Numerical Simulation of Thermomechanical Processes Coupled with Microstructure Evolution

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The finite element method is already used in metal forming at an industrial scale. However, progress is needed regarding the microstructure optimization of components produced by metal-forming processes such as hot forging or rolling. This article presents mathematical models to predict microstructure evolution during hot working, showing the models' application coupled to thermomechanical processes' simulation software.

Metal forming is one of the most important fields in production technology. It's an interdisciplinary field, ranging from mechanical engineering to materials science. The aim of metal-forming processes isn't limited to obtaining useful geometries that apply plastic deformation to the material; it also involves controlling the final component's mechanical properties, which are directly controlled by the microstructure obtained during the formation process. Characteristics such as strength, elongation, toughness, and fatigue life can be improved by obtaining a finer and more homogenous grain distribution during the metal-forming process.

Software based on the finite element method (FEM) that are focused on metal-forming processes can provide technical results such as final geometry, temperature, strain and stress distributions, and forces required to produce a given shape. However, for information related to the microstructural evolution during hot working, it's necessary to incorporate mathematical models into FEM software that are able to describe the kinetics of recrystallization during the process, taking into consideration grain size refinement and grain growth. By incorporating such mathematical models, it's possible to predict the formation process as a whole, including the final microstructure obtained for the forged part, allowing process optimization that focuses on a higher-quality final product. With this in mind, here we review static and dynamic phenomena during hot working and propose the coupling of mathematical models for microstructure evolution kinetics to FEM software.

Microstructure Evolution During Hot Working

At low temperatures, work-hardening mechanisms such as increasing dislocation density lead to an increase in stress necessary for further deformation. However, in processes carried out at high temperatures, such as hot forging and rolling, diffusion processes become important, and microstructural phenomena, such as recrystallization and recovery, can occur, modifying the material flow behavior. These phenomena that occur during deformation are known as dynamic recovery and dynamic recrystallization.[1,2]

For metals, especially those with high-stacking fault energy, above 0.1 joules per square meter ($J.m^{-2}$), work hardening is limited by dynamic recovery. Dynamic recovery can be conceptualized as a dynamic equilibrium between the rates of generation and annihilation of dislocations during deformation, resulting in a continuous rearrangement of these dislocations, which leads to a softening of the material, limiting the effect of work hardening.[3,4]

For materials that exhibit low-stacking fault energy, as is the case of steel in the austenitic phase, dynamic recovery is less effective. In these materials, the softening main mechanism is dynamic

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recrystallization, reducing flow stress and grain size.

As the material is deformed, a large number of defects are generated. These defects, which aren't completely eliminated by dynamic recovery, increase the thermodynamic potential for the onset of recrystallization. As soon as a critical deformation is reached (φ_c) the nucleation of new grains free of deformation starts along preferential sites such as grain boundaries.[2] This phenomenon generates a strong softening of the flow stress at the same time that it provides a strong grain-size refinement. Besides the chemical composition and initial microstructure, dynamic recrystallization is strongly dependent on the temperature, strain, and strain rate applied to the material.[3–5] Figure 1 illustrates the change in the flow curve of a typical plain steel according to microstructural change occurring during hot working.

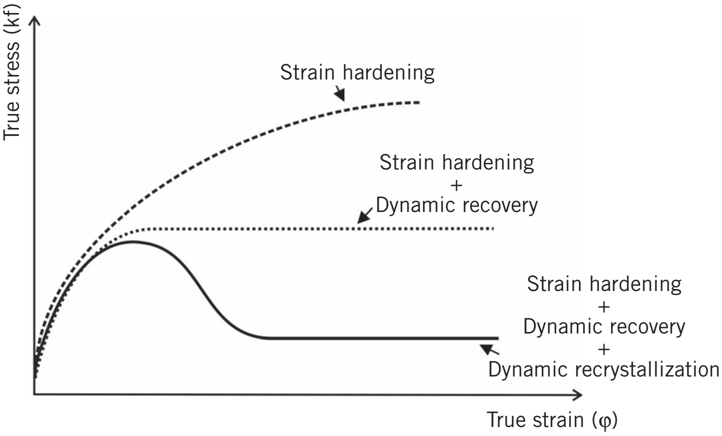

Figure 1. Changes in the flow curve of a plain steel during hot working, for different hardening/softening mechanisms involved.

