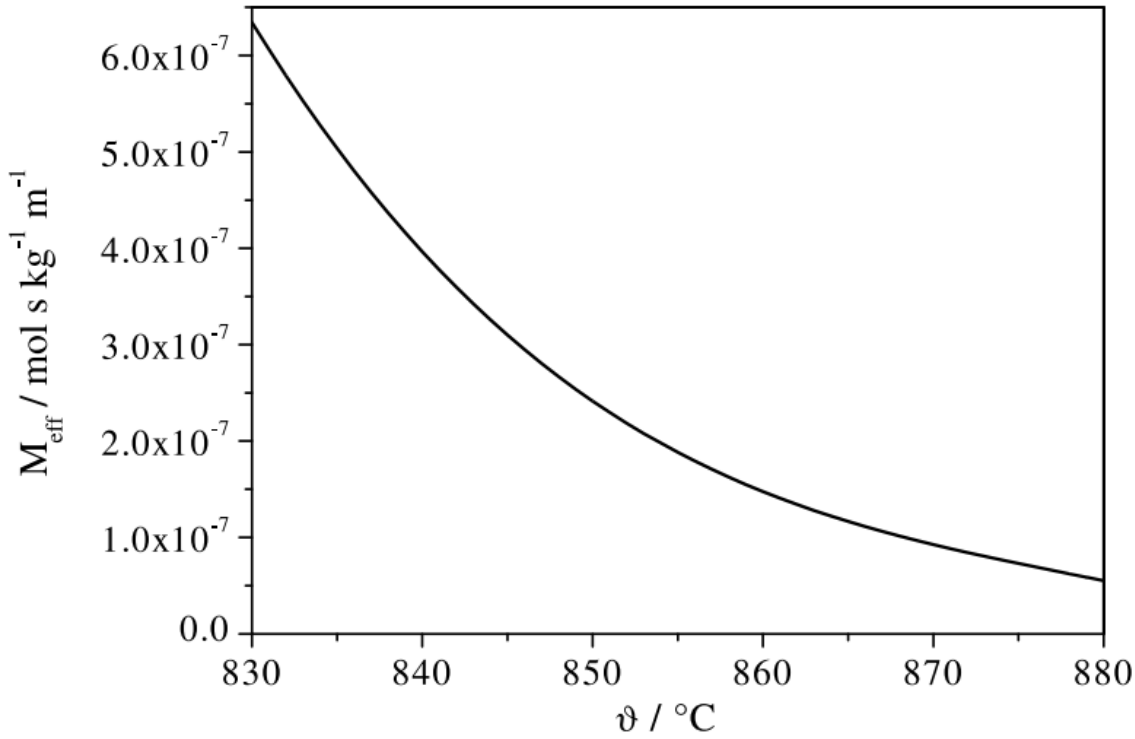


Fig. 5. Master curve for the effective mobility as a function of temperature assuming planar growth.

They provide a rough estimate that $v_{n,int}$ is expected to be significantly lower than bulk diffusion normalized velocity $v_{n,\gamma}$, possibly by a factor of a hundred to a thousand, assuming a normalization factor D_{int} / δ that is orders of magnitude larger than D_{Mn^γ} / a . This indicates that substitutional diffusion across the interface occurs on a similar time scale as interface motion, implying that transformation kinetics might be influenced by solute segregation to the moving interface.

To account for this, they propose modifying Equation (1) as presented earlier in this

term paper, introducing a solute drag pressure term ($\Delta\rho_{sd}$). This modified equation (12) allows for a more explicit consideration of solute drag effects on interface mobility.

$$v = M(\Delta\rho - \Delta\rho_{sd}) \quad (12)$$

An Arrhenius relationship explains how temperature influences intrinsic mobility (M), a critical element in ferrite transition. See below equation (13). Pre-exponential factor (M_0) is usually recognized to be roughly 140 kJ/mol; nevertheless, it varies significantly in the literature (4800 mol s /kg .m to 0.058 mol s /kg .m). To determine the role of M_0 , more research is needed.

