Simulation of Stainless Steel Tube Extrusion

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Luleå, Sweden, 2006
ABSTRACT

The simulation of hot extrusion processes is a difficult and challenging problem in process modeling. This is due to very large deformations, high strain rates and large temperature changes during the process. Computer models that with sufficient accuracy can describe the material behavior during extrusion can be very useful in process and product development. Today, the process development in industrial extrusion is to a great extent based on trial and error and often involves full size experiments. Numerical simulations can most likely replace many of these experiments, which are often both expensive and time consuming. The motivation for this research project is a request for accurate finite element models that can be used in process design and development of stainless steel tube extrusion. The models will be used to investigate the effect of different process parameters on the quality of the extruded tube.

In the work presented in this thesis, thermo-mechanically coupled simulations of glass-lubricated tube extrusion were performed. Finite element models in two and three dimensions were developed for extrusion problems with radial symmetry. Simulations were carried out using the commercial code MSC.Marc, which is a Lagrangian finite element code. Frequent remeshing was therefore needed during the analyses. The models were validated by comparing predicted values of extrusion force and exit surface temperature with measurements from an industrial extrusion press. The two-dimensional model was shown to provide good and fast solutions to extrusion problems with radial symmetry. A two-dimensional model is sufficient for many applications and this model is planned to be used for solving processing problems further on. For the three-dimensional model it was concluded that a very fine mesh would be needed to successfully predict the extrusion force using four-node tetrahedrons. This would result in unacceptably long computational times. The future work will be aiming at improving the three-dimensional model in order obtain accurate results within a reasonable time.

To obtain reliable simulation results a good constitutive model is crucial. This work has focused on the use of physically based material models, which are based on the underlying physical processes that cause the deformation. It is expected that these models can be extrapolated to a wider range of strains, strain rates and temperatures than more commonly used empirical models, provided that the correct physical processes are described by the model and that no new phenomena occurs. Physically based models are of special interest for steel extrusion simulations since the process is carried out at higher strain rates than what are normally used in mechanical laboratory tests. A dislocation density-based material model for the AISI type 316L stainless steel was used in the finite element simulations included in this thesis. The material model was calibrated by data from compression tests performed at different temperatures and strain rates.

Keywords: Extrusion, finite element method, stainless steel, physically based material model, dislocation density
The work presented in this thesis has been carried out at Dalarna University in Borlänge and Sandvik Materials Technology in Sandviken. The financial support was provided by the Swedish Knowledge Foundation (KK-stiftelsen), the Swedish Steel Producer’s Association (Jernkontoret) and Sandvik Materials Technology.

First and foremost I would like to express my gratitude to my supervisor, Professor Lars-Erik Lindgren, for his continuous support and guidance during the course of this work.

I would also like to thank my colleagues, both at Dalarna University and Sandvik, for creating a good atmosphere at work. I am especially grateful to Erika Hedblom, who has been my supervisor at Sandvik during these years. Thank you, Erika, for always taking time to listen and giving good advice.

Finally, I would like to thank my family and my friends for their encouragement and support. A special thanks to Robert for his nutritious cooking and for putting up with me. Thank you for being in my life.

Sofia Hansson
Borlänge, February 2006
THESIS

This thesis consists of an introduction and the following appended papers:

**Paper A**
Physically based material model in finite element simulation of extrusion of stainless steel tubes
Sofia Hansson and Konstantin Domkin
Conference Proceedings of the 8th International Conference on Technology of Plasticity (ICTP), Verona, Italy, 2005

**Paper B**
Dislocations, vacancies and solute diffusion in physically based plasticity model for AISI 316L
Lars-Erik Lindgren, Konstantin Domkin and Sofia Hansson
Manuscript to be submitted to an international journal

**Paper C**
A three-dimensional finite element simulation of stainless steel tube extrusion using a physically based material model
Sofia Hansson
1 Introduction

The importance of modeling and simulation in the metal-forming industry has increased heavily during the last decades. Process simulation is now accepted as an important tool for product and process development. Unfortunately, the introduction of computer simulation in extrusion technology has not been as fast as in other parts of the manufacturing industry. This is mainly due to particular difficulties in these simulations. Extrusion processes are associated with very large deformations, high strain rates and complex contact conditions. In addition, steel extrusion often involves large temperature changes during the process. From a simulation point of view this makes extrusion a challenging task.

Today, the process development in industrial extrusion is to a great extent based on trial and error and often involves full size experiments. Numerical simulations can most likely replace many of these experiments, which are often both expensive and time consuming. The motivation for this research project is a request for accurate finite element (FE) models that can be used in process design and development of stainless steel tube extrusion. Computer simulations can be used to get a better understanding of the mechanisms involved in the tube extrusion process and improve the quality of the extruded product.

1.1 Aim and scope of the current work

The main objective of this work is to use FE simulations to study the process of stainless steel tube extrusion in order to increase the understanding of the process and to investigate the effect of different process parameters on the quality of the extruded tube. Of special interest is the problem of eccentricity and how to control the dimensions of the extrudate. An accurate extrusion model would, however, have a wide field of application. Simulations could be very useful in die design and for introduction of new materials and tube dimensions.

The approach that is used in the research work is to start with relatively simple FE models and gradually extend the degree of difficulty in these models. Commercial FE codes are to be used for the simulations, extended by user subroutines if necessary. The implicit FE code MSC.Marc has been used in the papers that are appended to this thesis. Important parts of the model development are to correctly model the boundary conditions and material behavior for the process.

1.2 The extrusion process

A patent granted in 1797 by Joseph Bramah described a press in which lead was forced through a die. This was the earliest consideration of the principle of extrusion which must therefore be considered a modern process compared to other metal-forming processes like rolling and forging. With the development of aluminum, which was commercially available in 1886, the extrusion process was established as an important industrial process (Sheppard, 1999). Today, extrusion is used in the manufacturing of many different products of different materials, but the major field of application is in the aluminum
industry. In the production of complex shapes from aluminum billets, no other process can compete with extrusion.

The principle of extrusion is generally very simple. A billet is placed in a closed container and squeezed through a die by a ram. The design of the die opening determines the cross-section of the extruded product. When extruding tubes, a mandrel is inserted in the middle of the die. Unlike most other deformation processes, all principal stresses are compressive during extrusion. Tensile stresses are only present in a small region at the exit of the die surface. When a material is plastically deformed under this state of multiaxial compression, very high strains can be reached since the workability is high at high hydrostatic pressure. The risk of metal rupture is reduced and materials, which would crack in other processes, can be extruded without problems (Laue and Stenger, 1976).

Extrusion is in most cases a hot working operation but can also be carried out in cold mode. The working temperatures in hot extrusion are typically 0.7-0.9 $T_M$, where $T_M$ is the melting temperature. This is higher than in forging and hot rolling which are normally carried out between 0.6-0.8 $T_M$. Aluminum alloys are hot extruded at about 450-500 °C and steels at 1100-1300 °C. The strains involved in extrusion are large, often of order 1, and the strain rate range is 0.1-10$^2$ s$^{-1}$ (Frost and Ashby, 1982). There are many different methods of extrusion but a characterization is often made with respect to the direction of the extrusion relative to the ram. In direct or forward extrusion the flow of material is in the same direction as the motion of the ram. The opposite is called indirect or backward extrusion and the ram that is used in that case has a hollow shape. Direct extrusion and indirect extrusion are the two basic methods of working. The major difference between the methods is that there is no friction between the container and the billet surface in indirect extrusion. This means that the load required for extrusion is decreased compared with the direct mode and the pressure is independent of the billet length. In spite of the advantages using the indirect mode, the direct process is more widely utilized. This is partly because extrusion presses for indirect extrusion are difficult to construct (Sheppard, 1999).

Extrusion is a discontinuous process and the second billet is not loaded until the first billet is extruded. During start-up of extrusion, the extrusion load increases as the material is forced to fill the container and flow out of the die. After the transient start-up phase the process is often considered to be steady-state. In reality the process is never in a steady-state phase since the contact conditions are changing and the temperature varies during the process. Steady-state may however be a good approximation if the friction is negligible and the temperature changes are small. The material flow is steady-state during the greater part of the extrusion process. When the billet has been extruded to a small discard there is high resistance to radial flow towards the center and the load increases heavily. Extrusion is then interrupted.

Depending on the method of extrusion, material and lubrication, considerable differences in flow behavior can be observed during the process. Experimental methods have been used to detect the various flow patterns that exist in extrusion and the flow patterns have been classified into four categories: S, A, B and C (Laue and Stenger, 1976). A schematic diagram of the flow patterns is given in Figure 1.
Figure 1. Different types of material flow in extrusion (Laue and Stenger, 1976).

The maximum uniformity of flow is seen in type S. The flow is frictionless, both at the container wall and at the die, and the deformation zone is localized directly in front of the die. This type of flow characterizes very effective lubrication, for example glass lubrication in steel extrusion, or indirect extrusion using a die lubricant. Flow pattern of type A is typical for lubricated extrusion of soft alloys such as lead and tin, while B is seen in most aluminum alloys. For type A, B and C, an area of inactive material can be seen inside the container and close to the die. This material zone is called the dead metal zone and remains still throughout the whole process.

If possible, lubrication in extrusion is generally avoided. If container lubrication not results in a completely homogenous material flow, the effect of lubrication is only damaging to the surface quality of the extruded product. This is often the case in aluminum extrusion, where the reduction in extrusion load due to lubrication does not compensate for the surface damage that occurs. The dead metal zone is in that case utilized to produce products with high surface quality. The design of the die is important, especially when aluminum shapes are extruded. Complex shapes often require very complex dies with portholes, channels and welding chambers.

1.3 Extrusion of stainless steel tubes

It was not until 1950 that the metal forming process of extrusion was successfully applied to the steel industry. The possibility to extrude steel, and particularly stainless steel, arose with the introduction of the UGINE-Séjournet process. Séjournet discovered that steels can be extruded if molten glass is used as lubrication. Today the UGINE-Séjournet process is the most important method for steel extrusion. In the manufacturing of seamless tubes, direct extrusion is often used in combination with other processes like forging, piercing and rolling. Steel extrusion is performed at high temperature and associated with high thermal stresses in the tools, leading to wear problems. The extrusion speed must be high since the billet loses heat rapidly. The exit speed is typically 1-2 m/s for high alloyed steels (Laue and Stenger, 1976).

In glass-lubricated extrusion, there is a layer of glass between the billet and the container, between the billet and the mandrel, and between the billet and the die. Each billet is heated to the extrusion temperature and then rolled in a powder of glass during transportation to the extrusion chamber. Glass powder is also applied inside the billet to assure good lubrication between billet and mandrel. Lubrication through the die is provided by a thick disc of compacted glass, the glass pad, which is placed between the billet and the die. During extrusion, the glass pad is pressed against the die by the hot metal. The glass pad
will deform with the billet and melt progressively to surround the extrusion with a lubricant glass film. The principle of tube extrusion by the Ugine-Sejournét process is shown in Figure 2. The glass layer on the finished product is very thin and is easily removed after cooling.

Figure 2. Glass-lubricated tube extrusion (Baqué et al, 1975).

Attempts have been made to understand the film formation of the glass lubricant (e.g. Séjournet, 1954). Baqué et al (1975) proposed a theoretical model of the lubrication mechanism including progressive melting, hydrodynamic flow and stability of the film. Still, the behavior of the glass lubricant, and especially the glass pad, during extrusion is not fully understood. A general observation is, however, that the metal flow is almost frictionless when glass is used as lubrication (e.g. Hughes et al, 1974). Compared to aluminum extrusion, no dead metal zone is observed in glass-lubricated extrusion. Another important lubricating effect of the glass is the thermal insulation that prevents the tooling from overheating.

The main goal in tube extrusion is to manufacture consistent products with minimal dimensional variation. One particular dimensional problem is referred to as eccentricity, i.e. the hole in the extrudate is not centered along the centerline of the billet outer diameter. Some amount of eccentricity is always produced when tubes are manufactured but the dimensional variations of the extrudate can be minimized, for example by tight control of process parameters and material flow in the process. In the work by Pugliano and Misiolek (1994) it is proposed that the major causes of eccentricity in stainless steel tubing are billet temperature gradients, billet preparation, equipment misalignment and improper lubrication. Eccentricity can be due to either one or a combination of these variables. Good quality of the die is also essential to achieve tubes with tight dimensional tolerances and good surface quality. Since the die is subjected to very high temperature and pressure, a new die has to be inserted for each extrusion. The used dies can in most cases be ground and reused.

2 Modeling and simulation of extrusion

Analytical solutions for metal-forming problems such as extrusion are very difficult to obtain due to the complexity of the problems. In practice, such methods can only be used for very simple geometries and boundary conditions. Analytic solution methods to metal-forming problems are treated in, for example, Hosford and Caddell (1983). In extrusion,
analytical methods are in principle only applicable for analyses of the steady-state phase. Still, the current understanding of many important phenomena that occurs during extrusion is based on various analytical methods. If numerical methods are used instead, the important initial non-steady state of extrusion can also be analyzed. The distribution and evolution of stress, strain and temperature during the whole process can be studied in detail.

2.1 Lagrangian, Eulerian and ALE formulations

There are mainly three different types of FE codes that are utilized in extrusion simulation: Lagrangian, Eulerian and arbitrary Lagrangian Eulerian (ALE) codes. The appropriate approach is determined by the problem to be solved and to some extent the computer resources available. The details of Lagrangian, Eulerian and ALE formulations are given in, for example, Belytschko et al (2000).

In Lagrangian codes, the mesh moves with the material and deforms with the material flow. The quadrature points also move with the material which means that the constitutive equations are evaluated at the same material points through the whole analysis. In Lagrangian meshes it is common to distinguish between updated Lagrangian and total Lagrangian formulations. The dependent variables are functions of the material (Lagrangian) coordinates and time in both formulations. In the total Lagrangian formulation, the weak form involves integrals over the initial configuration and the derivatives are taken with respect to the material coordinates. The updated Lagrangian formulation means that the derivatives are taken with respect to the spatial (Eulerian) coordinates and the weak form involves integrals over the current, deformed configuration. Both the total Lagrangian and the updated Lagrangian formulations are treated thoroughly in Belytschko et al (2000). The Lagrangian approach is very useful for extrusion analyses. Using this formulation the thermo-mechanical history during the process can be studied directly and the free surface of the extrudate can be followed. The limitations of the Lagrangian description appear when the deformations are large. Large strains and deformations often lead to excessive distortion of the elements which implies bad or non-converging solutions. If the mesh is distorted, mesh refinement or remeshing is often required to obtain a solution. When remeshing is utilized, a new mesh is constructed and a mapping is performed to transfer data from the deformed mesh to the new mesh. In many commercial software packages, the remeshing technique has been automatized and can be controlled based on user defined criteria. Every remeshing involves interpolation and extrapolation of element variables which may accumulate errors in the solution. Remeshing is also a computer intensive step and reduces the computational efficiency. Meshing and remeshing are often especially problematic in structural parts of small dimensions. If it is possible, frequent remeshing should therefore be avoided.

An alternative to the Lagrangian approach is the Eulerian formulation where the nodes and elements are fixed in space and the material flows through the mesh. In this formulation, the dependent variables are functions of the spatial (Eulerian) coordinates and time. The Eulerian method has a wide field of application in fluid mechanics but it is also suitable for many extrusion problems. For instance, the material flow and temperature evolution in the container and through the die can be effectively studied using an Eulerian FE code. The
major advantage of this formulation is that the problem with mesh distortion is avoided and large deformations can be simulated with a low computational cost. Using an Eulerian approach, it is however difficult to model the free surface of the extrudate after it has left the die. Another drawback is that the treatment of constitutive equations is complicated due to flow of material through the elements. Treatment of moving boundaries and interfaces is also difficult using Eulerian elements (Belytschko et al, 2000).

The ALE methods are arbitrary combinations of the Lagrangian and Eulerian formulations and were developed in an attempt to bring the advantages with both formulations together. In an ALE formulation the displacements of material and mesh are decoupled and the mesh can move independently of the material. Thus both the motion of the mesh and the material must be described. The ALE formulation was originally developed for modeling of fluid-structure interaction and motion of free surfaces in fluid mechanics (e.g. Hughes et al, 1981). A couple of years later the method was introduced for metal-forming applications. Mesh distortion can generally be avoided using an ALE approach, but in practice it is difficult for the user to choose a mesh motion that eliminates severe mesh distortions. The general ALE formulation in solid mechanics is presented by Gadala and Wang (1998), together with practical applications of the ALE formulation in metal-forming. The punch indentation process and metal extrusion process were simulated and it was shown that load fluctuations, which is pertinent to the updated Lagrangian formulation and the way that mesh updating and boundary conditions are handled in this formulation, can be completely eliminated using the ALE approach.

In recent years other methods such as the natural element method (NEM) have shown promising results for metal-forming applications. NEM is a member of the family of meshless methods (e.g. Lu et al. 1994) and is also known as the natural neighbor Galerkin method since it uses natural neighbor-based interpolation schemes to construct the space of trial and test functions of the Galerkin method. With this approach, it is possible to use an updated Lagrangian formulation without having problems with mesh distortion. A study of the potential to use the natural element method in three-dimensional simulation of aluminum extrusion is given in the work by Alfaro et al (2005). They concluded that NEM has a large potential for simulating large deformation processes. It was also shown that the high computational cost of NEM, which is somewhat bigger than for FEM, is not a large problem for extrusion applications. There may, however, be complications if NEM is to be used for extrusion of thin-walled products. For that purpose, other techniques may be more appropriate.