Recrystallization Kinetics

For metal-forming processes such as hot forging and rolling, control of recrystallization and related conditions can provide a higher quality product. Through mathematical models it's possible to predict the material microstructural evolution during the forming process, describing the kinetics of dynamic recrystallization, static, and changes in grain size.

The combination of temperature, strain rate, and activation energy can be described by introducing the Zener-Hollomon parameter[6,7]

$$Z = \dot{\varphi} \cdot \exp\left(\frac{Q_{DRX}}{R \cdot T}\right),$$

Where $\dot{\varphi}$ = strain rate (s^{-1}), T = forming temperature in kelvins (K), Q = activation energy in joules per mole ($J \cdot mol^{-1}$), and R = universal gas constant ($8{,}314\ J \cdot mol^{-1} \cdot K^{-1}$).

Dynamically recrystallized grain size is directly dependent on parameter Z, and it can be calculated as follows[7]:

$$d_{DRX} = b \cdot Z^{b_2}.$$

The dynamic recrystallization (DRX) kinetics follows a modified Avrami-type equation, and it can be calculated as follows[6,7]:

$$X_{DRX} = 1 - \exp\left(d_1 \cdot \left(\frac{\varphi - \varphi_c}{\varphi_{ss} - \varphi_c}\right)^{d_2}\right),$$

where φ_c = critical strain to onset of dynamic recrystallization, φ_{ss} = strain to onset of steady-state, d_0 = initial austenitic grain size (μm), and d_1 and d_2 = material-dependent parameters.

The critical strain φ_c corresponds to a critical dislocation density required to initiate dynamic recrystallization and it can be obtained by

$$\varphi_c = 5{,}6 \cdot 10^{-4} \cdot d_0^{0{,}3} \cdot Z^{0{,}17}.$$

Not all work hardening can be eliminated during hot forming. After forming, or between different stages during the process, microstructural phenomena continue eliminating the work hardening until reaching the steady state of microstructural organization. These phenomena are the static recovery and static recrystallization.[8] The static recrystallization (SRX) kinetics also follows a modified Avrami-type equation and it can be calculated as follows[8,9]:

$$X_{SRX} = 1 - \exp\left(-0{,}693 \cdot \left(\frac{t}{t_{0{,}5}}\right)^k\right),$$

where $t_{0,5}$ is the time needed for 50-percent static recrystallization, and it can be obtained by

$$t_{0{,}5} = f_1 \cdot d_0^{f_2} \cdot \varphi^{f_s} \cdot \exp\left(\frac{Q_{SRX}}{R \cdot T}\right).$$

Static recrystallized grain size can be calculated by

$$d_{SRX} = C_1 \cdot d_0^{c_2} \cdot \varphi^{c_s} \cdot Z_m^{c_5},$$

where d_0 = initial austenitic grain size (μm), t = time interval between forming stages (s), and k, c_i, f_i = material-dependent parameters.

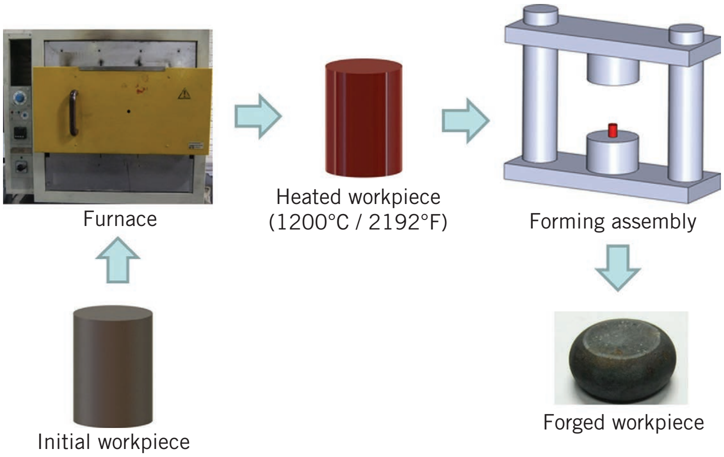

Figure 2. Typical steps for a hot upsetting test.

