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Grain Boundary Effects on Mechanical Properties: Design Approaches in Steel

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Abstract

For Poly-crystalline metals, Grain boundary design plays an important role to achieve desired mechanical properties in the final product form which may be a hot rolled or cold rolled coil. The fundamental mechanical properties are yield and tensile strengths, elongation and formability where grain refinement is particularly attractive mechanism for property design. Grain boundary strengthening provides benefits both in terms of fracture toughness and mechanical behavior at lower temperatures particularly in case of hot rolled high strength structural and line pipe steels. For cold rolled steels, grain boundary effects play a crucial role in critical automotive application steels such as Bake Hardening Index in Bake-hardening Steels. Additionally, deep drawability and formability characteristics are also strongly dependent upon grain size. Mechanical properties in steels are controlled majorly by two techniques - chemical composition and Steel processing parameters. Through first method of chemical composition control, during hot rolling, the control of austenite grain size is accomplished, alongside retardation of phase transformation to lower temperature. In second method, steel manufacturing process parameters i.e. hot rolling and coil cooling parameters, cold reduction, and subsequent heat treatment parameters such as annealing play an important role.

Keywords: thermomechanical processing, recrystallization, mean flow stress, hot rolling process modeling, steel design, grain boundary strengthening, mechanical properties

1. Microstructural evolution during thermomechanical processing of steel

1.1 Thermomechanical processing in hot rolling mill

Thermomechanical processing in hot rolling mill in general involves rolling of slabs or blooms to thinner sections which are classified as plate or coils by inducing reduction in thickness by rolling at controlled elevated temperatures to achieve desired mechanical properties.

As shown in **Figure 1**, typical thermomechanical hot rolling process can be divided into five basic processes.

Figure 1.
Typical setup of hot strip rolling mill.

1.1.1 Reheating of slabs

The first step involves heating up of slabs to remove dendritic segregation and facilitate solutionizing of microalloying element which is intended to precipitate during hot rolling, contributing to the strength of the material.

1.1.2 Rough rolling

Before inducing final reductions at finish rolling mill, slab is first introduced to be rolled in the roughing stands where thickness of slab is reduced from 200 to 300 mm to about 50 mm in several passes, usually four or five. In the roughing process, the width increases in each pass and is controlled by vertical edge rollers. Since the temperatures are high, recrystallization takes place during this process.

1.1.3 Finish rolling

Finishing mill is generally a tandem rolling mill consisting of 5–7 rolling stands. The finishing temperature is dependent upon the rolling speed. The interpass heating, or cooling is also controlled during rolling.

1.1.4 Accelerated cooling

After finish rolling, the hot rolled coil is subjected to cooling on runout table where water is sprayed on the top and bottom of the steel at a steady flow rate to induce phase and microstructure control leading to increased strengths.

1.2 Types of hot rolling approaches

The hot rolling process can be divided approaches based upon requirement of properties. They are chiefly identified as conventional controlled rolling (CCR) and recrystallization controlled rolling (RCR) (**Figure 2**). The recrystallization rolling requires rolling at high temperatures that leads to recrystallization and control of grain size. The process is designed to have mechanisms that inhibit grain growth after recrystallization. The conventional controlled rolling approach requires rolling in no-recrystallization zone, leading to unrecrystallized grains which ultimately lead to finer sizes after phase transformation (**Figure 2**).

The conventional controlled rolling shall be presented in detail as RCR has been mainly used for higher gauge rolling, i.e., plate mills or mills with lower rolling load capacities.

Figure 2.
 Recrystallization controlled rolling and conventional controlled rolling.

In general, in hot rolling method of conventional controlled rolling (CCR), methods of achieving strength would largely be dependent upon the grain size control of austenitic phase and eventually the phase transformation which is controlled by means of addition of microalloying elements in steel chemistry alongside or singly with application thermomechanical treatment practices during rolling.

The basic underlying principle of CCR is obtaining steel which possess both high toughness and strength through grain refinement. The successive methods to achieve finer grains are carried out as explained below:

1. Repeated deformation in roughing mill at recrystallization temperature range. Here, the austenitic grains are refined due to recrystallization.
2. Finish rolling which induces the successive heavy reduction in the non-recrystallization zone, i.e., rolling just above the non-recrystallization temperature T_{NR} . During finish rolling gamma (austenite) grains are forced to elongate in rolling direction, creating annealing twin deformation bands to cause alpha (ferrite) to form with a very fine size. Thus, by inducing numerous nucleation sites for alpha grains, its size is restricted.
3. Accelerated cooling that additionally promotes refinement of the ferrite grain size and restricts formation of pearlite.
4. Addition of microalloying elements also helps in enhancing strength by restricting movement of grain boundaries by formation of precipitates and restricting transformation of gamma phase.