2.2 Extrusion models

There are rather few papers published about extrusion of stainless steel tubes and hardly any of these concerns finite element simulations. This is simply because there are not many tube manufacturers around the world that produce stainless steel tubes through extrusion. In the aluminum industry, on the other hand, extensive activities have been devoted to modeling and simulation, and in the recent years great progress has been made in this area. Many modeling issues are similar for extrusion of aluminum and steel. Large deformations and high strain rates are present in both processes which lead to problems with mesh distortion if a Lagrangian FE code is utilized. Some of the differences between aluminum
and steel extrusion, besides the material properties, are the temperature and lubrication conditions. Aluminum is extruded with tool temperatures that are close to the temperature of the billet and with lower ram speeds than in steel extrusion. The billet temperature is much higher when steel is extruded and the temperature changes during the process are large. Extrusion of aluminum is generally carried out without lubrication and with the formation of a dead metal zone, while the metal flow in glass-lubricated steel extrusion is almost frictionless. In the manufacturing of aluminum shapes the dies can be very complex with portholes, channels and welding chambers. The die in steel extrusion has a simple geometry but can be difficult to model due to the melting glass pad.

Temperature is a very important parameter in extrusion and particularly in steel extrusion where the temperature difference between tooling and workpiece is large. Temperature changes during the process depend on the billet temperature, the heat transfer between the billet and the tools, and the heat generated by deformation and friction. If the temperature is too low, the extrusion pressures can become very high. High temperatures on the other hand may lead to problems with surface cracks. An understanding of the temperature changes during extrusion is therefore important. Damodaran and Shivpuri (1997) developed a simple numerical model for quick real time analyses of temperatures and pressures during glass-lubricated hot extrusion. Heat transfer was modeled using a finite difference technique. Given some process parameters and material data, the model predicts the exit temperature of the extrudate and the extrusion pressure. Temperatures and pressures were compared with results from two-dimensional FE simulations.

As mentioned in the previous section the metal flow is almost frictionless with glass lubrication but the exact conditions are uncertain. One particular problem in modeling is that the die profile is difficult to determine. The die profile with the metal is partly defined by the lubricating glass pad which melts progressively during extrusion. In order to simulate the process, an assumption of the shape of the glass pad has to be done. One solution to this problem is to examine the butt-end of the extrudate in order to determine the path of the metal flow (e.g. Damodaran et al, 2004). In Paper C, which is appended to this thesis, the die profile was determined by investigations of so-called stickers, i.e. billets that were stuck in the press and only partly extruded. A cross-section of a stainless steel sticker is shown in Figure 3.

Figure 3. Cross-section of a partly extruded tube.
The billet and the tube, together with the mandrel, can be seen in the figure. The large reduction associated with tube extrusion is clearly seen in the photograph.

Damodaran and Shivpuri (2004) investigated the prediction and control of part distortion during glass-lubricated hot extrusion of titanium alloys. A finite element model was constructed that included induction heating, billet transfer, glass lubrication and metal flow. Because of unreasonable simulation times the three-dimensional deformation was modeled using a two-dimensional approach. Slices from the three-dimensional model were taken at different locations and each slice was treated independently of each other (plane strain). The FE model was used in a sensitivity analysis where the effect of process and design parameters on metal flow and extrudate distortion was evaluated. The results showed that the distortion was more sensitive to die design than to parameters as extrusion speed and soaking temperature. Model predictions were validated by industrial experiments. Design charts for extrusion processes were developed based on FE analysis by Arif (2003). Cold direct extrusion of steel rods was modeled in two dimensions using four-node quadrilateral elements. 90 simulations were carried out using various combinations of process parameters defining the material properties, contact condition, geometry of the billet and geometry of the die.

A large amount of papers that uses the finite element method to simulate aluminum extrusion have been published in the recent decade. Zhou et al (2003) used an updated Lagrangian approach to simulate a whole cycle of three-dimensional extrusion of a solid cross-shaped aluminum profile. They concluded that it is feasible to perform whole cycle extrusion simulations if the extrudate has a high degree of symmetry and a wall thickness acceptable for meshing and remeshing. The billet length-to-diameter ratio was 4 in this study and the wall thickness 6 mm. Advantage of symmetry was taken and only one eight of the billet and extrudate was modeled. Many non-steady characteristics were revealed even in the expected steady state. This indicates that the process is non-steady through the whole extrusion cycle. Thus, an Eulerian or an ALE approach would not be able to accurately describe the dynamics of the process.

Three-dimensional extrusion of flat sections from hard deformable aluminum alloys was modeled in the work by Libura et al (2005). The commercial FE code DEFORM 3D based on Lagrangian formulation was used for the simulations. Four-node tetrahedral elements were used in the discretization and only a quarter of the total assembly was modeled due to symmetry. The aim of the work was to investigate material flow, stress state, temperature distributions and force parameters while using dies of special geometry. Li et al (2002) used DEFORM 3D to investigate the metal flow behavior, exit velocities and heat transfer for aluminum extrusions with three-dimensional complex geometries. Experiments were also carried out in an extrusion plant on a production scale. The results showed that distortion of the extrudates can be related to inhomogeneous metal flow and even a slight inhomogeneity of metal flow can have a significant effect on the final extruded shape. Good agreement was reached between simulations and experiments. The work by Li et al (2002) is an example of how numerical analyses can be used to improve and optimize die and extrusion design processes. Multi-hole die extrusion of aluminum was modeled and simulated in two and three dimensions by Peng et al (2004). The influence of number and distribution of die holes on the extrusion parameters were investigated. Material flow pattern, extrusion load and recrystallized grain size could effectively be obtained from the
simulations. Recrystallization control, prevention of surface cracks and control of material flow in hot aluminum extrusion were analyzed using FE simulations by Duan et al. Models for recrystallization and damage criteria were integrated into the commercial codes FORGE2 and FORGE3 through user subroutines.

Examples of simulations in which the ALE formulation is utilized are given in the doctoral thesis by Lof (2000). Extrusion of aluminum shapes was analyzed and part of the work was focused on modeling of the bearing area. With the ALE formulation it was possible to set the mesh inside the die and the bearing channel to be fixed in an Eulerian description. At the same time it could be avoided that material flowed out of the mesh at the free surfaces.

2.3 Model validation

To be able to trust results from numerical simulations, validation of the models is necessary. The best way of validation is to test and measure on the real object. Unfortunately, there are limitations of the measuring possibilities in many production presses. The exit surface temperatures are often the only temperatures that can be measured during the extrusion process. The extrusion force can be recorded and used for validation together with the geometries of the extruded product. Since full size experiments can be difficult and expensive, physical modeling has become a popular method to study the extrusion process. The idea in physical modeling is to find a soft model material, such as wax and plasticine, with similar deformation behavior as the real material and study extrusion of the model material in a laboratory press. However, it is very difficult to find a model material that deforms and behaves analogous to the real material. It is also complicated to set up an experiment with similar process conditions as in the real extrusion process. The technique with model material is a cheap and fast method to perform extrusion experiments, but the results may not always be applicable on the real process.

Arentoft et al (2000) compared results from physical modeling of cold mild steel extrusion with FE predictions. The material flow was studied in axisymmetric simulations and experiments. Filia wax was the base component in the model material and kaolin, lanolin, silicon, M1 and harpix was added to change the material properties. Physical and numerical modeling of aluminium extrusion has been performed by Libura et al (2005), among others. Sofuoglu and Gedikli (2004) simulated extrusion of solid cylindrical billets of plasticine via physical modelling and FEM. Various extrusion ratios and die angles were tested in the work. The numerical model was axisymmetric with quadrilateral elements and the analyses were performed in the FE code ANSYS. The extrusion load-ram displacement curves from the numerical analyses were found to be close to the experimental curves.

3 Constitutive modeling

A major challenge in the simulation of metal-forming processes is to correctly model the material behavior. A good constitutive model, which accurately reflects the changes in material properties, is crucial to the reliability of the final simulation result. The mathematical descriptions of the material response to various loadings are called constitutive models. In one-dimension, the constitutive relation is the same as the stress-strain law for the material. The field of constitutive modeling is generally approached from
a phenomenological viewpoint. The material response on a macroscopic level is then considered, without taken into account the micro-level phenomena that cause the material behavior. In these material models empirical relationships are used to describe experimental data and the models are referred to as empirical or engineering. Another approach is to use constitutive models that are microstructure-related and formulate mathematical descriptions based on the underlying physical processes of the deformation. These models are called physically based models but, so far, these models are rarely utilized in metal-forming simulations.

Constitutive modeling is one of the most intensive research fields within solid mechanics and there is an extensive amount of literature available on the subject. Different types of elastic and inelastic models are, for example, covered in the book by Lemaitre and Chaboche (1990). Constitutive models are often treated together with corresponding numerical strategies. A model that is formulated for a non-linear material results in a non-linear boundary value problem that has to be solved numerically. Computational aspects of inelasticity are treated in Simo and Hughes (1998).

The stress is a function of the elastic strains and the inelastic strains, which can be thermal and plastic/viscoplastic in the current context. The plastic/viscoplastic strains remain after unloading. An elasto-plastic material is based on the definition of a yield surface. The stress state cannot be outside this surface, see below. This is the approach that is used in the current work. The elasto-viscoplastic model gives the plastic strain rate as a function of how far outside a flow surface it is. The flow surface then plays a similar role as the yield surface in a plasticity model.

The theory of plasticity includes four major parts as described in Belytschko et al, (2000).

1. A decomposition of each strain increment into an elastic, reversible part and a plastic, irreversible part.
2. A yield function \( f(\sigma, q_\text{int}) \) which governs the onset and development of plastic deformation; \( q_\text{int} \) are a set of internal variables. This function is used to determine the amount of plastic flow.
3. A flow rule which governs the plastic flow, i.e. determines the direction of the plastic strain increments.
4. Evolution equations for internal variables, including a strain-hardening relation which governs the evolution of the yield function.

Rigid-viscoplastic models are quite common in simulation of aluminum extrusion (e.g. Li, 2002). In this model it is assumed that the stresses are mainly dependent on the strain rate. The material is treated as a fluid, often a non-Newtonian fluid. Since the elastic effects are neglected it is not possible to determine for example spring back or residual stresses accurately. The elastic deformations may however have a significant effect on the results. Lof, for example, showed that the elastic effects are important in parallel bearings.

A general problem in material modeling is the lack of material data. This is a particular problem in extrusion and other metal-forming applications that are performed at high strain rates and high temperatures. It is very difficult to perform controlled mechanical tests at these conditions and the available data has to be extrapolated. The validity of an empirical
material model is often limited outside the range of deformation conditions in which it was calibrated. Thus, physically based models are interesting for extrusion applications. It is expected that these models can be extrapolated to a wider range of strains, strain rates and temperatures than empirical models, provided that the correct physical processes are described by the model and that no new phenomena occurs. Another advantage with the physically based models is that data from other sources than mechanical testing can be utilized for the material parameter fitting.

### 3.1 Physically based models

Generally, the strength of a solid depends on strain, strain rate and temperature. The strength is determined by processes on the atomic scale that causes flow. Examples of such atomistic processes are: the glide motion of dislocation lines, their coupled glide and climb, the diffusive flow of individual atoms, grain boundary sliding and mechanical twinning (Frost and Ashby, 1982). The mechanisms of plasticity, the range of dominance of each mechanism and the rates of flow that they produce are presented in deformation-mechanism maps for different materials in Frost and Ashby (1982).

Within physically based modeling it is distinguished between explicit and implicit models. In implicit physically based models the form of the constitutive equation is given by theory of the physical processes that causes the deformation. The other option is to explicitly include physical models as evolution equations in the constitutive model.

The microstructure of a crystalline material can be modeled directly as in discrete dislocation dynamics and crystal plasticity, or indirectly as in dislocation density-based models. Direct calculations of action and interaction of dislocations are however extremely computer intensive. Today, the only approach that is applicable for use in simulation of metal-forming are models based on the concept of dislocation density. Dislocation density-based models have been developed by Bergström (1983), among others.

In the papers that are appended to this thesis, a dislocation density-based model was used to model the deformation behavior of AISI 316L during extrusion. The AISI type 316L material is an austenitic stainless steel (fcc-structure) which is characterized by low stacking fault energy. The model that is described in paper B shares its basic features with the model in Cheng et al (2001). The dislocation density is explicitly computed via evolution equations and the yield limit is obtained from this density. The model is based on two deformation mechanisms: low-temperature plasticity by dislocation glide (limited by a lattice resistance and discrete obstacles) and power-law creep by dislocation glide or glide plus climb. These mechanisms are explained in Frost and Ashby (1982) and in Paper B.

The performance of constitutive models based on dislocation density depends to a high extent on the deformation mechanisms that are included in the model, if these mechanisms are well understood and if adequate equations are found to describe them. A review of the current state in physically based modeling of metal plasticity and the implementation of these models into FE codes are given in the work by Domkin (2005).
4 Friction modeling

Friction is a complex physical phenomenon that depends on parameters like material, surface roughness, lubrication, temperature and pressure. The effects of friction in metal-forming simulations are commonly accounted for either by Coulomb friction models or through constant shear friction models. These friction laws are available in most commercial FE codes.

The Coulomb model can be described by

\[ \| \sigma_t \| < \mu \sigma_n \quad \text{ (stick)} \]  
\[ \sigma_t = -\mu \sigma_n \cdot \hat{t} \quad \text{ (slip)} \]

where \( \sigma_t \) is the tangential (friction) stress, \( \sigma_n \) is the normal stress, \( \hat{t} \) is a tangential vector in the direction of the relative velocity and \( \mu \) is the friction coefficient (MSC.Software, 2005). One limitation of this model appears when the normal stress becomes large. Using the Coulomb model, it is possible to develop high frictional shear stresses and the model may not correlate well with experimental observations.

A common alternative to the Coulomb friction model is the shear friction model. In this model the frictional stress is a direct function of the material equivalent stress or flow stress. The shear friction model is characterized by

\[ \| \sigma_t \| < m \frac{\sigma}{\sqrt{3}} \quad \text{ (stick)} \]  
\[ \sigma_t = -m \frac{\sigma}{\sqrt{3}} \cdot \hat{t} \quad \text{ (slip)} \]

where \( \sigma \) is the equivalent stress and \( m \) the shear friction factor (MSC.Software, 2005).

The Coulomb friction model and the shear friction model have about the same popularity in extrusion simulations. The Coulomb model was used successfully by Sofuoglu and Gedikli (2004) and Arentoft (2000), among others. The shear type friction model was utilized, for instance, in the work by Zhou et al (2003), Libura et al (2005) and Damodaran and Shivpuri (2004). It is very difficult to determine the friction coefficient during extrusion experimentally. The estimates that are used in simulation of hot aluminum extrusion vary a lot. In the papers that are appended to this thesis, the Coulomb friction model has been adopted. The coefficient of friction is low, in the order of \( \mu \approx 0.02 \), in glass-lubricated steel extrusion.
5 Summary of appended papers

Three papers are appended with this thesis. A summary of each paper is given below.

5.1 Paper A

Extrusion of stainless steel tubes is here simulated using an axisymmetric FE model with thermo-dynamical coupling. The tools are modeled as rigid bodies with heat transfer properties. The material is assumed to be elastic-plastic with isotropic hardening and the von Mises yield criterion is used. The flow stress is predicted by a dislocation density-based material model for the austenitic stainless steel 316L, which is implemented in a user subroutine for the commercial FE code MSC.Marc. Temperature and strain rate dependency in the model is introduced by the concept of short-range and long-range interactions of dislocations and obstacles. The evolution equation for the dislocation density accounts for static and dynamic recovery controlled by diffusional climb and interactions with vacancies. The material model is calibrated by comparison with results from compression tests at different temperatures and strain rates. In total, five model parameters are found by curve fitting. The simulation results reveal that the billet is exposed to large temperature changes during the extrusion process. Extrusion force and exit surface temperature predicted by the extrusion model are in good agreement with experimental measurements obtained in a production press.

5.2 Paper B

In this paper, an advanced dislocation density-based model is formulated in order to describe the plastic behavior of the austenitic stainless steel AISI 316L from room temperature up to 1300 °C. The model is based on a coupled set of evolution equations for dislocation density and vacancy concentration. In contrast to the model used in Paper A and Paper C, this model includes the effect of diffusing solutes in an attempt to describe dynamic strain ageing. This model is applicable to a wider temperature range than is needed for extrusion simulations. The model requires 11 parameters to be determined from mechanical testing. These parameters are found by comparison with a set of compression tests using a custom optimization toolbox for Matlab. An extensive overview of the field of dislocation processes and modeling is given in this work. The paper also describes the numerical algorithm that is used to solve the strongly nonlinear relations efficiently. This numerical procedure is applicable for use in user subroutines in FE codes.

5.3 Paper C

In this paper, the extrusion model is extended to three dimensions. A thermo-mechanically coupled FE analysis of tube extrusion is carried out, using the same dislocation density-based material model for AISI 316L as in Paper A. A rotational symmetric problem is considered and only a quarter of the geometry is modeled. Discretization is performed using four-node tetrahedrons. The tube dimensions are changed a little compared to Paper A. A tube with larger wall thickness is used to make meshing and remeshing somewhat easier. The path of the metal flow, i.e. the shape of the glass pad, is determined by examination of cross sections of stickers. The extrusion force predicted by the three-dimensional model is compared to experimental measurements and numerical force predictions from axisymmetric, two-dimensional simulations. The results indicate that the
extrusion model is essentially correct but a very fine mesh would be needed to accurately predict the extrusion force in three dimensions using linear four-node tetrahedrons.