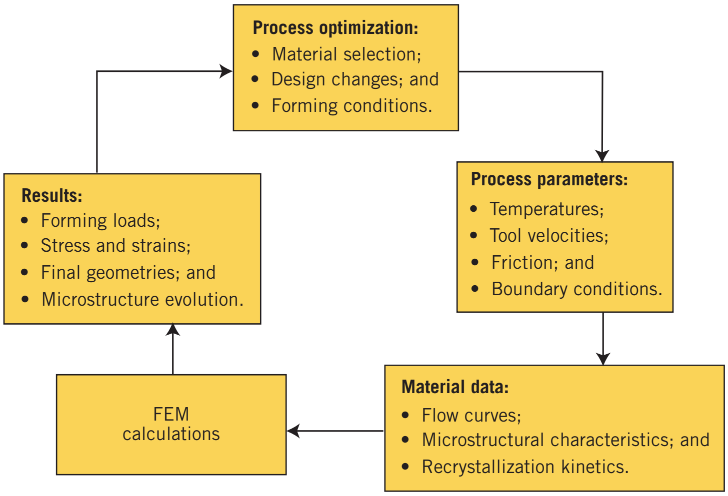

Figure 3. Flow chart for steps in an integrated thermomechanical and microstructure simulation.

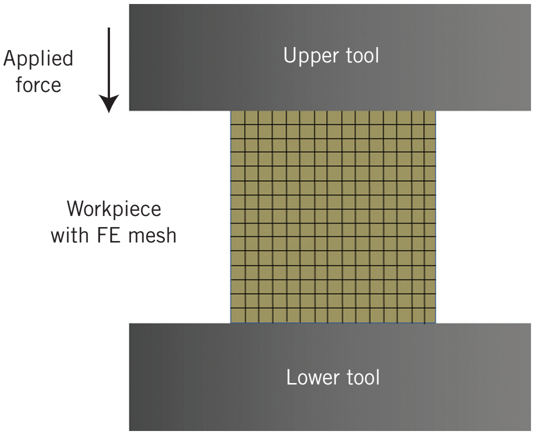

Figure 4. Numerical model used for the simulation.

After recrystallization, grain growth occurs if the material is still exposed to high temperatures. According to Sellars, grain growth can be calculated as follows[10]:

$$d_{gg} = d_0^{hd_2} + h \cdot d_3 \cdot t \cdot \exp\left(\frac{-Q_{gg}}{R \cdot T}\right).$$

The material-dependent parameters presented in the aforementioned equations $\{a_i, b_i, c_i, d_i, e_i, f_i, g_i, \ldots\}$ are related to changes in material microstructure during deformation and should be experimentally determined using regression analysis and metallographic techniques. Methods to determine these parameters are described in the literature.[9–12]

By incorporating the aforementioned mathematical models presented in numerical simulation software, it's possible to predict by the FEM the microstructure evolution during hot working.

Materials and Methods

Here, we'll provide further details about our approach.

Simulated Upsetting Test with Microstructure Evolution

To demonstrate the application of the FEM in a metal-forming process with microstructure prediction, we simulated an upsetting test, which is the simplest operation of open die forging. During the upsetting test, the workpiece is compressed between two flat dies, reducing its height and causing the flow of material in the transverse direction, increasing its diameter. This is equivalent to a conventional compression test, but it's usually carried out at high temperatures. Figure 2 illustrates the basic steps of the hot upsetting test usually carried out in industrial environments.

The flow curves and microstructural parameters of DIN 42CrMo4 steel were collected and inserted into the software. The software used was Programmer's Environment for Pre-Postprocessing/Larstran (PEP/Larstran), which is an open source academic software developed at the University of Aachen, Germany. PEP/Larstran works coupled with the microstructure module called Strucsim. For each increment of the forming process, simulation iterations between the thermomechanical and microstructure modules are executed. The thermomechanical module feeds the microstructure module with the instantaneous values of equivalent strain, strain rate, and temperature. The microstructure module then calculates the microstructural evolution depending on the values fed in, and taking into account the

Table 1. Parameters used for the simulation.