2. Recrystallization phenomenon during rolling

Static recrystallization is likely favored phenomenon in steels during roughing passes and for plain carbon steels it continues between finishing passes as well. The static recrystallization is favored by low alloying levels and high temperatures, strains, and strain rates.

The recovery is suppressed during finish interpasses, but as dislocation density is increasing on account of work hardening at finish rolling, dynamic recrystallization (**Figure 3**) is initiated after surpassing a critical strain value ϵ_C . Dynamic recrystallization is markedly identified by necklace-type grain structure. After dynamic

recrystallization during rolling pass, the recrystallized nuclei continue to grow after the deformation ends, leading to a phenomenon called metadynamic recrystallization.

In controlled rolling process CCR, the addition of microalloying elements is deliberate to prevent static recrystallization. However, at low rolling temperatures, increased strain rates and lower interpass times coupled with lower precipitation, dynamic recrystallization is favored. As shown in **Figure 3**, the strain accumulates to peak stress and then decreases which differs on basis of type of steel.

There has been an established relationship [1] between the maximum peak stress σ_p and the limiting Zener-Hollomon parameter Z which is given by

$$[\sinh(\alpha \sigma_p)]^{n'} = AZ \quad (1)$$

typical values of $n' = 4.5$ and $A = 0.12$.

$$Z = \dot{\epsilon} \cdot \exp\left(\frac{300000}{RT}\right) \quad (2)$$

while Sun and Hawbolt [2] have reported peak Z dependent on initial grain size d_0

$$Z_{LIM} = 5 \times 10^5 \cdot \exp(-0.0155 d_0) \quad (3)$$

The maximum peak strain ϵ_p [2] that can be reached for given temperature T , strain rate $\dot{\epsilon}$, and strain ϵ has been established as

$$\epsilon_p = 1.32 \times 10^{-2} d_0^{0.174} \dot{\epsilon}^{0.165} \exp\left(\frac{2930}{T}\right) \quad (4)$$

The dynamic recrystallization threshold strain ϵ_c will initiate when strain reaches 0.7 times the value of ϵ_p .

2.1 Determining rolling parameters for hot rolling

In order to obtain good dimensional tolerance and optimum mechanical properties after rolling, optimum rolling parameters need to be established. The usual

Figure 3.
Stress-strain distribution with onset of recrystallization during rolling pass.

method is to achieve this to calculate the dynamic mean flow stresses (MFS) at each rolling stand of roughing mill and more importantly at finish rolling mill. The MFS is chiefly dependent upon the alloying elements, rolling reduction, and temperature at each rolling pass and based upon these factors several models have been proposed [3].

A most widely used method, simplified rolling load versus inverse temperature, is plotted to determine the rolling conditions and has been depicted in **Figure 4**. When the mean flow stress, which is directly related to mill rolling load value, is plotted against the inverse absolute temperature, a slope kink signifying end of static recrystallization is observed. If rolling is accomplished below this temperature represented as T_{NR} (temperature of no further recrystallization), there is a sudden jump in mean flow stress which is due to additive nature of work hardening induced in each pass [4].

The onset of recrystallization during finish rolling is controlled largely by rolling interpass time. It has been reported [4] that for interpass intervals significantly longer than 1 second, static recrystallization takes place, whereas those involving interpass times of 15–100 ms, dynamic or metadynamic recrystallization is favored. Another important factor to include is consideration of strain-induced precipitation, which inhibits recrystallization phenomenon.

When high strength low-alloyed steels are finish rolled, an additive buildup of strain causes an increase in MFS consecutively after each pass. When a critical strain value is surpassed, dynamic recrystallization is initiated, and a small drop in load caused by metadynamic recrystallization is observed during end of rolling. In carbon-manganese grades, this may be associated with the austenite to ferrite transformation.

2.2 Modeling the mean flow stress to estimate the critical rolling parameters

As thermomechanical processing involves microstructural evolution in terms of static and dynamic recrystallization that takes place during the rolling process, the mean flow stress shall also depend upon these considerations also.

A model equation for mean flow stress prediction for carbon-manganese grades by Misaka [5] has been proposed as below:

$$MFS_{MISAKA} = e^{(0.126 - 1.75 [C] + 0.594 [C]^2 + \frac{2851 + 2698[C] - 1120[C]^2}{T})} \quad (5)$$

Figure 4.
Plot of mean flow stress versus inverse of absolute temperature.

Various researchers (Siciliano et al. [3], Sun and Hawbolt [2]) have worked upon refinement of the equation to include effect of recrystallization that would affect the value of MFS.

Recrystallization criteria are a function of initial grain size d_0 , strain $\dot{\epsilon}$, strain rate $\dot{\epsilon}$, and temperature T during rolling and are initiated when the strain at a pass exceeds critical strain ϵ_C favored by appropriate temperature.