6 Discussion and future work

The aim of the current work is to model and simulate the process of stainless steel tube extrusion using the finite element method. A special request is to use the simulations for eccentricity studies, i.e. to evaluate the effect of certain process parameters on the final dimensions of the extruded tube. For this purpose the extrusion model must be fully three-dimensional. In the work presented in this thesis, extrusion has been modeled and simulated using two- and three-dimensional models with radial symmetry. These models are steps on the way towards a fully three-dimensional model and can also be very useful in product and process development.

The two-dimensional model has been shown to provide good and fast solutions to extrusion problems with radial symmetry. The computational times for these simulations are typically an hour or less, while a three-dimensional simulation often runs for a couple of days, even though symmetry is utilized. A two-dimensional model is sufficient in many applications and this model is planned to be used for solving processing problems further on.

In three dimensions, extrusion simulation is very computer intensive and still a challenging task. One of the problems is that there are few types of elements that can be used with remeshing in three dimensions in most commercial FE codes. Good remeshing routines for hexahedral elements would be very useful for this type of simulation. Another drawback is that global adaptive remeshing is not yet supported in parallel mode in the used FE code. This means that the computational times can not be reduced by use of multiple processors. It was shown in Paper C that a very fine mesh of four-node tetrahedrons would be needed to receive good results regarding the extrusion force for a rotational symmetric problem in three dimensions. To use this approach in a fully three-dimensional model would result in unacceptably long computational times. The future work will be aiming at improving the three-dimensional model in order obtain accurate results at reasonable computational times. The possibility to utilize other element types will be evaluated.

The work so far has been focused only on the austenitic stainless steel 316L and dislocation density-based material models. It is expected that these models can be extrapolated to a wider range of strains, strain rates and temperatures than more commonly used empirical models. This holds if the correct physical processes are described by the model and no new phenomena occurs. Extrusion is generally carried out at higher strain rates than can be used in mechanical laboratory tests and data from the mechanical tests have to be extrapolated. The use of physically based models in extrusion simulations is therefore motivated. The dislocation density-based model for AISI 316L could be improved and extended to include dynamic recrystallization and deformation twinning. Especially dynamic recrystallization should be important for extrusion purposes. Further on, more effort will be put on simulation of extrusion of other materials, for example duplex stainless steels.
The accuracy of the simulations depends on the assumed boundary conditions and how well these conditions describe the real process. Many process parameters, such as thermal and frictional conditions, are difficult to determine correctly. In the future it will be important to acquire more experimental data from the process. Additional experimental measurements will also be necessary for further validation of the models.

7 References


PHYSICALLY BASED MATERIAL MODEL IN FINITE ELEMENT SIMULATION OF EXTRUSION OF STAINLESS STEEL TUBES

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Summary

Stainless steel tube extrusion is a metal-forming process associated with large deformations, high strain rates and high temperatures. The finite element method provides a powerful tool for analysis of phenomena that occur during extrusion. In the present study, a dislocation density-based material model for the AISI type 316L stainless steel is implemented in a user subroutine for the commercial finite element code MSC.Marc. The model is calibrated using results from compression tests at different temperatures and strain rates. A thermo-mechanically coupled axisymmetric FE model is utilized to simulate the extrusion process. Model predictions of extrusion force and exit surface temperature are in good agreement with experimental values.

Keywords: physically based material model, extrusion, stainless steel, finite element

1 Introduction

Process simulation has become an important tool in design and development of extrusion and other manufacturing processes. A key obstacle is that the simulation of hot extrusion processes is quite difficult due to the significant deformations of the workpiece. To model the metal flow during extrusion, continuous remeshing is needed. Another main challenge when simulating manufacturing processes is to accurately model the material behavior. A good constitutive model, which correctly reflects the changes in material properties, is crucial to the reliability of the final simulation result. For processes associated with large deformations, high strain rates and high temperatures, such as extrusion, extrapolation from existing material data is often necessary. Physically based models [1,2] are of particular interest as it is expected that these models can more accurately describe the material behavior over a larger range of strains, strain rates and temperatures. Material parameter fitting can be simplified since data from other tests than mechanical testing can supply information.

In the present study, a dislocation density-based material model for the AISI type 316L stainless steel was implemented into a finite element code and applied to the stainless steel tube extrusion process. In order to validate the simulation results, exit surface temperature and extrusion pressure were measured during extrusion in a 14.5 MN extrusion press.
2 Stainless steel tube extrusion

The basic principle of extrusion is very straightforward. A billet is placed in a closed container and squeezed through a die to reduce the cross-section area and increase the length of the billet. The design of the die opening determines the cross-section of the extruded product. When extruding tubes, a mandrel is inserted in the middle of the die. Today, the most important method for steel extrusion is the Ugine-Séjournet process, where molten glass is used as lubrication [3]. The principles of this process are shown in Figure 1.

![Figure 1: Glass-lubricated tube extrusion.](image)

In glass-lubricated extrusion, there is a layer of glass between the billet and the container, between the billet and the mandrel, and between the billet and the die. Each heated billet is coated with powdered glass during transportation to the extrusion chamber. Glass powder is also applied inside the billet to assure good lubrication between billet and mandrel. Lubrication through the die is provided by a disc of compacted glass, the glass pad, which is placed between the billet and the die, see Figure 1. During extrusion, the glass pad is pressed against the die by the hot metal. The glass pad will deform with the billet and melt progressively to surround the extrusion with a lubricant glass film. The glass-lubricated extrusion process has been studied by Baqué, Pantin and Jacob [4] among others. Generally, it is quite difficult to predict the shape of the interface between the glass pad and the die. However, in FE analysis of extrusion, an assumption of the shape of the glass pad has to be done since it forms the die profile with the metal. One solution is to examine the butt of the extrudate to determine the path of the metal flow [5].

3 Methods and models

3.1 Mechanical testing

In order to calibrate the material model, compression tests were conducted over a temperature range of 1100-1300 °C at strain rates of 0.01, 1 and 10 s⁻¹. The experimental steel was of AISI type 316L, i.e. an austenitic stainless steel. The nominal chemical composition of the test material is given in Table 1. Cylindrical specimens of 10 mm diameter and 12 mm height were used for the hot compression tests.
The temperature was recorded during the test to see whether there was a temperature rise due to plastic dissipated energy.

**Table 1: Chemical composition of experimental steel (wt %).**

<table>
<thead>
<tr>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Cu</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.009</td>
<td>0.27</td>
<td>1.74</td>
<td>0.030</td>
<td>0.024</td>
<td>16.82</td>
<td>10.26</td>
<td>2.08</td>
<td>0.31</td>
<td>0.029</td>
</tr>
</tbody>
</table>

### 3.2 Material model

The yield limit is assumed to consist of two components:

$$\sigma_y = \sigma^* + \sigma_g$$,  \hspace{1cm}  (1)

where $\sigma^*$ is the friction stress and $\sigma_g$ is an athermal component. The friction stress accounts for the short-range interactions between dislocations and discrete obstacles. The process is thermally activated and characterized by the free energy, $\Delta F$, required to overcome the lattice resistance or obstacles without aid from external stress. Relation of the friction stress to the effective plastic strain rate, $\dot{\varepsilon}^p$, and temperature, $T$, is derived from the expression of the activation energy $\Delta F$ [2]. The classical Orowan equation is used for the dislocation velocity and the strain rate. The resulting expression can be written as

$$\sigma^* = \dot{\varepsilon}^p \left[ 1 - \left( \frac{kT}{\Delta F} \ln \frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0} \right)^{\frac{1}{q}} \right]^{\frac{1}{q}}$$,  \hspace{1cm}  (2)

where $\dot{\varepsilon}$ is the athermal flow strength and $k$ is the Boltzmann’s constant. The parameters $p$ and $q$ are chosen as 1. The reference strain rate, $\dot{\varepsilon}_0$, depends on the density of mobile dislocations and is assumed be constant. In the equation above, the non-dimensional parameters $\dot{\varepsilon}_0$ and $\Delta F$ are introduced as $\dot{\varepsilon} = \dot{\varepsilon}_0 G$ and $\Delta F = \Delta F_0 G b^2$, where $G$ is the shear modulus, and $b$ is the magnitude of the Burger’s vector.

The athermal component in Equation 1, $\sigma_g$, is a result of the long-range interactions with the dislocation substructure. It is expressed via the density of immobile dislocations, $\rho$, as

$$\sigma_g = m \alpha G b \sqrt{\rho}$$,  \hspace{1cm}  (3)

where $m$ is the average Taylor orientation factor and $\alpha = 1$ is a proportionality factor. To establish a relationship between dislocation density and plastic deformation, an evolution equation is utilized,
\[ \dot{\rho} = U \dot{\rho}^0 - \Omega \rho^2, \tag{4} \]

where \( U \) is the dislocation multiplication parameter, which can be related to the mean free path, \( \Lambda \), by \[6\]

\[ U = \frac{m}{b \Lambda}. \tag{5} \]

The remobilization parameter, \( \Omega \), accounts for the static and dynamic recovery controlled by diffusional climb and interactions with vacancies \[7\],

\[ \Omega = 2D_0^* \frac{Gb^3}{kT} = 2D_0^* \frac{c_{\infty}}{c_{\infty}^0} \frac{Q_v}{kT} \frac{Gb^3}{kT}. \tag{6} \]

Here, the self-diffusivity coefficient, \( D_0^* \), is related to the vacancy migration and vacancy self-diffusion, and \( Q_v \) is the combined activation energy of vacancy formation and vacancy migration. In the present formulation of the model, the vacancy concentration, \( c_{\infty} \), is assumed not to deviate from that of the thermal equilibrium at the current temperature, i.e. \( c_{\infty} = c_{\infty}^0(T) \).

The parameters of the model were obtained by fitting it to the compression tests introduced in the previous section. The values of the parameters are summarized in Table 2. The experimental yield stress curves and corresponding curves predicted by the model are presented in Figure 2. Predicted curves for the strain rate of 100 s\(^{-1}\) are also shown for comparison since such high strain rates are quite common in extrusion processes.

**Table 2: Model parameters for AISI 316L stainless steel.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burger’s vector, ( b )</td>
<td>2.58 \times 10^{-10} m</td>
</tr>
<tr>
<td>Athermal strength coefficient, ( c_0 )</td>
<td>0.003</td>
</tr>
<tr>
<td>Free energy coefficient, ( \Delta_0 )</td>
<td>0.6</td>
</tr>
<tr>
<td>Reference strain rate, ( \dot{\varepsilon}_{\text{ref}} )</td>
<td>( 10^6 ) s(^{-1})</td>
</tr>
<tr>
<td>Average Taylor factor, ( m )</td>
<td>3.06</td>
</tr>
<tr>
<td>Self-diffusivity coefficient, ( D_0^* )</td>
<td>4.15 \times 10^4 m(^2)/s</td>
</tr>
<tr>
<td>Vacancy activation energy, ( Q_v )</td>
<td>5.07 \times 10^{-19} J</td>
</tr>
<tr>
<td>Mean free path, ( \Lambda )</td>
<td>53 \times 10^{-6} m at ( T = 1100 )°C, 167 \times 10^{-6} m at ( T = 1300 )°C</td>
</tr>
</tbody>
</table>
The material model was implemented in the commercial finite element code MSC.Marc using the YIEL user subroutine, which computes the yield stress as a function of the current plastic strain, strain rate and temperature. In this context, the dislocation density is treated as an internal state variable and computed by numerical integration of the evolution equation.

3.3 FE model

The extrusion process was modeled with an axisymmetric FE model due to rotational symmetry in loading and workpiece. The implicit FE code MSC.Marc was used for the simulations. The behavior of the metal during extrusion was simulated in a thermo-mechanically coupled analysis. The extrusion process parameters and thermal initial conditions are summarized in Table 3. Since steady-state condition is the dominating phase in tube extrusion, only part of the total billet length was considered. The billet length considered was long enough to correctly simulate the start-up of extrusion until steady-state was obtained. The billet consisted of four-node quadratic elements together with a few three-node triangular elements. Due to the large deformations of the billet, the elements became heavily distorted and remeshing was required frequently during analysis. Automatic remeshing schemes, based on given remeshing criteria, are available in MSC.Marc and were used successfully.

The glass pad was modeled as a rigid surface with a constant temperature of 1100 °C. The shape of the glass pad is an approximation based on an earlier study where the amount of glass used during extrusion was weighed. In accordance with those measurements an assumed profile of the glass pad during extrusion was constructed. The other tools, i.e. die, container, mandrel and pressure pad, were modeled as rigid bodies with heat transfer properties. When glass lubrication is used, the metal flow is almost frictionless and a constant Coulomb friction coefficient of 0.03 was assumed at the above contact areas. Between the billet and the ram the friction factor was set to 0.35.

1 In the original published paper there is an error in Figure 2. The correct figure is shown here.
Table 3: Extrusion process parameters and initial conditions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Billet material</td>
<td>AISI 316L</td>
</tr>
<tr>
<td>Container, die, mandrel, ram material</td>
<td>AISI H13</td>
</tr>
<tr>
<td>Ram speed</td>
<td>93 mm/s</td>
</tr>
<tr>
<td>Container diameter</td>
<td>125.3 mm</td>
</tr>
<tr>
<td>Billet inner diameter</td>
<td>33 mm</td>
</tr>
<tr>
<td>Billet outer diameter</td>
<td>121 mm</td>
</tr>
<tr>
<td>Billet length</td>
<td>421 mm</td>
</tr>
<tr>
<td>Tube outer diameter</td>
<td>33.2 mm</td>
</tr>
<tr>
<td>Tube wall thickness</td>
<td>3.5 mm</td>
</tr>
<tr>
<td>Billet initial temperature</td>
<td>1150 °C</td>
</tr>
<tr>
<td>Die initial temperature</td>
<td>20 °C</td>
</tr>
<tr>
<td>Container initial temperature</td>
<td>200 °C</td>
</tr>
<tr>
<td>Mandrel initial temperature</td>
<td>100 °C</td>
</tr>
<tr>
<td>Ram initial temperature</td>
<td>20 °C</td>
</tr>
</tbody>
</table>

The surface and contact heat transfer coefficients were assumed to be 0.66 kW/m²/°C and 9 kW/m²/°C, respectively [8]. Thermal conductivity and specific heat capacity data for different temperatures were obtained from literature [9].

4 Results and discussion

The material model with the chosen parameter set somewhat underestimates the stress in the case of \( T = 1100 \, ^\circ\text{C} \) and rate = \( 10 \, \text{s}^{-1} \), see Figure 2a. The agreement with the other measured curves is satisfactory. The reason for the variation of the mean free path with temperature does not have an apparent physical foundation, but in terms of the presented model it accounts for a weaker hardening rate at higher temperatures. The values of the parameters found from curve-fitting are physically reasonable and in the same order of magnitude as those found in literature.

Figure 3: Plastic strain rate distribution in extrusion simulation.
After the start-up of the extrusion process, the metal flow conditions soon stabilized. In the FE simulation, steady state was reached within a ram travel distance of only 13 mm. During steady state, the maximum effective plastic strain rate in the deformation zone was approximately 240 s\(^{-1}\). The plastic strain rate distribution in the extrusion model is shown in Figure 3.

The billet temperature in the deformation zone increased markedly due to heat generation by the plastic deformation. A maximum temperature of 1290 °C was recorded. The back end of the billet, on the other hand, was heavily chilled due to contact with the tooling. Temperatures as low as 760 °C were observed. There are some uncertainties with this result. Heat transfer between the billet and the tooling was difficult to model due to large temperature gradients. These gradients resulted in discretization errors of temperature at the interface nodes. The heat transfer coefficients may also be outside the margin of error.

The exit surface temperatures, evaluated from the FE simulation, are shown in Figure 4 together with values obtained from experiments in a production extrusion press. 425 mm of extruded tube was considered in the numerical model. Temperatures from the FE model seem to agree quite well with the temperatures measured in the production extrusion press at the beginning of extrusion. The maximum difference in temperature between model and experiment was measured to 40 °C, which corresponds to an error of 3.2%. After 0.15 s, the difference between predicted and measured exit temperature was 22 °C. One source of this difference in temperature stems from the experimental measurements of the temperature profile since the sensitive nature of installing the optical pyrometer makes it susceptible to error. However, this exit surface temperature is the only temperature available for measurements during extrusion. There are also uncertainties in the model due to errors in the thermal initial conditions. The billet initial temperature, for example, is modeled as uniform, while in reality, temperature gradients exist.

![Figure 4: Exit surface temperature during extrusion.](image-url)
The extrusion force predicted by the FE model was 11.0 MN compared to the experimentally obtained value of 11.5 MN; a difference of approximately 4.4%, which must be considered acceptable. As mentioned earlier, the shape of the glass pad against the billet and the die needs further investigations and analyses. The underestimation of the force may also be due to the extremely low friction factor used.

5 Conclusions

The stress-strain curves of AISI 316L, obtained from compression tests at temperatures 1100 ºC and 1300 ºC, were well described by the dislocation density-based material model. Application to an axisymmetric FE analysis of glass-lubricated tube extrusion showed that the model performs well for these simulations. The extrusion pressure and the exit surface temperatures predicted by the FE model were in good agreement with the experimental measurements.

6 Acknowledgements

The financial support from the Swedish Knowledge Foundation (KK-stiftelsen) and the Swedish Steel Producers’ Association (Jernkontoret) is gratefully acknowledged.