Parameter	Value
Material	DIN 42CrMo4 steel
Friction coefficient	0.3
Reduction in height	25 mm
Workpiece temperature	900° C
Tool speed	3.7 mm/s
Mesh	Hexaedric 8 nodes
Number of elements	2,280

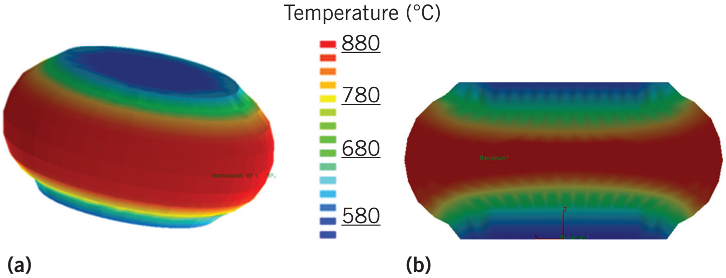

Figure 5. Temperature field (a) in the entire workpiece, and (b) through the longitudinal section.

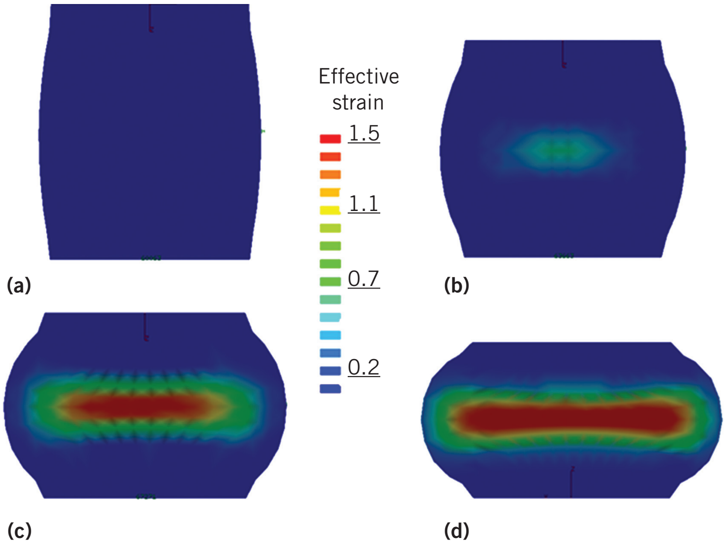

Figure 6. Longitudinal section showing equivalent strain distribution at (a) 25 percent, (b) 50 percent, (c) 75 percent, and (d) 100 percent of the process.

previous microstructural state. The flow chart in Figure 3 illustrates the steps for incorporating the mathematical models, process parameters, and material data into the PEP/Larstran.

Figure 4 illustrates the numerical model used to simulate the upsetting test. The numerical model reproduces usual test conditions, using the parameters shown in Table 1.

The upsetting test's purpose is mainly to demonstrate the change in grain size of the material due to dynamic recrystallization. It's known that homogeneous and finer-grain distribution provides a better mechanical behavior, especially for components that are exposed to cyclic loads (fatigue). As previously mentioned, by controlling the recrystallization phenomena during the process, it's possible to obtain a large grain refinement.

Results and Discussion

Figure 5 illustrates the temperature field in the workpiece after the process. Numerical simulation results show a loss of temperature in the upper and lower faces due to heat conduction between the workpiece and tools.

As expected, the workpiece has a barrel shape due to the frictional forces existing between the workpiece and tool surfaces, restricting material flow along this region.

Figures 6a through 6d illustrate the effective strain field across the workpiece during the process's different stages. We can observe how the degree of strain becomes more intense along the reduction in height, especially in the workpiece's central region. The regions of restricted flow (between the workpiece and tool surfaces) show smaller strain intensity. These behaviors are expected—however, only through the FEM is it possible to precisely quantify the profile of strain intensities throughout the workpiece, which is important in optimizing the mechanical behavior, because it directly influences the component's final microstructure (see Figure 7).