2.2.1 Critical strain evaluation for static recrystallization

If d_0 is the initial grain size, the critical strain to initiate dynamic crystallization is given by

$$\epsilon_C = 5.6 \times 10^{-4} d_0^{0.3} Z^{0.17} \quad (6)$$

where Z is Zener-Holloman parameter defined by

$$Z = \dot{\epsilon} \cdot \exp\left(\frac{300000}{RT}\right) \quad (7)$$

To calculate type of crystallization that occurs at a particular pass, the strain values need to be compared against critical strain value.

2.2.2 Grain size evaluation for static recrystallization

If ϵ_a (strain at a pass) is less than the critical strain ϵ_c , static recrystallization is favored, leading to grain size governed by the equation:

$$d_{SRX} = 343 \epsilon^{-0.5} d_0^{0.4} \exp\left(\frac{-45000}{RT}\right) \quad (8)$$

Time for 50% completion of recrystallization (static) is

$$t_{0.5}^{SRX} = 2.3 \times 10^{-15} \epsilon^{-2.5} d_0^2 \exp\left(\frac{230000}{RT}\right) \quad (9)$$

Grain growth during interpass time t_{ip} is governed by

$$d^2 = d_{SRX}^2 + 4 \times 10^7 (t_{ip} - 4.32 t_{0.5}) \exp\left(\frac{-113000}{RT}\right) \quad (10)$$

2.2.3 Grain size evaluation for dynamic recrystallization

If ϵ_a (strain at a pass) is greater than the critical strain ϵ_c , dynamic recrystallization is favored, leading to grain size governed by equation:

$$d_{MDRX} = 2.6 \times 10^4 Z^{-0.23} \quad (11)$$

Time for 50% completion of recrystallization (dynamic) is

$$t_{0.5}^{MDRX} = 1.1 \times Z^{-0.8} \exp\left(\frac{230000}{RT}\right) \quad (12)$$

Grain growth during interpass time t_{ip} is governed by

$$d^2 = d_{MDRX}^2 + 1.2 \times 10^7 (t_{ip} - 2.65 t_{0.5}) \exp\left(\frac{-113000}{RT}\right) \quad (13)$$

2.2.4 Evaluation for work hardening and fractional softening

Accumulated strain ϵ_a at each pass is governed by the following equation:

$$\epsilon_a = \epsilon_n + (1 - X)\epsilon_{n-1} \quad (14)$$

where fractional softening X is governed by recrystallization:

$$X = 1 - \exp\left(0.693 \left[\frac{t}{t_{0.5}}\right]^q\right) \quad (15)$$

The value of q shall depend upon the type of recrystallization.

For static recrystallization (SRX), $q = 1.0$.

For metadynamic recrystallization (MDRX), $q = 1.5$.

2.2.5 Evaluation for predicting mean flow stress (MFS) in each rolling pass

The modified mean flow stress modeling equation incorporating effect of manganese addition shall be

$$MFS = (0.78 + 0.137[Mn])X MFS_{MISAKA} X 9.8 X (1 - X_{DYN}) + K\sigma_{SS}X_{DYN} \quad (16)$$

where X_{DYN} is

$$X_{DYN} = 1 - \exp\left(0.693 \left[\frac{\epsilon - \epsilon_c}{\epsilon_{0.5}}\right]^2\right), \quad (17)$$

where

$$\epsilon_{0.5} = 1.44 \times 10^{-3} \dot{\epsilon}^{0.05} d_0^{0.25} \exp\left(\frac{6420}{T}\right), \quad (18)$$

and where σ_{SS} is defined as steady state of stress after peak stress is achieved:

$$\sigma_{SS} = 7.2 \dot{\epsilon} \exp\left(\frac{300000}{RT}\right)^{0.09} \quad (19)$$

3. Effect of chemical composition

High-strength steel requires tensile properties as main requirement, whereas the requirements such as weldability and ductility are also of chief importance. Therefore, carbon which is the chief source of strength should not exceed very high values, and hence high-strength steel requires addition of alloying elements.

The addition of microalloying elements can be divided into two categories [6]:

1. Microalloying elements: niobium, vanadium, titanium, aluminum, and boron.
2. Substitutional elements: silicon, manganese, molybdenum, copper, nickel, and chromium.

3.1 Addition of niobium, titanium, and vanadium

Microalloying elements such as niobium, titanium, and vanadium are principally carbide-forming elements. Although the addition of these elements in steel raises its A_{r3} temperature, they retard austenite transformation to ferrite by restricting carbon diffusion. Strengthening by addition of one or all of niobium, vanadium, or titanium has shown a remarkable increase in strength of steel. The strengthening phenomenon is caused by fine precipitation of nitrides, carbides, or carbonitrides which are coherent with ferrite matrix but induce strengthening by impeding dislocation movement.