7 References

Paper B
Dislocations, vacancies and solute diffusion in a physically based plasticity model for AISI 316L

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³Sandvik Materials Technology, 811 81 Sandviken, Sweden

1 Introduction

The description of material behaviour is crucial for all simulations of material deformation processes. The use of simulations to study manufacturing, [1, 2], includes additional complications due to the changing microstructure of the material. Therefore, it is preferable to use physically based models that can catch the essential phenomena dominating the deformation based on the underlying physics of the deformation, Kocks & Mecking [3], coupled to microstructure evolution. However, the models must still be tractable for large scale computations. Additional advantages of using physically based models is expected to be a larger domain of validity as well as the possibility to utilise other information from other sources than mechanical testing to determine the model parameters.

This study is part of a project aiming at developing a material model for describing the plastic behaviour of AISI 316L for a large range of temperatures, strains and strain rates. The material has fcc structure and a low stacking fault energy (SFE). The current scope is limited to temperatures from room temperature (RT) up to 1300°C, strains up to 0.6 and strain rates from 0.0005 up to 10 s⁻¹. This also includes the phenomenon of dynamic strain ageing (DSA). The paper gives an overview of the formulation and relevant publications. The model shares its basic features with the model in Cheng, Nemat-Nasser and Guo [4]. Some submodels are different and the effect of excess vacancies on diffusion processes is included. The chosen model is based on a coupled set of evolution equations for dislocation density and (mono) vacancy concentration. Furthermore, it includes the effect of diffusing solutes in order to describe DSA. The model parameters are calibrated by comparison with a set of compression tests. It has been decided to avoid adjusting physical quantities like diffusivities etc in the parameter fitting procedure.

The paper also describes the numerical algorithm used to solve these strongly nonlinear relations in an efficient manner applicable for user routines in finite element codes. The model has been formulated in a way that alleviates the replacements of different sub-models of the material model. Thus the proposed formulation is a platform for further development.

2 Overview of deformation behaviour

The inelastic deformation depends on the interaction between dislocations and the microstructure of the material. This structure is evolving during the deformation. Hardening as well as recovery processes may occur. This is also affected by the strain rate and temperature. The active mechanisms depend on the current structure of the material and applied stress or strain rate at the given temperature. An overview of the dominating deformation mechanisms can be outlined in a deformation map [5, 6]. The inelastic deformations that are of concern when constructing these maps [6] are shown in Table 1. The model presented in this paper is based on the dislocation mechanism, #2 and 4 in the table. The tests that are used to calibrate the model are compressive tests and the time scale of creep processes is not evaluated. It should be noted that twinning is not included in the current model.
Table 1. Mechanisms for inelastic deformations.

<table>
<thead>
<tr>
<th>#</th>
<th>Deformation mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Collapse at the ideal strength when the ideal shear strength is exceeded.</td>
</tr>
<tr>
<td>2</td>
<td>Low-temperature plasticity by dislocation glide: a) limited by a lattice resistance or Peierl’s stress; b) limited by discrete obstacles; c) limited by phonon or other drags; and d) influenced by adiabatic heating. This plasticity is mainly obstacle-limited in the case of austenitic stainless steels [5].</td>
</tr>
<tr>
<td>3</td>
<td>Low-temperature plasticity by twinning</td>
</tr>
<tr>
<td>4</td>
<td>Power-law creep by dislocation glide or glide plus climb: a) limited by glide processes; b) limited by lattice-diffusion controlled climb (high-temperature creep); c) limited by core-diffusion controlled climb (low-temperature creep); d) power-law break down creep at transition from dislocation glide plus climb to glide alone at higher stresses; e) Harper-Dorn creep; and f) creep accompanied by dynamic recrystallisation.</td>
</tr>
<tr>
<td>5</td>
<td>Diffusional flow: a) limited by lattice diffusion (Nabarro-Herring creep) at higher temperatures; b) limited by boundary diffusion (Coble creep) at lower temperatures; and c) interface-reaction controlled diffusional flow.</td>
</tr>
</tbody>
</table>

3 Dislocation density model

3.1 Physically based models

Physically based models are formulated on the underlying physical processes causing the deformation in contrast to empirical models of a more curve-fitting nature. Due to the need for averaging and also limited knowledge some relations for these processes may be phenomenological. Two different types of physically based models exist. One option is to explicitly include the physical model as an evolution equation in the constitutive model. This is the approach in the current paper. The other possibility is to determine the form of the constitutive equation based on knowledge about the physical process causing the deformation. The latter is a so-called “model-based-phenomenology”, Frost and Ashby [6]. The same hardening model can be obtained from empirical models and models based on dislocation mechanisms as in the case of power law creep. However, in general it is expected that the physically based models can have a larger range of validity than purely empirical equations that do not consider the underlying physical process.

The focus in this study is on dislocation density models that can be used to describe the hardening behaviour of the material. The evolution of the flow stress during the deformation determines the isotropic hardening of the material. We will not account for back-stresses, kinematic hardening, in this study.

3.2 Plasticity and dislocations

The current study uses the concept of rate-independent plasticity and a yield surface. It is an approximation where the plastic strains are assumed to develop instantaneously in such a way that the stress state stays on the yield surface during a plastic process. The applied stress is then equal to the yield stress during a plastic deformation. The processes that determine this yield surface are rate-dependent. Therefore, we will have a rate-dependent yield limit applied in the context of rate-independent plasticity.

The yield limit is assumed to consist of two components [7].

\[ \sigma_y = \sigma_G + \sigma^* \]  (1)
where \( \sigma_v \) is due to long-range interactions with the dislocation substructure. It is an athermal stress contribution. The second term, \( \sigma^* \), is the short-range interactions. It is a friction stress needed to move dislocations through the lattice and to pass short-range obstacles. Thermal vibrations can assist the stress to overcome these obstacles.

The long-range term in Eq. (1) is written as

\[
\sigma_v = m \alpha G_b \sqrt{\rho}
\]

where \( m \) is the Taylor orientation factor translating the effect of the resolved shear stress in different slip systems into effective stress and strain quantities. It depends on the crystal structure and is affected by texture. It is assumed to be constant and is 3.06 for fcc crystals \[8\]. \( \alpha \) is a proportionality factor, \( \rho \) is the dislocation density and \( G \) is the temperature dependent shear modulus. We will assume \( \alpha \) to be constant although it is known to depend on the dislocation substructure \[9\]. This dependency is not so important \[3\]. We will ignore the temperature dependency of Burger’s vector \( b \). Variants of Eq. (2) have been used when different dislocations densities are accounted for \[10-14\]. The model for the evolution of the dislocation density needed for Eq. (2) is formulated in the next section.

The second term in Eq. (1), the short-range stress component, is obtained as described below. The dislocation velocity is related to the plastic strain rate via the Orowan equation

\[
\dot{\varepsilon} = \frac{m b \nu}{m} \varepsilon_{\text{eff}}
\]

where \( \varepsilon_{\text{eff}} \) is the effective stress due to the applied load, \( \sigma_v \) is long-range stresses. The form of the function \( f \) and \( \Delta G \) depend on the stresses, type of obstacle etc. The stress available to move the dislocation is thus the applied stress minus the long-range flow stress component. The effective stress is assumed, in the theory of plasticity, to be equal to the flow stress during the deformation

\[
\bar{\sigma} = \sigma_y
\]

and then Eq. (1) gives

\[
\sigma^* = \sigma_y - \sigma_v
\]

Combining Eq.s (6-8) gives
The short-range stress component of the yield stress requires a model that determines $f$ and $\Delta G$. This is discussed in chapter 3.4.

The flow stress variation with the control variables temperature, strain and strain-rate is further complicated by dynamic ageing. It is due to diffusion of solute atoms that affects the plastic deformation. Several mechanisms are proposed based on drag effects on moving dislocations and thereby the short-range stress component or the pinning of dislocations and thereby the long-range stress component [10, 18-20]. Probably, both phenomena are present simultaneously. The latter effect is chosen for the model in this study and the phenomenon is discussed in chapter 3.4.

Models for the dislocation evolution are discussed next and thereafter models for the short-range component are described.

### 3.3 Evolution of density of immobile dislocations

The direct simulation of the process, in the spirit of discrete dislocation dynamics, is costly to compute. Hence, an average treatment of dislocation processes is favourable, and the concept of dislocation density is found useful. The dislocation density based models are formulated at the macro level, i.e. all the quantities (like dislocation densities, flow stress etc) are calculated for a representative material volume that can be considered homogeneous. Every dislocation model considers at least two different densities, mobile and immobile dislocations. That is the case for the model by Bergström [8, 21-23] and this is also the case in the current study. Zikry [24] traces evolution of the dislocation densities in different slip systems and their interactions and effect on the long-range stress component, Eq. (2). Mughrabi [13, 14] and Estrin [25] use two types of densities for immobile dislocations, channels and walls. They can also accommodate cell size and width as variables to describe hardening behaviour or, as in [26], cell area density and cell fraction. The channels are low density volumes whereas the walls are dense dislocation walls in the substructure created by the dislocations. They have separate, and coupled, evolution equations. A similar approach was also used by Nes [10]. This split into two different densities for immobile dislocations corresponds to the use of separate densities for statistically stored dislocations (SSD) and geometrically necessary dislocations (GND) that have separate evolution equations [27, 28]. SSD is the minimum density of dislocations needed to accommodate a given strain gradient and GND represents dislocations that are needed to preserve lattice compatibility [29]. They accumulate near grain boundaries whereas the SSD are stored in grain interiors. Evers et al. [30, 31] used an model with GND and SSD for each slip direction and a complex model for their interaction. Mugrabi [32] discusses the association with SSD and GND densities with gradient plasticity models. Seefeld and Klimanek [33] set up a coupled set of differential equations for mobile and immobile dislocations combined with disinclination densities.

The use of two different densities for immobile dislocations is used to model back-stress and pertaining kinematic hardening in [34, 35]. Peeters et al. [36, 37] introduced a third type of directional sensitive dislocation density in order to include the effect of deformation path changes.

The basic evolution equations for different dislocation densities do all have the same characteristics, storage and recovery processes. This kind of evolution equation is derived for each type of dislocation density. They may be expressed in the form of “hardening term – recovery term”

$$\dot{\rho}_i = \dot{\rho}_i^{(+)} - \dot{\rho}_i^{(-)}$$  \hspace{1cm} (10)

where $\rho_i$ denotes a specific dislocation density. In the following we have $i=m$ for mobile dislocations and $i=i$ for immobile dislocations.
The model used in the current approach [8, 21, 22, 38] is based on the assumption that the mobile dislocation density is stress and strain independent and much smaller than the immobile one [4, 12, 39]. This is expressed as

\[ \rho = \rho_i + \rho_n \]
\[ \rho_n \ll \rho_i \]  \hspace{1cm} (11)

\[ \frac{\partial \rho_n}{\partial \sigma} \approx 0, \quad \frac{\partial \rho_n}{\partial \varepsilon^p} \approx 0 \]

Thus transients when changing stress [15, 17] that are associated with changes in the mobile dislocation density, like Lüder's band formation, can not be modelled with the assumptions above.

The immobile dislocation density is used in Eq. (2) for the long-range stress contribution to the flow stress.

\[ \sigma_0 = m a G b \sqrt{\rho_i} \]  \hspace{1cm} (12)

We will in the following describe the evolution equations for the density of immobile dislocations, \( \rho_i \). The initial dislocation density is denoted as \( \rho_i(0) = \rho_{i0} \).

### 3.3.1 Hardening

It is assumed that mobile dislocations move, on average, a distance (mean free path), \( \Lambda \), before they are immobilised or annihilated. The density of mobile dislocations and their average velocity are related to the plastic strain rate according to Eq. (3). The increase in the immobile dislocation density is also assumed to be proportional to the plastic strain rate [8, 11, 40-42]

\[ \rho_i^{(c)} = \frac{m}{b} \frac{1}{\Lambda} \dot{\varepsilon}^p \]  \hspace{1cm} (13)

where \( m \) is the Taylor orientation factor, 3.06 for fcc crystals [8]. This factor is evolving with the deformation but is assumed to be constant in the current model. The mean free path, \( \Lambda \), is assumed to be a combination of the distance between grain boundaries, \( g \), and dislocation subcell or subgrain diameter, \( s \),

\[ \frac{1}{\Lambda} = \left( \frac{1}{g} + \frac{1}{s} + \text{others} \right) \]  \hspace{1cm} (14)

where “others” denotes contributions from varying types of obstacles like precipitates [43] or the distance between martensite lathes [44]. The initial grain size is \( g_0 \) and it is assumed to be constant in the current model. Models for recrystallisation and grain growth can be included and used to modify the grain size term in Eq. (14). The effect of grain size on flow stress, the Petch-Hall effect, is accounted for via this equation and its effect depends on whether it will be masked by the other terms or not [45, 46]. Karaman et al. [47] consider twins as permeable obstacles to dislocations although they included this effect in a separate term and not via Eq. (14).

The formation and decrease in size of subcells is one sequence of dislocation patterns that are formed during straining [48]. Holt [49] derives a relation between dislocation subcell diameter and dislocation density

\[ s = K_s \frac{1}{\sqrt{\rho_i}} \]  \hspace{1cm} (15)

The analysis by Holt also indicates the approximate value of the parameter \( K_s \) by relating the dislocation density to the long-range stress component, Eq. (2), and plotting this for a number of
materials. Holt [49] states that the Eq. (15) is not valid when the dislocation mobility is low or when it is high.

The subcell formation is a complex process in which dislocations form different low energy structures [34, 35, 50, 51]. Despite these complications the relation proposed by Holt has been found to be useful, e.g. [52, 53]. Michel et al. [54] found $K_c$ to be 16 for AISI 316 from room temperature up to 816ºC. Raj and Pharr [55] analysed a large amount of data and noticed that there is a support for a linear relation between flow stress and subcell size in many cases. They evaluated a somewhat more general relation

$$s = K_c \frac{1}{\rho_i^{n/2}}$$

(16)

The best fit to data gave the exponent $n$ the value of 0.84. A statistical correlation was found between $K_c$ and $n$

$$\log K_c = -3.0n + 4.37 - \log[(am)^{b^{-1}}]$$

(17)

However, their analysis of the uncertainties in data lead Raj and Pharr to recommend the use of $n=1$. Thus, they obtained Eq. (15) and a $K_c$ in the same order as Holt [49]. Raj and Pharr [55] noticed that the case of austenitic stainless steel AISI 316 from [56] was a clear exception with $n=1.52$. Kuhlmann-Wilsdorf [45] discusses the microstructure evolution and, of particular interest in this study, how material with fcc structure first forms a Taylor lattice that becomes a carpet structure and then a cell structure. The Taylor lattice has long glide paths, i.e. a large $K_c$ in Eq. (15). One discussed example is $\alpha$-brass with $K_c=250$. Hansen [57] draws the conclusion that, due to the complex geometry of formed cells or subgrains, $K_c$ should not be considered as a true constant. The review by Gil Sevillano et al. [9] states that larger strains are required to develop a cellular substructure and that a decrease in stacking fault energy (SFE) or temperature or a higher strain rate gives a more uniform dislocation distribution in fcc materials compared to bcc materials. Higher SFE and higher temperatures give larger cells [58]. Furthermore, they observed that the complexity in the substructure formation in low SFE metals [59] accounts for the lack in quantitative data to be used to formulate models. The temperature influence is small until it reaches about half homologous temperature. The deformation changes character from planar slip to cross-slip as the stacking fault increases with increasing temperature [60]. It was also noted in [60] that cell formation is difficult for strain below 0.25 and also that planar slip was found at 823 K due to dynamic strain ageing (DSA).

We, like in [61], consider $s$ to be a characteristic length in general applicable for other dislocation substructures than cells. It describes the effect of the dislocation structure on the mean free path of a dislocation and may therefore not directly be related to a geometric measure. This can also be motivated from the observations that a glide dislocation may pass several cells before it is trapped [3, 62]. Seefeld and Klímanek [33] also includes a factor for the probability that a dislocation is trapped in a cell wall. The parameter $s$ is taken as a combination of a geometric measure between obstacles to dislocation motion and their strength. One possibility is to use Eq. (15) and allow the value of $K_c$ to depend on temperature and plastic strain rate in an ad-hoc manner in lack of models for substructure formation. Thus strain rate and temperature will affect the dislocation storage via this part of the model. This was noted by Gil Sevillano et al. [9] as a deficit of the original proposal by Bergström. In this study we will assume that $K_c$ is dependent on temperature only. We also introduce a lower limit for the subcell size, $s_\ell$, and then Eq. (15) is written as

$$s = K_c \frac{1}{\sqrt{\rho_i}} + s_\ell$$

(18)
3.3.2 Recovery

Different processes may contribute to the reduction in the dislocation density. The formulations by Bergström [8] and Estrin [41], for example, lead to a remobilisation of dislocations proportional to the current immobile dislocation density

\[ \rho_i^{(c)} = \Omega \rho_i^{\ast} \]  

(19)

where \( \Omega \) is a recovery function. This kind of models can only accommodate dynamic recovery due to the strain-rate term in Eq. (19). Engberg [63] reviews different models for recovery that also can be used for static recovery. and Nes [10] formulates a recovery proportional to \( \rho_i^{\ast} \) with cross-slip controlled recovery having \( x=1 \) and climb controlled having \( x=2 \). Li [64] assumes diffusional climb controlled recovery leading to a formulation in the format

\[ \rho_i^{(c)} = \Omega (\rho_i^2 - \rho_{eq}^2) \]  

(20)

where \( \rho_{eq} \) is an equilibrium value towards which the density decreases.