$$M = M_0 \exp(-Q_M / RT) \quad (13)$$

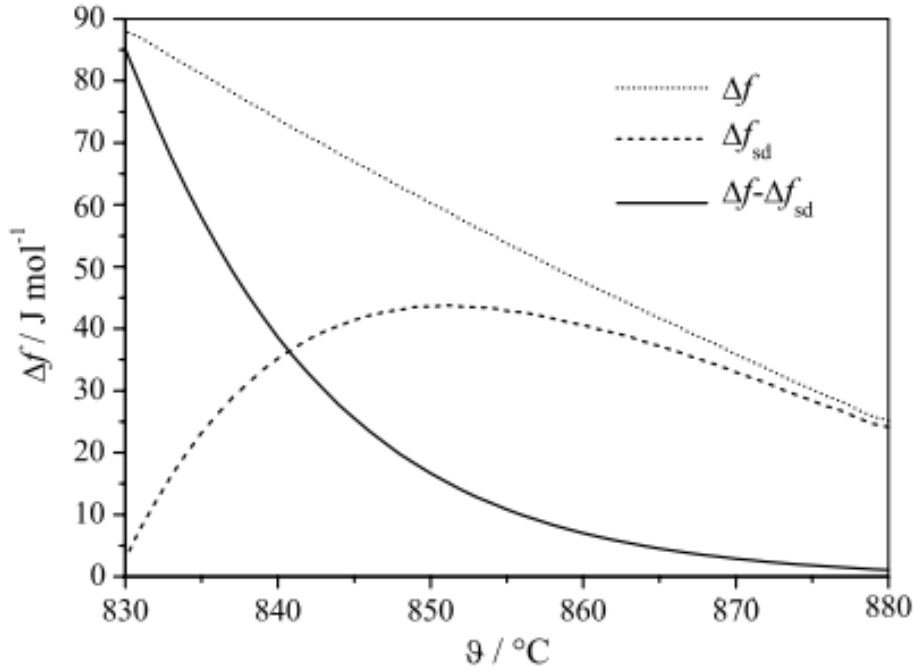


Fig. 6. Effective driving pressure $\Delta f - \Delta f_{sd}$ and its contributions (Δf , Δf_{sd}) as a function of temperature.

Based on the effective mobility (M_{eff}), the researchers computed the force opposing transformation (solute drag pressure, Δp_{sd}). By presuming that the intrinsic mobility at a given temperature is represented by the largest M_{eff} value, they calculated a lower bound for the intrinsic mobility (M_0).

They discovered an increase at lower temperatures by analyzing the effective driving force, which is the difference between the driving force and solute drag. The solute drag, the opposite force, peaked at middle temperatures.

Finally, they investigated the relationship between this opposing force and the transformation rate (normalized velocity, $v_{n,\text{int}}$) by examining how it is affected by the diffusion coefficient at the interface, which is thought to follow an Arrhenius relationship as discussed in [22].

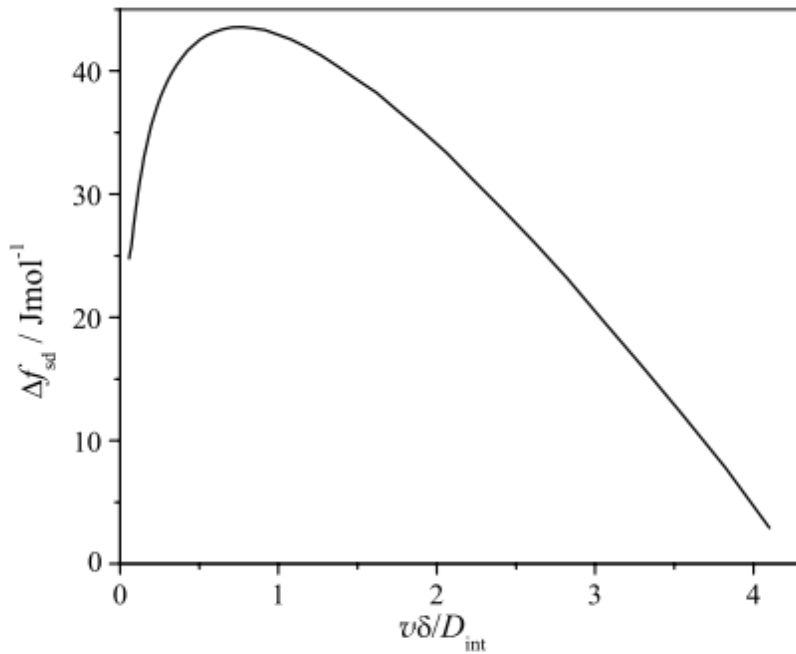


Fig. 7. Solute drag pressure Δf_{sd} as a function of the normalized velocity $v_{n,\text{int}}$.

The authors [22, 23] related the binding energy (E_b) of solute atoms at the interface to the opposite force, or solute drag. They estimated E_b to be around $-3RT$, or negative three times the ideal gas constant multiplied by temperature, based on previous studies and accepted values for Mn-segregation.

4. Conclusions & Outlook :-

The effective mobility of the γ/α interface during phase transformation in ultra-low carbon low alloy steel is estimated using data obtained from dilatometer tests. Unlike spherical growth, planar growth of ferrite results in a mobility independent of the cooling rate. Consequently, ferrite forms plates at low volume fractions, & the material transforms through a process of thickening & coalescing these plates. Despite being a thermally activated quantity, effective mobilities decrease with increasing temperature, which is quite consistent with that reported in [7]. The assumption of ferrite growing as spheres is not supported by the analysis, [9-12] suggesting that solute drag of Mn may contribute to the decrease in effective mobility with temperature.

Estimating Solute Drag Pressure :-

The solute drag pressure is estimated by replacing the effective mobility with an effective driving pressure, which relies on the selection of the intrinsic mobility, an unknown quantity.

Nonetheless, evaluation of experimental data narrows down the possible range of the pre-exponential factor of the intrinsic mobility [8-12], indicating solute drag

behavior consistent with analyses reported in previous studies [23, 24].

Prospective Routes for Research :-

The study finally concludes by mentioning that future research in this field should focus on gaining deep understanding of interface migration & solute interface interaction to gain deeper insights into underlying physics. While in situ studies of this phenomenon are currently beyond experimental capabilities, yet transformation studies & analyses on selected steels & model alloys could provide us, useful insights into trends of solute interface interaction with systematic changes in composition. Additionally, establishing natural & realistic austenite-ferrite phase arrangements presents a challenge for describing overall kinetics of transformation across a range of ferrite volume fractions.

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