Figure 7 illustrates the numerical results for the recrystallized fraction and average grain size. As we mentioned, after a critical degree of strain, dynamic recrystallization occurs, which is the nucleation of new grains free of strain in the material during the process. This dynamic recrystallization depends on the degree of strain imposed on the material, which can be seen in Figure 7. Note that in the center of the workpiece shown in Figure 7a, where the degree of strain is higher, the recrystallized fraction reaches 1.0, which means that the material is fully recrystallized. The recrystallized fraction tends to decrease as it moves away from the central region to a minimum value near the surface,

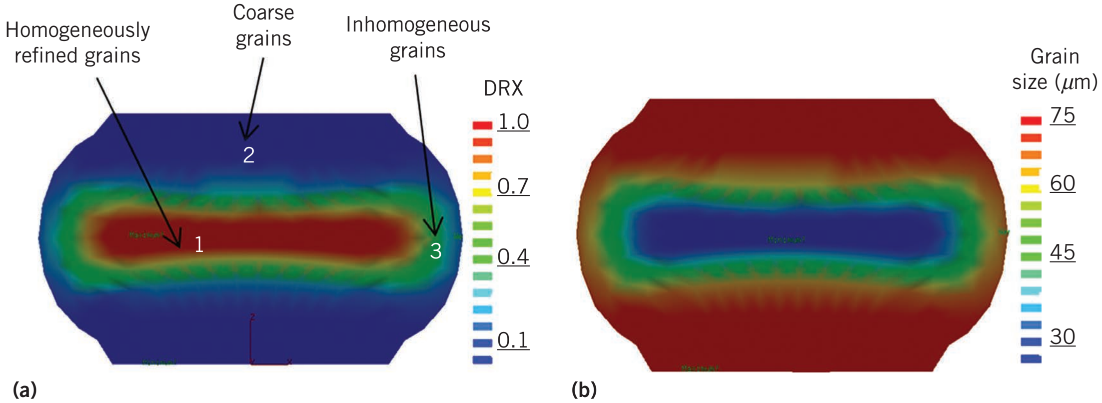

Figure 7. Longitudinal cutting illustrating (a) recrystallized fraction (DRX) and (b) average grain size.

precisely at the region where smaller strains are found. Dynamic recrystallization provides grain size refinement in the workpiece's central region. The grain size decreases from an initial value of 75 μm to about 30 μm, as Figure 7b shows.

According to numerical results, we expect that in the workpiece's center (point 1 in Figure 7a) grain size distribution will be finer and homogeneous. Close to the contact surfaces between the workpiece and tools, where the strain is smaller, we expect a coarser grain distribution (point 2 in Figure 7a), while at point 3 in Figure 7a we expect an inhomogeneous microstructure consisting of both coarse and fine grains, because recrystallization is only partial in this region. This microstructure distribution is usually the distribution observed experimentally.[13]

This is a simple but useful case study to demonstrate the relevance of the FEM for metal forming, both for researchers and for the industrial environment. Possibly by reducing the interfacial friction as well as different tool shapes, it could provide different results—perhaps a more homogeneous recrystallization through the workpiece's entire longitudinal section. All these aspects can be predicted by numerical simulation applied to metal forming, eliminating costs with tooling and laborious experimental procedures.

As the example demonstrated in this article, by controlling the parameters that directly influence the material microstructure's evolution, it's possible to optimize the process seeking to obtain a homogeneous and refined microstructure, and consequently improve the final product's mechanical performance. However, as with most metal-forming processes, it's difficult to work with high temperatures, and there are high costs involved in tooling for the production of large components. These factors make it difficult to perform the optimization process through experimental and trial-and-error stages.

Therefore, it's crucial to employ better research efforts that optimize mathematical models to predict microstructure evolution implemented in FEM systems applied in the metal-forming industry. Such efforts enable a clearer understanding of the factors that influence metallurgical phenomena during metal-forming processes, which in turn helps metal-forming industries have complete control of the process, and obtain a product with a homogeneous and refined microstructure. This leads to optimal mechanical performance from a higher-quality product.

Acknowledgments

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