Siwecki and Engberg [43] use a model for the recovery by climb accounting for the interaction with vacancies [65]. If the inclusion of the effect of precipitates is excluded from the model in Siwecki and Engberg [43], then it can be written as

\[ \rho_i^{(c)} = c_c D_m \frac{Gh^3}{kT} \rho_i^2 \]  

(21)

where \( c_c D_m \) is a product of the fraction of vacancies, \( c_c \), and the diffusivity of migration, \( D_m \), and \( c_c \) is a material parameter.

Militzer et al. [66] use a quite similar formulation based on Sandström and Lagneborg [40] and Mecking and Estrin [67] with a modification of the diffusivity that is consistent with the formulation in chapter 3.5,

\[ \rho_i^{(c)} = 2D_c \frac{c_c}{c_c^0} \frac{Gh^3}{kT} \rho_i^2 = 2D_c \frac{c_c}{c_c^0} \frac{Gh^3}{kT} \rho_i^2 \]  

(22)

where \( c_c^0 \) is the thermal equilibrium vacancy concentration. The model in Lúkac and Balik [68] for climb recovery can be reformulated to a similar expression and with a multiplying parameter, like \( c_c \) in Eq. (21), that must be fitted with experiments.

The model in Eq. (22) is combined with Eq. (20) to give

\[ \rho_i^{(c)} = 2D_c \frac{c_c}{c_c^0} \frac{Gh^3}{kT} \left( \rho_i^2 - \rho_{eq}^2 \right) \]  

(23)

Solid-solution for steels like 316L may reduce the possibility for partial dislocations to unite in order to climb. This is believed to be, in co-operation with formation of fine subgrains, a reason for the high creep strength of 18-8 austenite stainless steel [62, 69, 70]. The creep rates are reduced [62] with a factor of

\[ (\gamma/Gh)^{0.3} \]  

(24)

where \( \gamma \) is the stacking-fault energy. The stacking fault energy for 316 is 23 ml/m² [71]. Therefore, we introduce a material parameter into Eq. (23) in the same way as in Eq. (21) giving

\[ \rho_i^{(c)} = 2c_c D_c \frac{c_c}{c_c^0} \frac{Gh^3}{kT} \left( \rho_i^2 - \rho_{eq}^2 \right) \]  

(25)
The difference between this expression and Eq. (21) is the temperature dependent equilibrium vacancy concentration, \( c_v^e \), discussed later.

### 3.4 Mobile dislocations

The short-range stress is the component of the flow stress that moves the mobile dislocations through the lattice with its obstacles etc. There is the resistance of the lattice itself, the Peierl’s stress \[72\], which is not believed to be the controlling factor for fcc metals \[12, 15\]. Schoeck \[15\] notices that the different models used for thermal activation all lead to a reaction rate of the form of Eq. (9),

\[
\tilde{\dot{\varepsilon}}^p = f(\sigma^*) e^{-\Delta G/kT}
\]

[Frost and Ashby \[6\] discuss different mechanisms controlling the dislocation glide in a crystal structure. A general formula for the activation energy, also in \[73, 74\], is

\[
\Delta G = \Delta F \left[ 1 - \left( \frac{\sigma^*}{\dot{\varepsilon}} \right)^p \right]^q
\]

(26)

\( \Delta F \) is the free energy required to overcome the lattice resistance or obstacles without aid from external stress. The quantity \( \dot{\varepsilon} \) is the athermal flow strength that must be exceeded in order to move the dislocation across the barrier without aid of thermal energy. It reflects not only the strength but also the density and arrangement of the obstacles. The conditions for the exponents in Eq. (26) are

\[
0 \leq p \leq 1
\]

\[
1 \leq q \leq 2
\]

(27)

The stress dependency in the pre-exponential term \( f(\sigma^*) \) in Eq. (9) can be ignored when the activation energy is large. It arises from the variation of the mobile dislocation density \[6, 17, 42\] and thus assuming it is constant is consistent with the assumption of stress independent mobile dislocation density in Eq. (5). It is assumed in this study, like in \[16, 42, 73, 75\], that this is the case for the deformation process that has the largest contribution to the friction stress. The function \( f(\sigma^*) \) is then treated as a constant and Eq. (9) can be combined with Eq. (26) to

\[
\tilde{\dot{\varepsilon}}^p = \tilde{\dot{\varepsilon}}_{ref} e^{\frac{\Delta F}{kT} \left[ \left( \frac{\sigma^*}{\dot{\varepsilon}} \right)^p \right]^q}
\]

(28)

where the reference strain rate, \( \tilde{\dot{\varepsilon}}_{ref} \), is constant as motivated above. Comparing with Eq. (5) gives that

\[
\tilde{\dot{\varepsilon}}_{ref} = \frac{\rho_s A b \nu_a}{m}
\]

(29)

Eq. (28) can be rewritten to give the friction stress as a function of the effective plastic strain rate

\[
\sigma^* = \tilde{\dot{\varepsilon}} \left( 1 - \left( \frac{kT}{\Delta F} \ln \left( \frac{\tilde{\dot{\varepsilon}}_{ref}}{\tilde{\dot{\varepsilon}}^p} \right) \right)^{1/p} \right)^{1/q}
\]

(30)

Nemat-Nasser and Guo \[73\] used the values \( p=2/3 \) and \( q=2 \). Uenishi and Teodosiu \[16\] used \( p=1/2 \) and \( q=1 \) and Follansbee \[75\] used \( p=1/2 \) and \( q=3/2 \). The influence of the coefficients \( p \) and \( q \) is small when the activation energy \( \Delta F \) is large \[6\] as in the case of obstacle limited dislocation glide. Therefore Frost and Ashby \[6\] propose the values \( p=q=1 \), which is also used in
this study. Table 2 lists approximate ranges for the activation energy and athermal strength for different obstacles. This study utilises only one obstacle activation energy although there may exist a range of obstacles of various types [76].

Table 2. Activation energy for different obstacles (from [6]).

<table>
<thead>
<tr>
<th>Obstacle strength</th>
<th>$\Delta F$</th>
<th>$\dot{\tau}$</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong</td>
<td>$2Gb^3$</td>
<td>$\frac{Gb}{l}$</td>
<td>Dispersions; large or strong precipitates (spacing $l$)</td>
</tr>
<tr>
<td>Medium</td>
<td>$0.2-1.0Gb^3$</td>
<td>$\simeq \frac{Gb}{l}$</td>
<td>Small or weak precipitates (spacing $l$)</td>
</tr>
<tr>
<td>Weak</td>
<td>$&lt;0.2Gb^3$</td>
<td>$&lt;\frac{Gb}{l}$</td>
<td>Lattice resistance; solution hardening (solute spacing $l$)</td>
</tr>
</tbody>
</table>

The stress needed for moving the dislocation in the lattice with different short-range obstacles is further influenced by dynamic strain ageing (DSA) or the Portevin-Le Chatelier effect (PLC). Then [4, 7, 77-80] presence of solute atoms can influence the stress needed to move the dislocations. The solute atoms can also affect the immobilisation and remobilisation of dislocations [41]. This was utilised by Bergström [38] and van Liempt et al. [23] to model strain-ageing by changing the evolution im mobile dislocation density. Their approach is not used in the current study.

If the dislocation velocity is low, i.e. the plastic strain rate is small, then the solute atoms can move with the dislocation without any problem. When the strain rate is higher, then there is an additional stress that must be overcome to move the dislocation. When the dislocation moves even faster, then the solute atoms are passed like fixed obstacles and the drag stress is reduced. DSA can be manifested as peaks or plateau in the variation of flow stress with temperature and negative strain rate sensitivity (SRS). It exhibits itself as serrations on the stress-strain curve. The aim in the current study is only to be able to represent the global response and not these serrations.

The DSA effect is believed to be caused by diffusion of C and N atoms but also by the solutes Cr and Ni at higher temperatures [78, 80, 81]. Cheng et al. [4] modified the $\dot{\tau}$ and $\Delta F$ in Eq. (30) for the activation energy whereas Rizzi and Hähner [77] added a transient term to the activation energy in order to model DSA. Both approaches give an increase in flow stress when the strain rate is low, in relation to the diffusion of solute atoms. None of the models do account for the observed influence of accumulated strain [80, 82] for triggering DSA. The model by Cheng et al. [4] modified the $\dot{\tau}$ and $\Delta F$ in Eq. (30) by

$$\dot{\tau} = \dot{\tau}_0 \sqrt{\frac{c^\gamma}{c_0^\gamma}} \sqrt{\frac{\rho}{\rho_0}}$$

(31)

and

$$\Delta F = \Delta F_0 \sqrt{\frac{c^\gamma}{c_0^\gamma}}$$

(32)

where $c^\gamma$ is the solute concentration, $\gamma$ denotes the solute atom, of the dislocation and $c_0^\gamma$ is the bulk solute concentration corresponding to the evaluated $\Delta F_0$. Eq. (31) is further simplified by
removing the effect of bowing out of the dislocations accounted for by the dislocation density term $\sqrt{\rho/\rho_0}$. Then the expression will be identical to the original equation when $c^\gamma = c^\gamma_{ref}$. We introduce the following scaling of the obstacle parameters

$$\tilde{c} = \tau G \frac{c^\gamma}{c^\gamma_{ref}}$$  \hspace{1cm} (33)$$

and

$$\Delta F_0 = \Delta f Gb^3 \frac{c^\gamma}{c^\gamma_{ref}}$$  \hspace{1cm} (34)$$

Thus we will use

$$\sigma^* = \tau G \frac{c^\gamma}{c^\gamma_{ref}} \left( 1 - \frac{kT}{\Delta f Gb^3} \ln \left( \frac{\dot{c}^\gamma_{ref}}{c^\gamma_{ref}} \right) \right)$$  \hspace{1cm} (35)$$

Diffusion of solutes for obtaining $c^\gamma$ is discussed in chapter 3.6. There is a lower limit of the plastic strain rate in this model giving zero friction stress. It is

$$\dot{\varepsilon}_{min} = \dot{\varepsilon}_{ref} \frac{\Delta G_0}{kT} \frac{c^\gamma}{c^\gamma_{ref}}$$  \hspace{1cm} (36)$$

### 3.5 Vacancy migration and generation

The existence and motion of vacancies is coupled with the recovery of dislocations as well as the diffusion of solute atoms. Creation of vacancies increases the entropy but requires energy. This leads to an equilibrium level of vacancies when a crystal is retained a sufficient time at a given temperature. Changing the temperature or deforming the material generates excess vacancies. The models considered here are only concerned with mono-vacancies. Haasen [12] gives a coupled set of evolution equations for vacancies and divacancies. However, that formulation does not account for generation of vacancies by plastic deformation.

The relation for the equilibrium concentration at a given temperature is [7, 12]

$$c_{eq}^V = e^\frac{Q_v}{kT} \frac{\dot{Q}_v}{\dot{Q}_\nu} = c_{eq}^V e^\frac{Q_v}{kT}$$  \hspace{1cm} (37)$$

where $Q_v$ is the activation energy for forming a vacancy and $\Delta S_{eq}$ is the increase in entropy when creating a vacancy.

The self-diffusion coefficient can be written as [7]

$$D_v = a^2 \nu e^\frac{\Delta S_{eq}}{k} \frac{Q_v}{\dot{Q}_\nu} = D_{eq} e^\frac{Q_v}{kT}$$  \hspace{1cm} (38)$$

where $a$ is the lattice constant, $\nu$ is the lattice vibration frequency, $\Delta S_{eq}$ is the entropy increase and $Q_{eq}$ is the energy barrier for the jumping of an atom into a vacancy. The parameters given in the last equality in Eq. (38) are those obtained from measurements. Using Eq. (37) the self-diffusivity can be written as
Thus the self-diffusivity is proportional to the equilibrium concentration of vacancies. We assume that the diffusivity at non-equilibrium vacancy concentrations can be written as

\[ D'_v = \frac{c}{c_{eq}} D \]  

(40)

The vacancy migration is used in the model below for vacancy annihilation. It is the part of the self-diffusion associated with the motion of existing vacancies. Thus it is written as

\[ D_{vm} = a' \nu e\frac{c}{c_{eq}} = D_{vo} e\frac{c}{c_{eq}} \]  

(41)

The model in Siwecki and Engberg [43] for vacancy generation and recovery is written as

\[ \dot{c}_v = [c_i b \kappa - c_c \dot{c}_c, D_c (c_c - c_c^eq)] \sqrt{\rho} \]  

(42)

Militzer et al. [66] use a similar model

\[ \dot{c}_v^eq = \dot{c}_v - \dot{c}_v^eq = \left[ \chi \frac{b h}{Q_s} + \zeta \frac{c_i}{4b^3}, \frac{\Omega_0}{b} \right] \frac{\dot{\sigma}}{\kappa^2} - D_{vo} \left( \frac{1}{\kappa^2 + \frac{1}{g^2}} \right) (c_c - c_c^eq) \]  

(43)

where \( \Omega_0 \) is the atomic volume and \( c_i \) is the concentration of thermal jogs. The term \( \kappa \) depends on the subcell formation of the dislocations and can from [67] be found to be

\[ \kappa = K_c \]  

(44)

We therefore rewrite the equation by introducing the subcell size, \( s \), from Holt’s relation discussed earlier. This gives

\[ \dot{c}_v^eq = \dot{c}_v - \dot{c}_v^eq = \left[ \chi \frac{b h}{Q_s} + \zeta \frac{c_i}{4b^3}, \frac{\Omega_0}{b} \right] \frac{\dot{\sigma}}{\kappa^2} - D_{vo} \left( \frac{1}{\kappa^2 + \frac{1}{g^2}} \right) (c_c - c_c^eq) \]  

(45)

The factor \( \chi \) in the mechanical production term, \( \chi \sigma \dot{\sigma} \), is the fraction of the mechanical work spent for the vacancy formation [67]. Militzer et al. assume

\[ \chi \approx 0.1 \]  

(46)

The concentration of thermal jogs is given by

\[ c_j = \sqrt{\frac{Q_s}{\Omega_0}} \]  

(47)

where the formation energy is approximated as

\[ Q_s = \frac{Gb^3}{4\pi(1-v)} \]  

(48)

and \( v \) is Poisson’s ratio.

The parameter \( \zeta \) describes the neutralisation effect by vacancy emitting and absorbing jogs. It is given as

\[ \zeta = \begin{cases} 
0.5 - \zeta_0 c_j & \text{if } c_j \leq 0.5/\zeta_0 \\
0 & \text{if } c_j > 0.5/\zeta_0 
\end{cases} \]  

(49)
The rate of change in equilibrium concentration in Eq. (43) is only due to change in temperature

\[ \dot{c}_v^{eq} = c_v^{eq} \left( \frac{Q_v}{T^2} \right)^T \]  

We assume that the stress in Eq. (43) is equal to the effective stress, which is equal to the flow stress during a plastic deformation. Then we have

\[ \dot{c}_v^{eq} = \left[ \frac{\sigma}{Q_v} + \frac{\gamma}{Q_v} \right] \frac{\Omega}{b} \dot{\gamma} - D_{\text{eff}} \left( \frac{1}{s} + \frac{1}{g} \right) \left( c^* - c_v^{eq} \right) \]  

This equation is chosen as the model for vacancy generation and recovery. Further simplification makes it possible to relate to the model in Eq. (42). Excluding the effect of thermal jogs, taking Eq. (12) and ignoring the short-range component of the flow stress leads to

\[ \dot{c}_v^{eq} = \frac{\alpha G \Omega}{Q_v} b \tilde{\gamma} \sqrt{\rho_c} - D_{\text{eff}} \left( \frac{1}{s} + \frac{1}{g} \right) \left( c^* - c_v^{eq} \right) \]  

The first part in the first term above can be directly identified with \( c_1 \) in Eq. (42). The second term has a similar structure as the second term in Eq. (42).

An additional remark can be made regarding Eq. (52). Militzer et al. [66] refer to Mecking and Estrin [67]. The latter reference also supports the possibility to relate the recovery term of the vacancy concentration with the mean free path of a moving dislocation, Eq. (14). Then one could also write

\[ \dot{c}_v^{eq} = \frac{\alpha G \Omega}{Q_v} b \tilde{\gamma} \sqrt{\rho_c} - D_{\text{eff}} \left( \frac{1}{s} + \frac{1}{g} \right) \left( c^* - c_v^{eq} \right) \]  

### 3.6 Diffusion of solutes

The diffusion of solute atoms affects the motion of dislocations as discussed earlier. In the studied material the largest amount of solute atoms are Cr and Ni. The diffusivity is affected by the deformation due to creation of vacancies and dislocations [83-87]. The latter is called pipe diffusion. Diffusion is also easy along grain boundaries. The relative effects of the different contributions from lattice, pipe and grain boundary diffusion vary with temperature as they have different activation energies. However, the effect of solutes on mobile dislocations is only dependent on lattice diffusion as they only move within a grain or subcell before they are immobilised.