One of the most significant effect of adding individually or simultaneous addition of V, Nb, and Ti is to decrease recrystallization temperature. Which contributes in generating a finer size of gamma (austenite) grains during finish rolling.

The two principal mechanisms that inhibit recrystallization and eventually grain growth are particle pinning and solute drag.

The grain boundary movement can be accounted on strain-induced precipitation of micro carbides on gamma grain boundaries that limit the gamma grain size. Addition of titanium or niobium helps in suppressing gamma grain growth by means of nitride or carbonitride precipitates which are majorly present at grain boundaries and inhibit their movement.

In the case of vanadium addition, addition of nitrogen can be helpful in increasing the strength and toughness. The vanadium nitride precipitates are useful in imparting strength to the steel. The addition of nitrogen however attributes to poor weldability. Likewise, the strengthening may be achieved by adding niobium, but a higher niobium content is bound to give poor weldability. Hence the conventional methods require simultaneous addition of V and Nb.

3.2 Manganese-based strengthening

The improvement of toughness can be achieved through addition of manganese that leads to decrease in A_{r3} temperature. Due to decrease in A_{r3} coupled with low coiling temperatures, the alpha (ferrite) grains are refined, thus increasing the strength. Additionally, the fine precipitate size is contributed by niobium carbonitrides and vanadium nitrides.

4. Effect of controlled hot rolling parameters

4.1 Reheating temperatures at reheating furnace

In general, austenitic grains starts to recrystallize at temperatures above 1050°C. Since an initial finer gamma grain size is helpful in creating a final finer size of alpha, lower reheating temperatures are effective. Also, the microalloying elements also add to refinement of the austenitic grain size by means of undissolved carbides and nitrides that restrict initial austenitic grain size.

Eventually, a lower slab reheating temperature by contributing fine austenitic grain size and lower temperature rolling at roughing mill will induce even finer grain size by reduction at lower temperatures.

4.2 Repeated recrystallization in roughing mill

Due to repeated reduction in roughing mill, both recrystallization and precipitation are competing phenomena. However, at higher temperatures

recrystallization will be the first phenomenon. As a basic principle of controlled rolling demands that precipitation should occur during finish rolling, it has been recommended to have higher roughing temperatures along with short rougher interpass intervals.

The gamma grain is refined by repeated static recrystallization caused during roughing mill action. Increasing rolling strain has marked effects on facilitating static recrystallization caused by higher dislocation density and increased nucleation sites caused by fine size of austenite which in turn leads to softening of material. However, there is a limiting value of grain refinement.

4.3 Finish rolling at no-recrystallization temperatures

As has been elucidated above, no-recrystallization temperature (T_{NR}) is important in design of controlled rolling process. This temperature determines where strain is multiplied for austenite grains, leading to strain-induced precipitation of carbonitrides as well as enhanced sites for a fine-grain size ferrite to be nucleated at the sites. Hot rolling being a dynamic process, no-recrystallization temperature depends upon deformation parameters. The influencing factors for T_{NR} are composition of the steel, strain values applied in each pass, the strain rate, and the rolling interpass time [7, 8].

During finish rolling the value of T_{NR} tends to dynamically lower down as the strain value or the reduction increases. This phenomenon is attributable on account of static recrystallization caused by increased recrystallization sites owing to finer grains and higher dislocation density induced during each rolling pass.

The strain rate value is also a determining factor for the onset of dynamic recovery and facilitates static recrystallization which eventually decreases the T_{NR} .

During controlled rolling, the interpass time during each rolling reduction also plays an important role as the prime requirement is to roll below T_{NR} temperatures. The precipitation kinetics are accelerated due to strains induced when rolling below T_{NR} . A lower interpass time is preferable as higher interpass will lead to coarsening of precipitate sizes as well as increased tendency of recrystallization detrimental to final strength value of steel.

4.4 Accelerated cooling

The runout table and the coiler in general act like post heat treatment unit which makes possible to achieve phase transformation through control of cooling to generate coils with varied properties and microstructures.

Accelerated cooling after hot rolling leads to further refinement of grains and phase control, leading to enhancement of properties. The phenomenon for strengthening of microstructure is phase transformations in terms of microstructures avoiding pearlitic transformations, precipitation strengthening through carbides, and nitride precipitates which along with controlled cooling rates lead to the refinement of grain size in the resulting microstructure. The accelerated cooling may be classified into two techniques—continuous accelerated cooling and interrupted accelerated cooling.

The final mechanical properties after accelerated cooling are majorly influenced by the alloying content and hot rolling parameters.

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