The equation for the temperature dependency of the diffusion is

\[ D_l^\gamma = D_0^\gamma e^{\frac{Q_l^\gamma}{RT}} \]  

where \( l \) denotes lattice diffusion and \( \gamma \) is a symbol for the diffusing atom. Diffusivities are measured at an equilibrium value of vacancies and we assume similar to the Eq. (40) that it increases linearly with the vacancy concentration as

\[ D_l^\gamma = \frac{c_v^{eq}}{c_v^{eq}} D_l^\gamma \]  

The diffusion of the solute atoms into the dislocations is dependent on two time scales. The characteristic time of the diffusion process is denoted \( t_D \). The dislocation motion is characterised
by the waiting time at obstacles, $t_w$. Assuming the time of flight between obstacles is negligible and using Eqs (3) and (29) give

$$t_w = \frac{\Lambda}{\bar{F}} = \frac{\dot{\epsilon}_{\text{ref}}}{\bar{F} \mu} \tag{56}$$

The characteristic time for diffusion of solutes is assumed to be [4]

$$t_0 = \frac{1}{KD_{\gamma}^*} \tag{57}$$

where $D_{\gamma}^*$ is proportional to the vacancy concentration, Eq. (55). $K$ is a parameter to be determined. The influence of the interaction energy between the solute and the dislocation is only accounted for via $K$. The evolution equation for the solute concentration is taken from [4]

$$c' = c_0' + \left(c'_0 - c_0\right) \left[1 - \exp\left(-\left(h_0 \frac{t}{t_0}\right)^\xi\right)\right] \tag{58}$$

where $c'_0$ is a saturation value, $c_0'$ is the bulk concentration of the solute in [4] and $h_0$ is a parameter to be determined. $\xi$ is $1/3$ for pipe diffusion along dislocation line and $2/3$ for volume diffusion in the lattice, which is the case in the DSA model. The assumption in Eq. (57) makes it possible to write

$$c' = c_0' + \left(c'_0 - c_0\right) \left[1 - \exp\left(-\left(h D_{\gamma}^* t_s\right)^\xi\right)\right] \tag{59}$$

where $h$ is a combination of $h_0$ and $K$. The Burgers vector is introduced in order to make $h$ non-dimensional. The model has been formulated for the case of several solutes in [4].

4 Stress update algorithm

The model for the yield stress will be used in a strain-stress algorithm in finite element codes. The radial return method and other similar algorithms are commonly used [88-91] for this purpose. They all need to update the stress and internal state variables from the control variables of a thermo-mechanical problem, i.e. from given increments in total strains, temperature and time, Figure 1. The lower box in Figure 1 illustrates the role of the logic described below for updating the flow stress. The plastic strain is an internal variable common to most plasticity models. The current model requires two additional internal state variables, immobile dislocation density and vacancy concentration. They are determined by the control variables and by the effective plastic strain increment. In addition, further dependent internal variables are introduced in order to create a framework where it is straightforward to replace different submodels. Collectively all these internal variables are denoted by the vector $q$ in the formulas below.

Essential part of the stress-update algorithms is the solution of a non-linear equation known as the consistency condition [88-91] to compute the increment of effective plastic strain. It requires calculation of the yield stress and hardening modulus for the current iterative estimation of the plastic strain and internal variables. Moreover, the hardening modulus is also needed in the computation of the consistent tangent matrix of a stress-strain algorithm. This matrix is used in the implicit finite element codes in order to preserve the 2nd order rate of convergence of the full Newton-Raphson iterations for equilibrium [92]. The hardening modulus is defined as
It is derived analytically in Appendix 1. Alternatively it can be computed by a numerical perturbation, which can be straight-forward and efficient as there is only one independent variable involved, the effective plastic strain.

\[
H' = \frac{d\sigma_y(q)}{d\varepsilon_p} = \frac{\partial \sigma_y}{\partial q} \frac{dq}{d\Delta\varepsilon_p}
\]

(60)

Figure 1. Internal variables and yield stress in the context of finite element analysis.

The basic, essential internal variables needed for the model are the immobile dislocation density and the vacancy concentration, scaled by their initial or reference values as appropriate,

\[
q_0' = \left( \frac{\rho_i}{\rho_{i0}} \frac{c_v}{c_{v0}} \right)
\]

(61)

These are the only necessary state variables for the current model. We also introduce dependent internal variables; subcell size (s), mobile dislocation density (\(\rho_m\)), velocity of mobile dislocations (\(\bar{v}\)), solute concentration (\(c^s\)) and grain size (g). We write

\[
q_{m}' = \left( \frac{s - s_u}{s_0 - s_u} \frac{\rho_m}{\rho_{m0}} \frac{\bar{v}}{\bar{v}_{ref}} \frac{c^s}{g} \right)
\]

(62)

This makes it simple to use other relations for subcell formation, stress dependent mobile dislocation density etc. than those in this study. The current model uses constant grain size but it is possible to include grain growth and recrystallisation into the numerical scheme. Finally, we include the two components of the flow stress

\[
q_1' = \left( \frac{\sigma_s}{\sigma_{0,0}} \frac{\sigma_g}{\sigma_{0,0}} \right)
\]

(63)

into the vector of internal variables. It is then possible to have more elaborate relations for these variables as well. This is of particular interest for the short-range stress component (\(\sigma^s\)) where several other options are common.
We use the notation
\[ \mathbf{q}^T = [q_n^T \ q_m^T \ q_i^T] \quad (64) \]

The evolution of the essential internal state variables is governed by a coupled set of differential equations,
\[ \dot{\rho}_i = P_p \mathbf{\tilde{\epsilon}}^\rho + P_i \quad (65) \]
\[ \dot{c}_e = X_p \mathbf{\tilde{\epsilon}}^\rho + X_i \quad (66) \]

where Eqs. (13, 14) and Eq (25) give
\[ P_p = \frac{m}{b \Lambda} \quad (67) \]
\[ \frac{1}{\Lambda} = \frac{1}{g} + \frac{1}{s} \quad (68) \]
\[ P_i = -2c_e D_e \frac{c_e}{c_e^{eq}} G b^3 \left( \rho_i^e - \rho_n^e \right) \quad (69) \]

where \( \rho_n^e \) is set zero. Eqs (50-51) together with Eq. (1) give
\[ X_p = \frac{\Omega}{Q_i} \left( \sigma^* + \sigma_c \right) + c_i \frac{\Omega_c}{4b^2} \quad (70) \]
\[ X_i = -D_m \left( \frac{1}{g} + \frac{1}{s} \right) c_e - c_e^{eq} + c_e^{eq} \left( \frac{Q_i}{T} \right) \quad (71) \]

These evolution equations are solved incrementally by a fully implicit method. We assume constant plastic strain rate during the increment
\[ \mathbf{\tilde{\epsilon}}^\rho = \frac{\Delta \mathbf{\epsilon}^\rho}{\Delta t} \quad (72) \]

Thus we can write the system of evolution equations we have to solve as
\[ \Delta \rho_i = \sigma^* P_p \Delta \mathbf{\tilde{\epsilon}}^\rho + \sigma^* P_i \Delta t \quad (73) \]
\[ \Delta c_i = \sigma^* X_p \Delta \mathbf{\tilde{\epsilon}}^\rho + \sigma^* X_i \Delta t \quad (74) \]

where the left superscript denotes that all variables are evaluated at time \( \sigma^* t \) in the incremental procedure. Equations (73) and (74) is a set of nonlinear equations for \( ^{\sigma^*}q_{\sigma^*} \) that will be solved simultaneously with the submodel equations for \( ^{\sigma^*}q_{\sigma^*} \) and \( ^{\sigma^*}q_{\sigma^*} \). The left superscript \( n+1 \) is omitted in all the following equations in this section to simplify the writing. Equations (73) and (74) give
\[ H_1 = \Delta \rho_i - \frac{\rho_n^e}{P_p^e} \left[ P_p \mathbf{\tilde{\epsilon}}^\rho \Delta t + P_i \Delta t \right] = 0 \quad (75) \]
\[ H_2 = \Delta c_i - \frac{c_n^{eq}}{c_e^{eq}} \left[ X_p \mathbf{\tilde{\epsilon}}^\rho \Delta t + X_i \Delta t \right] = 0 \quad (76) \]

The model for formation of subcells by immobile forest dislocations, Eq. (18), is written as
\[ H_1 = \left( \frac{s - s_o}{s_u - s_o} \right) \sqrt{\frac{\rho}{\rho_o}} - 1 = 0 \]  
(77)

where we scaled with
\[ s_o - s_u = \frac{K_c}{\sqrt{\rho_o}} \]  
(78)

The mobile dislocation density is assumed to be independent of stress in the current model and the relation \( H_4 \) below is just used to compute this density. It can be used to evaluate the basic assumption of small mobile dislocation density compared with the immobile dislocation density or replaced with a more advanced model. Eq. (29) embodies the assumption of stress and strain independent mobile dislocation density corresponds to
\[ H_4 = \frac{\rho_a h \Lambda \nu_a}{m \bar{\varepsilon}_{ref}} - 1 = 0 \]  
(79)

The Orowan equation, Eq. (3), is rewritten in non-dimensional form as
\[ \frac{\dot{\varepsilon}^\varphi}{\bar{\varepsilon}_1} - \frac{h \rho_a \bar{\varepsilon}}{m \bar{\varepsilon}_{ref}} = 0 \]  
(80)

where we arbitrarily choose strain rate of \( 1 \text{ s}^{-1} \) as a reference. Furthermore, we define the reference dislocation velocity at this strain rate via the initial mobile dislocation density,
\[ \frac{h \rho_{a0} \bar{\varepsilon}_{ref}}{m} = \bar{\varepsilon}_1 = 1 \text{ s}^{-1} \]  
(81)

Combining the last two equations gives
\[ H_6 = \frac{\dot{\varepsilon}^\varphi}{\bar{\varepsilon}_1} - \frac{\rho_a h \Lambda \nu_a}{\rho_{a0} \bar{\varepsilon}_{ref}} = 0 \]  
(82)

The Cr and Ni solute atoms are combined in the diffusion model into one solute. This means that \( c^{Cr} \) is the sum of Cr and Ni concentrations. The diffusivity of Cr is used in the model. Then Eq. (59) gives
\[ H_8 = \left( c^{Cr} - c_0^{Cr} \right) - \left( c_0^{Cr} - c_0^{Cr} \right) \left( 1 - \exp \left( - \left( \frac{h D^{Cr} \tau_a}{b^2} \right) \right) \right) = 0 \]  
(83)

where
\[ D^{Cr} = \frac{c^{Cr}}{c_0^{Cr}} D^{Cr} = \frac{c^{Cr}}{c_0^{Cr}} D^{Cr} e^{\frac{E^{Cr}}{RT}} \]  
(84)

and
\[ \tau_a = \frac{\bar{\varepsilon}_{ref}}{\nu_a \bar{\varepsilon}^\varphi} \]  
[ Eq. (56) ]

The current model uses a constant grain size and thus the trivial relation is
\[ H_7 = \frac{\bar{g}}{g_o} - 1 = 0 \]  
(85)
The flow stress is a sum of the long-range and the short-range components, Eq. (1). They are directly included in the system of equations to be solved. The model for short range obstacles, Eq. (35), can be written as

$$H_s^* = \left( \frac{\sigma_s}{\tau_s G} \right)^p \left[ -\left( \frac{c^p}{c_{ref}^p} \right)^\beta - \left( \frac{c^p}{c_{ref}^p} \right)^\gamma \right] \frac{kT}{\Delta G_b} \ln \left( \frac{\dot{\varepsilon}_s}{\varepsilon_0} \right)^\delta = 0,$$  \hspace{1cm} (86)

where the bulk solute concentration, $c_{ref}^p$, is used as a reference concentration.

The model for the long-range stress component, Eq. (12), is

$$H_l = \frac{\sigma_{G,0}}{\sigma_{G,0}} - \frac{maG_b}{\sigma_{G,0}} \sqrt{\rho},$$  \hspace{1cm} (87)

where initial value of this stress component is used for scaling.

We combine the complete set of equations of the present model with 9 submodels in a compact vector form,

$$H(q, \Delta \varepsilon, \Delta t, T) = 0$$  \hspace{1cm} (88)

where the left superscript $n+1$ for the variables at the end of the increment is omitted. It is also left out in the equations below.

Variation of internal variables with the effective plastic strain is defined implicitly through this system of equations, Eq. (88), where the time step, $\Delta t$, and change in temperature are assumed to be given and fixed. For the present material model it is not feasible to derive analytical expression of such function, $q = q(\Delta \varepsilon)$. An iterative solution of the system of equations in Eq. (88) is required. Newton iterative procedure is used, with the given initial data for the beginning of the time step and change in control variables (Figure 1). The linearised system of equations for an iteration $(i)$ is written as

$$H_{(i)} + \frac{\partial H_{(i)}}{\partial q} \Delta q = 0$$  \hspace{1cm} (89)

where the subscript $(i)$ is an iteration counter and

$$H_{(i)} = H(q_{(i)}, \Delta \varepsilon, \Delta t, T).$$  \hspace{1cm} (90)

From Eq. (89) the iterative change in internal variables is computed as

$$\Delta q = -\left[ \frac{\partial H_{(i)}}{\partial q} \right]^{-1} H_{(i)}$$  \hspace{1cm} (91)

Then the variables are updated,

$$q_{(i+1)} = q_{(i)} + \Delta q$$  \hspace{1cm} (92)

The iterations are terminated when the iterative changes for the independent variables are small, $\delta q \leq TOL_1 * \rho_0$  \hspace{1cm} (93)

and

$$\delta c_v \leq TOL_2 * c_v^{ref}.$$.  \hspace{1cm} (94)
The matrix $\frac{\partial H((i))}{\partial q}$ is given in Appendix 1.

The iterations need a predictor for the first iteration and usually this can be taken as

$$q_{(i)} = ^*q$$

(95)

However, in the authors' experience with the present model, the Newton iterations in such cases tend to diverge, especially when increments are not very small. To prevent divergence during early iterations and to facilitate asymptotically quadratic convergence rate of the Newton method, a rough approximate solution is obtained first, which is then used to start the Newton iterations.

5 Experiments

A number of experiments were performed in order to characterise AISI 316L and to calibrate the dislocation-density model. Compression tests are the basis for the model development in the current study and the model parameters were calibrated by results from tests performed at different temperatures and strain rates. Tensile tests have been carried out for comparison. The chemical composition of the experimental steel is shown in Table 3.

Table 3. Chemical composition of AISI 316L [\%].

<table>
<thead>
<tr>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Cu</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.009</td>
<td>0.27</td>
<td>1.74</td>
<td>0.030</td>
<td>0.024</td>
<td>16.82</td>
<td>10.26</td>
<td>2.08</td>
<td>0.31</td>
<td>0.029</td>
</tr>
</tbody>
</table>

5.1 Experimental procedure

Compression tests were performed at several temperatures and strain rates up to a total strain of 0.6, as shown in Table 4. Furthermore, four tests were performed with a holding time of 300 s at a strain of 0.2 before the compression was continued to 0.6. These tests were performed with a strain rate of $0.01s^{-1}$ at the temperatures given in Table 4. Four strain rate jump tests were also carried out. The initial strain rate of $0.01 s^{-1}$ was then increased to $1 s^{-1}$ at a total strain of 0.1. After compression to a total strain of 0.3 the rate was reduced to $0.01 s^{-1}$ and the test continued until 0.6. The nominal temperatures for all tests can be seen in Table 4. The actual temperatures were recorded and used in the optimisation together with the computed true stress and strain data. The true strain was obtained from measurements of the diameter change during the test. At room temperature (RT), this was calibrated with a measurement of the change in length. This calibration was also used for the high temperature tests. Tests at RT, 800°C and 1100°C were performed both in tensile and compression mode.
The mechanical test specimens were machined from a hot rolled, round bar of diameter 127 mm, with the rolling direction of the bar corresponding to the loading axis of the test specimens. Cylindrical specimens of diameter 10 mm and height 12 mm were used for the compression tests performed at temperatures above 800°C. For tests conducted in the temperature range of RT-800°C, cylindrical specimens of diameter 6 mm and height 9 mm were used. The tensile test specimens were rods, 10 mm in diameter and 115 mm long, with threaded ends. To ensure a uniform deformation zone, the specimens were machined with a thinner central part of approximately 25 mm. The diameter of the deformation zone was 5 mm for the RT tests and 9.5 mm for the tests performed at elevated temperature. The tests were performed in a Gleeble 1500 thermomechanical simulator. Between the compression-test specimen and the tungsten carbide anvils, a graphite foil and a tantalum foil were inserted in order to reduce the friction and to prevent sticking, respectively. For the tests with high reheating temperature, above 900°C, the end surfaces of the specimens were coated with an electroplated nickel coating or a nickel foil in order to prevent carbon diffusion.

Each test specimen was first heated to 1100°C at a rate of 20°C/s where it was held for five minutes before it was cooled to the test temperature at a rate of 5°C/s. This procedure was carried out to ensure that all mechanical tests were performed with specimens of the same grain size. For comparison, one test at room temperature was performed both with and without the heating procedure. The resulting stress-strain curves were, however, very similar.

A grain size investigation was performed on the test specimens compressed at RT, 400°C, 800°C and 1300°C at a strain rate of 1 s⁻¹. A polished and etched cross-section of each specimen was studied in a light optical microscope (LOM) and the grain size was measured according to the mean linear intercept method [93]. To determine if any martensite had been induced during the mechanical tests, magnetic balance measurements were carried out. The tensile and compression test specimens tested at RT and the compression-test specimens tested at 400°C were analysed.

### 5.2 Experimental results

Some tests were duplicated and performed both in tensile and compression mode. The true stress-strain curves from these tests are shown in Figure 2. The tests with a strain rate of 10 s⁻¹ are not shown in the figure but they follow the same trend. Many tests have been duplicated as the results have been reproducible. Variations are less than 5%. The difference between tension and compression can also be seen in Figure 2.
Figure 2. Tensile and compression tests at 20°C, 800°C and 1100°C at strain rates of 0.01 s\(^{-1}\).

Figure 3 shows the results from compression tests in the temperature range RT-1100°C at a strain rate of 0.01 s\(^{-1}\). Four strain rate jump tests are also included.

Figure 3. Compressions test for different temperatures at strain rate 0.01 s\(^{-1}\) including four strain rate jump tests up to 1 s\(^{-1}\).
Figure 4 shows the results from compression tests in the temperature range RT-1100°C at a strain rate of 1 s⁻¹. Four strain rate jump tests, also shown in Figure 3, are included.

![Compression tests at different temperatures at strain rate 1 s⁻¹ including four strain rate jump tests from 0.01 to 1 s⁻¹.](image)

Compression-tested results at different temperatures at strain rate 10 s⁻¹ are given in Figure 5.

![Compression tests at different temperatures at strain rate 10 s⁻¹.](image)
The results from the compression tests, strain rate jump tests and holding tests at 900°C and 1100°C can be seen in Figure 6.

Figure 6. Compression tests at strain rate 0.01 s⁻¹, strain rate jump and holding tests for 900°C and 1100°C.

Figures 7-10 show compression tests at different strain rates at 400°C, 600°C, 700°C and 800°C, respectively. The serrated flow, characteristic for DSA, is clearly seen at low strain rates at these temperatures.

Figure 7. Compression tests at different strain rates at 400°C.
Figure 8. Compression tests at different strain rates at 600ºC.

Figure 9. Compression tests at different strain rates at 700ºC. The flow stress curves at the strain rates of 0.01 and 1 s\(^{-1}\) are near each other. The flow stress for the lower rate exhibits serrations whereas the curve for 1 s\(^{-1}\) is smooth.
Figure 10. Compression tests at different strain rates at 800°C.

The microstructural investigation revealed that a small amount of martensite had been induced in the test conducted at RT. Deformation twins were observed at 1300°C. As expected, the grain sizes were found to be in the same order of magnitude independent of testing temperature. The average grain size was 90 μm.

The results from the magnetic balance investigation are shown in Table 5. The compression test carried out at RT and strain rate 0.01 s⁻¹ was found to contain 8 % of a magnetic phase. In this case, the magnetic phase most certain is deformation induced martensite.

Table 5. Measurements of magnetic phase

<table>
<thead>
<tr>
<th>Test temperature [ºC]</th>
<th>Mechanical test type</th>
<th>Strain Rate [s⁻¹]</th>
<th>Amount of magnetic phase [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>Compression</td>
<td>0.01</td>
<td>8.0</td>
</tr>
<tr>
<td>20</td>
<td>Compression</td>
<td>1</td>
<td>3.7</td>
</tr>
<tr>
<td>20</td>
<td>Compression</td>
<td>10</td>
<td>1.1</td>
</tr>
<tr>
<td>20</td>
<td>Tensile</td>
<td>0.01</td>
<td>1.3</td>
</tr>
<tr>
<td>20</td>
<td>Tensile</td>
<td>1</td>
<td>1.5</td>
</tr>
<tr>
<td>20</td>
<td>Tensile</td>
<td>10</td>
<td>1.0</td>
</tr>
<tr>
<td>400</td>
<td>Compression</td>
<td>0.01</td>
<td>1.0</td>
</tr>
<tr>
<td>400</td>
<td>Compression</td>
<td>1</td>
<td>0.7</td>
</tr>
<tr>
<td>400</td>
<td>Compression</td>
<td>10</td>
<td>0.9</td>
</tr>
</tbody>
</table>
6 Parameter fitting procedure

The parameter determination is done by an error minimisation procedure using a developed Matlab toolbox also used in [2, 94, 95]. An error measure is minimised with respect to the material parameters. We minimise

$$e(p) \quad p \in \mathbb{R}^n$$

subject to constraints

$$L \leq p \leq U$$

where $p$ is a vector with the $n$ unknown parameters and $e$ is an error measure. $L$ and $U$ are lower and upper limits for the parameters.

We consider the problem as strain driven. The strain history is given as $n_{inc}$ number of strain increments. Bruhns and Anding [96] write the error measure as

$$e(p) = \frac{1}{2} r^T G r$$

where $G$ is a diagonal matrix with individual standard deviation errors for the measured data. The vector $r$ has the elements

$$r_i = (\sigma_i - \sigma_e)$$

where $i$

$$i = 1...n_{inc}$$

denotes the different sampling times of the strain during the tests. The matrix $G$ can also be used to make the error non-dimensional [97] and include user defined weight functions, $w(\varepsilon)$. We use

$$G_i = w_i \Delta \varepsilon_i \quad \text{(no summation on } i)$$

The weights $w_i$ make it possible to place more emphasis on more important parts of the measured data, see chapter 6.2. The overall logic of the parameter fitting is shown in Figure 11. $p_{final}$ is the material parameters that minimize the difference between computed $\sigma_i$ and measured stress $\sigma_e$.

![Diagram](image)

Figure 11. Parameter fitting procedure for minimisation of difference between measured and computed stress.
6.1 Parameter space for optimisation

The parameters to be determined from the mechanical tests are given in Table 6. Ranges are given when the parameters is unknown. These ranges are used as upper and lower limit in the parameter optimisation procedure described above.

It is assumed that Poisson’s ratio is constant $\nu = 0.3$ and we have

$$ G = \frac{E}{2(1 + \nu)} \quad (102) $$

Young’s modulus is assumed to be $2 \cdot 10^5$ MPa at room temperature and decreases linearly to $1.16 \cdot 10^5$ MPa at 1200 °C. This is consistent with the values in the report by Burgan [98] and also used by Frost and Ashby [6] for AISI 316. $G_{\text{ref}}$ is the shear modulus at 27 °C and its value is 81 GPa. These data are extrapolated down to $1.09 \cdot 10^5$ MPa at 1300 °C. The thermal expansion is also needed when computing the stress. It is given in Table 7.

Some physical constants that are used are given in Table 8. It also contains measured or approximated or assumed values for some parameters. $T_m$ is the melting temperature, 1440°C. The entropy increase due to the formation of a vacancy, Eq. (37), can be estimated from a simplified analysis for temperature higher than the Debye temperature to be in the order of $0.5k-2k$. We follow Militzer et al. [66] and assume $\Delta S_v = k$. Approximate relations [81] indicates that

$$ Q_{\text{sm}} = 0.4Q_v \quad (103) $$

and then

$$ Q_v = 0.6Q_v \quad (104) $$

This is in fair agreement with the data in Table 8.

We assume in this study that Cr and Ni are the important solutes causing DSA in the temperature range around 600°C. Their concentrations are added into one concentration denoted $c^{\text{Cr}}$. We assume lattice diffusion is dominating giving $\xi = 2/3$ and use the diffusivity for Cr in the model.
Table 6. Parameters to be determined.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Used in Eq. (#)</th>
<th>Value</th>
<th>Dimension</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>12, 87</td>
<td>0.4</td>
<td>-</td>
<td>[34, 35]</td>
</tr>
<tr>
<td>( K_c )</td>
<td>18, 78</td>
<td>-</td>
<td>-</td>
<td>See chapter 3.3.1.</td>
</tr>
<tr>
<td>( s_a )</td>
<td>18, 78</td>
<td>[m]</td>
<td>-</td>
<td>Moteff [99] give examples around 0.5 ( \mu )m.</td>
</tr>
<tr>
<td>( \rho_0 )</td>
<td>Initial and scaling value</td>
<td>( 1 \cdot 10^{10} \leq \rho_0 \leq 1 \cdot 10^{12} ) [m/m³]</td>
<td>-</td>
<td>The lower limit was used in [34].</td>
</tr>
<tr>
<td>( \epsilon_{r} )</td>
<td>25, 69</td>
<td>&lt;1</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( \tau_0 )</td>
<td>35, 86</td>
<td>0.001 ( \leq \tau_0 \leq 1 )</td>
<td>-</td>
<td>[6] used ( 6.5 \cdot 10^{-3} ) for AISI 316</td>
</tr>
<tr>
<td>( \Delta f_0 )</td>
<td>35, 86</td>
<td>0.1 ( \leq \Delta f_0 \leq 2 )</td>
<td>-</td>
<td>[6] used 0.5 for AISI 316</td>
</tr>
<tr>
<td>( p )</td>
<td>35, 86</td>
<td>0 ( \leq p \leq 1 )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( q )</td>
<td>35, 86</td>
<td>1 ( \leq q \leq 2 )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( c_{s}, c^{+} )</td>
<td>59, 83</td>
<td>( 1 &gt; c_{s}^{+} &gt; c^{+} )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( h )</td>
<td>59, 83</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

Table 7. Thermal dilatation

<table>
<thead>
<tr>
<th>Temperature [°C]</th>
<th>0</th>
<th>50</th>
<th>150</th>
<th>250</th>
<th>350</th>
<th>450</th>
<th>550</th>
<th>650</th>
<th>750</th>
<th>1500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal strain ([-\cdot]10^3)</td>
<td>0</td>
<td>0.58</td>
<td>1.73</td>
<td>3.18</td>
<td>4.75</td>
<td>6.43</td>
<td>8.12</td>
<td>9.88</td>
<td>11.6</td>
<td>2.49</td>
</tr>
</tbody>
</table>
Table 8. Known or assumed parameters.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Used in Eq. (#)</th>
<th>Value</th>
<th>Dimension</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>Boltzmann’s constant</td>
<td>$1.38 \times 10^{-23}$</td>
<td>[J/K]</td>
<td>-</td>
</tr>
<tr>
<td>$m$</td>
<td>Taylor factor</td>
<td>3.06</td>
<td>-</td>
<td>For fcc [6]</td>
</tr>
<tr>
<td>$b$</td>
<td>Burgers vector</td>
<td>$2.58 \times 10^{-10}$</td>
<td>[m]</td>
<td>For AISI 316 from [6]</td>
</tr>
<tr>
<td>$\nu_s$</td>
<td>29, 56, 79</td>
<td>1.10$^{12}$</td>
<td>-</td>
<td>[15]</td>
</tr>
<tr>
<td>$\tilde{\varepsilon}_{ref}$</td>
<td>29, 35, 56, 79, 86</td>
<td>1. $10^6$</td>
<td>[s$^{-1}$]</td>
<td>For AISI 316 from [6]</td>
</tr>
<tr>
<td>$e_{0}^{C}$</td>
<td>59, 83</td>
<td>0.27</td>
<td>-</td>
<td>Combined bulk fraction of Ni and Cr</td>
</tr>
<tr>
<td>$\Delta S_{cr}$</td>
<td>37 (gives $e_{0}^{C}$)</td>
<td>$k$</td>
<td>[J/K]</td>
<td>From [66]</td>
</tr>
<tr>
<td>$Q_{cr}$</td>
<td>37, 50-51, 70-71</td>
<td>$2.46 \times 10^{-19}$</td>
<td>[J]</td>
<td>From [66] and gives $e_{0}^{C}$</td>
</tr>
<tr>
<td>$D_{m0}$</td>
<td>41, 51, 71</td>
<td>$1.37 \times 10^{-5}$</td>
<td>[m$^2$/s]</td>
<td>Frost and Ashby [6]</td>
</tr>
<tr>
<td>$Q_{m}$</td>
<td>41, 51, 71</td>
<td>$2.38 \times 10^{-19}$</td>
<td>[J]</td>
<td>From [6].</td>
</tr>
<tr>
<td>$D_{m} = D_{m0} \tilde{e}_{cr}^{\alpha}$</td>
<td>38, 25, 69</td>
<td>$3.7 \times 10^{-5}$</td>
<td>[m$^2$/s]</td>
<td>Relation is derived from Eqns (38) and (41). Data is consistent with [100] and [6].</td>
</tr>
<tr>
<td>$Q_{t} = Q_{cr} + Q_{m}$</td>
<td>38, 25, 69</td>
<td>$4.65 \times 10^{-19}$</td>
<td>[J]</td>
<td>From [6], Kim [101], Perkins [100] give a similar value for the 18-8 steel</td>
</tr>
<tr>
<td>$\zeta_{0}$</td>
<td>49, 51, 70</td>
<td>10</td>
<td>-</td>
<td>From [66]</td>
</tr>
<tr>
<td>$Q_{0}$</td>
<td>47, 51, 70</td>
<td>[J]</td>
<td>From [66]</td>
<td></td>
</tr>
<tr>
<td>$\chi$</td>
<td>51, 70</td>
<td>0.1</td>
<td>[-]</td>
<td></td>
</tr>
<tr>
<td>$\Omega_{0}$</td>
<td>51, 70</td>
<td>$1.21 \times 10^{-24}$</td>
<td>[m$^3$]</td>
<td>From [6]</td>
</tr>
<tr>
<td>$D_{0t}^{(1)}$</td>
<td>54, 59, 83-84</td>
<td>$1.3 \times 10^{-5}$</td>
<td>[m$^2$/s]</td>
<td>Perkins [100]</td>
</tr>
<tr>
<td>$Q_{0}^{(1)}$</td>
<td>54, 59, 83-84</td>
<td>$4.37 \times 10^{-19}$</td>
<td>[J]</td>
<td>Perkins [100]</td>
</tr>
<tr>
<td>$\xi$</td>
<td>59, 83</td>
<td>2/3</td>
<td>[-]</td>
<td></td>
</tr>
<tr>
<td>$g_{0}$</td>
<td>85</td>
<td>$90 \times 10^{-6}$</td>
<td>[m]</td>
<td>Measured, see chapter 5.2.</td>
</tr>
</tbody>
</table>

$^{(1)}$The lattice diffusivity of Cr is used both for Cr and Ni.
6.2 Strategy for optimisation and found value of parameters

The basic approach is to use the physical constants in Table 8 without modifications. The divide and conquer strategy described below was used to determine the parameters in Table 6. The weighting function in Eq. (101) was set up so that the part of the strain-stress curve up to 0.2 was given five times larger weights than the last part of the curve. Thus more emphasis is placed on fitting this part of the curves when performing optimisations for the compression tests. The optimisation strategy can be summarised as

1. Determination of \( p, q, \alpha \) and \( \rho_0 \)

An evaluation of the virgin yield limits, \( \sigma_v(\bar{\varepsilon}^*, T) \), from all the compression tests at the different temperatures and strain rates was made. The virgin yield limit in the model depends on the parameters \( p, q, \tau_0, \Delta f_0, h, c_{sV}, \alpha \) and \( \rho_0 \). The tests at 200 and 400ºC show that the recovery, chapter 3.3.2, and the rate effects in the friction stress term, chapter 3.4, are negligible. These tests were used to evaluate the parameters for the long-range stress component and the pertaining hardening model. These parameters are \( \alpha, K_c, s_a \), and \( \rho_0 \). The last parameter does not affect the results much within the range that is possible\([1–100]\cdot10^{10}\). The higher value was chosen. The focus was on matching the initial slope of the curve as the model could not reproduce the complete curve. The the values for \( D \) and \( \rho_0 \) were fixed together with \( p \) and \( q \).

2. Determination of \( \tau_0, \Delta f_0 \) and \( c_{sV} \) and excluding DSA model.

Preliminary evaluation for all tests at each one of the test temperatures was done. This showed that the parameters \( \tau_0 \) and \( \Delta f_0 \) become quite stable and they were then taken as constant. It was found at this stage that the model for DSA did not work well. The value for the solute fraction in the mobile dislocation was assumed to be the bulk value (0.27) up to 400ºC and quite arbitrarily fixed to \( c_{sV} = 0.8 \) at higher temperatures.

3. Determination of \( K_c, s_a \), and \( c_\gamma \) versus temperature.

Evaluation of the remaining temperature dependent parameters \( K_c, s_a, c_\gamma \) separately for each test temperature. \( c_\gamma \) obtained a quite constant value for temperatures below 400ºC and is of no importance in the low temperature range as the recovery processes are negligible in these tests.

4. Demonstration of DSA model, \( h \)-term.

A test optimisation for determining \( h \) using \( c_{sV} = 0.8 \) was done at 800ºC.

Table 9. Obtained parameters.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( K_c ) (^{(1)} )</th>
<th>( s_a ) (^{(1)} )</th>
<th>( \rho_0 ) (^{(1)} )</th>
<th>( c_\gamma ) (^{(1)} )</th>
<th>( \tau_0 )</th>
<th>( \Delta f_0 )</th>
<th>( p )</th>
<th>( q )</th>
<th>( c_{sV} )</th>
<th>( h ) (^{(2)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^{(1)}\) See Table 10.

\(^{(2)}\) Only evaluated at 800 ºC.
Table 10. Obtained parameters that are taken as temperature dependent.

<table>
<thead>
<tr>
<th>T [ºC]</th>
<th>20</th>
<th>200</th>
<th>400</th>
<th>600</th>
<th>700</th>
<th>800</th>
<th>800^1^</th>
<th>900</th>
<th>1100</th>
<th>1300</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kc [-]</td>
<td>24</td>
<td>20</td>
<td>20</td>
<td>16</td>
<td>14.7</td>
<td>10</td>
<td>29</td>
<td>59</td>
<td>140</td>
<td>200</td>
</tr>
<tr>
<td>s_s [µm]</td>
<td>0.25</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>c_r [-]</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.003</td>
<td>0.007</td>
<td>0.01</td>
<td>0.01</td>
<td>0.018</td>
<td>0.01</td>
<td>0.04</td>
</tr>
</tbody>
</table>

^1^accounting for DSA with h=160

7 Comparison of model and experiments

The computed results using the parameters given in previous chapter are shown together with measurements below. Figure 12 shows them for the temperatures 20ºC, 200ºC, and 400ºC. Symbols denote experiments for the different strain rates (triangles 10s⁻¹, stars 1s⁻¹ and circles 0.01s⁻¹). Solid line is computed results for 0.01s⁻¹ and dashed line for dashed lined for 1s⁻¹ and dotted line for 10s⁻¹. The same for the tests in the temperature range 600 - 1300ºC is given in Figure 13-18, respectively. Figure 13 and Figure 14 have an additional strain rate of 0.0005s⁻¹.

And Figure 16 and Figure 17 includes rate jump tests and hold performed test as described earlier. These tests for lower temperatures were not included for comparison as these rate effects are small at the lower temperatures as can be seen in for example Figure 3. The DSA model is only utilised the stress-strain curves in Figure 19. This curve corresponds to the results in Figure 15 where the solute concentration was fixed to 0.8 for all rates. Further results for the DSA model at 800ºC are shown in the later figures. Solute concentration is shown in Figure 20, vacancy concentration in Figure 21. Figure 22 shows the computed dislocation density.

All figures use symbols for smoothed experimental values for the different strain rates. The dots are used for the strain rate 0.0005 s⁻¹, circles for 0.01 s⁻¹, stars for 1 s⁻¹ and triangles for 10 s⁻¹. Fat solid line is denotes computed results for 0.0005 s⁻¹, solid line for 0.01 s⁻¹, dashed line for 1 s⁻¹ and dotted line for 10 s⁻¹.

Figure 12. Smoothed measured data (symbols) and computed flow stress (lines) for 20, 200 and 400ºC, for strain rates 0.01 (blue), 1.0 (green) and 10 s⁻¹ (red). It is assumed that c_r = 0.27.
Figure 13. Smoothed measured data (symbols) and computed flow stress (lines) for 600°C. It is assumed that $c^{Cr} = 0.8$.

Figure 14. Smoothed measured data (symbols) and computed flow stress (lines) for 700°C. It is assumed that $c^{Cr} = 0.8$. 
Figure 15. Smoothed measured data (symbols) and computed flow stress (lines) for 800°C. It is assumed that $c_r = 0.8$.

Figure 16. Smoothed measured (symbols) and computed flow stress (lines) for 900°C. Strain rate jump test and hold test for this temperature are also shown. It is assumed that $c_r = 0.8$. 
Figure 17. Smoothed measured (symbols) and computed flow stress (lines) for 1100°C. Strain rate jump test and hold test for this temperature are also shown. It is assumed that $c^\eta = 0.8$.

Figure 18. Smoothed measured (symbols) and computed flow stress (lines) for 1300°C. It is assumed that $c^\eta = 0.8$. 

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Figure 19. Smoothed measured (symbols) and computed flow stress (lines) for 800°C including the DSA effect.

Figure 20. Computed solute concentration, $c^{Cr}$, for 800°C, including the DSA effect.
Figure 21. Computed vacancy concentration for 800°C including the DSA effect.

Figure 22. Computed dislocation density for 800°C including the DSA effect.
8 Discussions

8.1 Experiments

8.1.1 Tension-compression asymmetry
The difference between tensile and compressive tests in Figure 2 is yet to be explained. The difference seems to disappear at 1100°C. The same differences have been observed in earlier tests performed at Sandvik Materials Technology for Sanmac 316L. Then the difference disappeared at 800°C.

A difference in tensile and compressive behaviour was also found by Yapici et al. [102]. They produced test pieces by the equal channel angular extrusion (ECAE) process at 700°C and 800°C. These were quenched and then tested at room temperature. Asymmetry in tension and compression was also observed for test pieces produced at 700°C but not at 800°C. This asymmetry was not observed in as-received samples. They considered the asymmetry to be due to either texture or residual stresses. Twinning occurs more easily under tensile loading in the [1 1 1] direction of the crystal whereas the opposite holds for the [0 0 1] direction. However, their samples did not exhibit any texture and, based on further investigations, they concluded that the samples produced at 700°C had residual stresses causing the asymmetry.

Texture measurements have not been completed in the current study. The test pieces have not been produced in the same way as in [102] and tests in Figure 2 indicate about the same initial yield limit for compression and tension tests. The difference is mainly the hardening behaviour. Thus the difference can not be explained based on the current available information.

It should be noted that the model proposed in this paper has been calibrated using the compression tests. The model would have fitted the tensile tests better with their more linear hardening.

8.1.2 Rate dependency effects
The difference between the different strain rates for the test from RT up to 400°C is considered to be small, see Figure 3 and Figure 4.

8.1.3 Twinning
Twins have been observed even in the test performed at 1300°C. Moteff [99] observed twinning for cold-worked bar but not in cold-worked sheet of AISI 316. The first case had larger initial grain sizes. This is in agreement with Karaman et al. [47, 103]. El-Danaf et al. [104] performed compression tests for AISI 316L with a strain rate of 0.001 s\(^{-1}\) up to a total strain of 1.0. The samples had a grain size of 40 \(\mu\)m. They noticed primary twinning for strains between 0.1-0.25 leading to a reduced hardening rate. No increase in hardening due to twin intersections was observed. Yapici et al. [102] observed twinning in their tests at 700 and 800°C.

8.1.4 Dynamic strain aging
DSA can be seen in Figure 7-10. The temperature range is 400-800°C. Barnby [105] observed jerky flow for tensile tests of AISI 316 in the temperature range of 300-700°C for a strain rate of 0.00013 s\(^{-1}\). The material had a grain size of 180 \(\mu\)m. The rate dependency of the flow stress was small below 600°C. He observed a smooth region before DSA occurred and his analysis supported that vacancy assisted diffusion of Cr could cause this. Hong and Lee [80] studied AISI 316L. The specimens had an initial 17% cold work and were thereafter cyclically loaded. The strain rates were in the range of 0.0001 – 0.01s\(^{-1}\). They plotted the region of serrated flow versus strain rate and temperature. Lower rates gave a wider region shifted to lower temperatures for serrated flow. They also classified the serrations into different types. Mannan [106] investigated an AISI 316 steel and found that finer grains lowers the temperature interval for DSA. A grain
size of 0.04 mm gave a temperature range for DSA from 250 to 600°C whereas a grain size of 0.65 mm gave a range of 350-700°C. Yapici et al. [102] discuss the work of others. Interstitials and/or solutes cause DSA in the region of 300-900°C depending on strain rate.

8.2 Model versus experiments

8.2.1 Hardening
Comparisons between computed and measured stress-strain curves in chapter 7 show that they agree quite well at higher temperatures. The hardening evolution is more linear in the model, Figure 12, than in the measurements at lower temperatures. This is believed to be due to twinning that reduced the hardening [104]. The current model does not include twinning. The microstructure measurements also found twinning at higher temperatures. The agreement between tests and computations are probably due to a too large recovery in the model. The optimisation procedure could make the tests and computations agree by determining a large value for \( c_r \). The recovery term at low temperatures is negligible and thus no large \( c_r \) could make up for the missing twinning effect in the model.

The subcell formation model, Eq. (18), was found to work quite well despite the complexities discussed in chapter 3.3.1 when allowing \( K_c \) to be temperature dependent. The value for \( K_c \) may become different when extending the current model with a model for twinning.

No measurements of dislocation densities have been performed. Thus the computed dislocation densities and vacancy concentrations are not validated. Angella et al. [107] investigated the influence of grain size and shape by torsion tests of 316L around 1000ºC at a strain rate of 0.006 s\(^{-1}\). They found that \( \rho \) was 11·10\(^{14} \) m/m\(^3\) near grain boundaries and much lower in interior at \( \rho = 0.36 \). Sauzay et al. [108] performed cyclic tests and measured a dislocation density of 3·10\(^{13} \) m/m\(^3\) in the interior of grains.

8.2.2 Dynamic strain ageing
The model for solute diffusion is a large simplification of the actual phenomenon as Kubin et al point out [20]. An attempt is made to model DSA in the same manner as in Cheng et al. [4]. This model was extended with the effect of vacancy concentration on the diffusion of solutes. This was made in order to enable the triggering of DSA occurring after some strain. For example, Figure 10 shows that the flow stress for the test with a strain rate of 1 s\(^{-1}\) becomes larger than the flow stress for the rate 10 s\(^{-1}\) around a strain of 0.2. It was hoped that the increase in vacancy concentration would increase the diffusivity of the solutes so that DSA occurs at that instant. However, it was found that it is not possible to adjust the parameter \( h \) in Eq. (59) so that the solute only diffuses into the mobile dislocations for the lower rates and not the higher rates. This is due to the fact that the difference in the evolution of vacancy concentration for different strain rates is not large enough, Figure 21. Cheng et al. [4] used numerical values for the diffusivities that did not correspond to any real atoms which is in contrast to our approach to not calibrate the physical constants in Table 8. There are several simplifications in the phenomenological model for solute diffusion, Eq. (59) as well as in the assumption on how it affects the friction stress, Eq. (35). This would need improvement or the alternative approach of letting the solute diffusion pin dislocations, also discussed in chapter 3.4 can be used. The latter would mean that their effect would contribute to Eq. (13).
9 Conclusions

- A physically based constitutive model has been proposed and calibrated versus compression tests from RT up to 1300°C and for strain rates up to 10 s⁻¹. The model requires 11 parameters to be determined from mechanical testing. The overall agreement is good provided the strain is less than 0.25. The model can not represent the DSA behaviour as hoped.
- The inclusion of deformation due to twinning has been found to be an important extension in order to improve accuracy at higher strains.
- The model for dynamic strain aging is not sufficiently accurate.
- The numerical procedure has been adapted to what is needed in finite element simulation and is suitable for large scale computations as the computational overhead is negligible. The model with its submodels has been implemented in a flexible way that will alleviates future extensions/modifications.

10 Acknowledgements

The financial support from the Swedish Knowledge Foundation and Sandvik Materials Technology is gratefully acknowledged. Furthermore, the authors also express their appreciation to PhD Mahesh Somani and the staff at Mechanical Engineering Dept, University at Oulu, Oulu, Finland for performing the mechanical testing in an excellent way.

11 References


[64] Li, J., *Recrystallisation, Grain Growth and Textures*. 1966: ASM.


Appendix 1. Hardening modulus and derivatives involved in the solution of the evolution equations for internal variables

The hardening modulus is defined as
\[
H' = \frac{d\sigma_y(q)}{d\Delta^p} = \frac{\sigma_y}{\Delta^p} \frac{dq}{dH} \quad [\text{Eq. (60)}] 
\]

The linearisation of the hardening law, Eq. (88), in the converged state gives,
\[
\frac{\partial H}{\partial q} \approx \frac{\partial H}{\partial \Delta^p} \frac{d\Delta^p}{dq} = 0, \quad H_{ij} = 0 \quad \text{(A-1)}
\]

Hence the derivative of internal variables w.r.t. effective plastic strain is expressed as,
\[
\frac{d q}{d \Delta^p} = \left[ \frac{\partial H}{\partial q} \right]^{-1} \frac{\partial H}{\partial \Delta^p} \quad \text{(A-2)}
\]

The expression of the hardening modulus and also the iterative solution procedure for the internal variables in chapter 4 involves the derivatives which are given below. Derivatives not given are zero.

The internal variables are
\[
q^T = \begin{pmatrix}
\rho_e & c_e & s - s_e & s_e - s & \rho_{\alpha} & \rho_{\alpha} & \frac{\sigma^*}{\tau_G} & \frac{\sigma_{\alpha}}{\sigma_{\alpha,0}}
\end{pmatrix} \quad [\text{Eq. (64)}] 
\]

Because the scaling of internal variables is applied only for the solution of the system of equations, arbitrary scaling factors can be chosen. To simplify some formulas here we choose the current value of the shear modulus, \(G\), as one of the reference values.

The following derivative vector is trivially obtained from the Eq. (1) and Eq. (64),
\[
\frac{\partial \sigma_y}{\partial q} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \tau_G & \sigma_{\alpha,0}
\end{pmatrix} \quad \text{(A-3)}
\]

Evolution equation for the immobile dislocation density leads to
\[
H_1 = \frac{\Delta \rho}{\rho_0} - \frac{1}{s} \left[ \frac{m}{b} + \frac{1}{s} \right] \frac{1}{\Delta \Delta^p} - \frac{c_e}{s} - \frac{c_e \Delta^p}{s} \left( \frac{\rho^2}{\rho_e^2} \right) \Delta t = 0 \quad \text{(A-4)}
\]

which gives
\[
\frac{\partial H_1}{\partial q_1} = \frac{\partial H_1}{\partial \rho_e} \rho_e = 1 + 4c_e \Delta t \left( \frac{c_e \Delta^p}{s} \right) \rho_e \Delta t \quad \text{(A-5)}
\]

\[
\frac{\partial H_1}{\partial q_2} = \frac{\partial H_1}{\partial c_e} c_e \Delta t = 2c_e \Delta t \left( \frac{c_e \Delta^p}{s} \right) \rho_e \Delta t \quad \text{(A-6)}
\]
\[
\frac{\partial H_1}{\partial q_3} = \frac{\partial H_1}{\partial s}(s_0 - s_\alpha) = \frac{m}{b\rho_\alpha} \frac{(s_0 - s_\alpha)}{s^2} \Delta F^p \\
\frac{\partial H_1}{\partial q_7} = \frac{\partial H_1}{\partial g} g_0 = \frac{m}{b\rho_\alpha} \frac{g_0}{g^2} \Delta F^p \\
\frac{\partial H_1}{\partial \bar{F}^p} = \frac{1}{\Delta t} \frac{\partial H_1}{\partial \bar{F}^p} = -\frac{1}{\rho_\alpha} \bar{F}^p = -\frac{m}{\rho_\alpha} b\Delta
\] (A-7) (A-8) (A-9)

Evolution equation for the vacancy concentration leads to
\[
H_2 = \frac{\Delta c_v}{c_v^0} - \frac{1}{c_v^0} \left[ \frac{\Omega_0}{Q_{cf}} (\sigma^* + \sigma_g) \Delta F^p + \zeta \frac{c_i}{4b^2} \frac{\Omega_0}{b} \Delta F^p \\
- D_m \left( \frac{1}{g} \bar{F}^p + \frac{1}{s} \right) (c_v - c_v^\gamma) \Delta t + c_v^\gamma \left( \frac{Q_{cf}}{T} \right) \Delta t \right] = 0
\] (A-10)

which gives
\[
\frac{\partial H_2}{\partial q_2} = \frac{\partial H_2}{\partial c_v} c_v^0 = 1 + D_m \left( \frac{1}{g} \bar{F}^p + \frac{1}{s} \right) \Delta t \\
\frac{\partial H_2}{\partial q_3} = \frac{\partial H_2}{\partial s}(s_0 - s_\alpha) = -2 D_m \left( \frac{1}{g} \bar{F}^p + \frac{1}{s} \right) (c_v - c_v^\gamma) \Delta t \\
\frac{\partial H_2}{\partial q_7} = \frac{\partial H_2}{\partial g} g_0 = -2 D_m \left( \frac{1}{g} \bar{F}^p + \frac{1}{s} \right) (c_v - c_v^\gamma) \Delta t \\
\frac{\partial H_2}{\partial q_4} = \frac{\partial H_2}{\partial \sigma^*} \tau_\sigma G = -\chi \frac{\Omega_0}{c_v^0 Q_{cf}} \Delta F^p \cdot \tau_\sigma G \\
\frac{\partial H_2}{\partial q_5} = \frac{\partial H_2}{\partial \sigma_g} \sigma_g,0 = -\chi \frac{\Omega_0}{c_v^0 Q_{cf}} \Delta F^p \cdot \sigma_g,0 \\
\frac{\partial H_2}{\partial \bar{F}^p} = \frac{1}{\Delta t} \frac{\partial H_1}{\partial \bar{F}^p} = \frac{1}{c_v^0} \chi \frac{\Omega_0}{c_v^0 Q_{cf}} (\sigma^* + \sigma_g) - \zeta \frac{c_i}{4b^2} \frac{\Omega_0}{b}

Subcell size formation
\[
H_3 = \left( \frac{s_0 - s_\alpha}{s_0 - s_\alpha} \right) \left( \frac{\rho_\alpha}{\rho_\alpha} \right)^{1/2} - 1 = 0 \\
[ \text{Eq. (77)} \]

which gives
\[
\frac{\partial H_3}{\partial q_1} = \frac{\partial H_3}{\partial \rho_\alpha} \rho_\alpha = \frac{1}{2} \left( \frac{s_0 - s_\alpha}{s_0 - s_\alpha} \right) \left( \frac{\rho_\alpha}{\rho_\alpha} \right)^{-1/2} \\
\frac{\partial H_3}{\partial q_3} = \frac{\partial H_3}{\partial s}(s_0 - s_\alpha) \left( \frac{\rho_\alpha}{\rho_\alpha} \right)^{1/2}
\] (A-17) (A-18)

Mobile dislocation density relation
\[ H_i = \frac{\rho_i b \Lambda v_i}{m \bar{\Sigma}_{\text{ref}}} - 1 = 0 \]  

[ Eq. (79) ]

which gives

\[ \frac{\partial H_i}{\partial q_i} = \frac{\partial H_i}{\partial \rho_i} \rho_i \frac{\bar{\Sigma}_{\text{ref}}}{m \bar{\Sigma}_{\text{ref}}} = \frac{\rho_i b \Lambda v_i}{m \bar{\Sigma}_{\text{ref}}} \]  

(A-19)

\[ \frac{\partial H_i}{\partial q_i} = \frac{\partial H_i}{\partial q_0} (q_0 - s_u) = \frac{\rho_i b \Lambda v_i}{m \bar{\Sigma}_{\text{ref}}} \frac{\Lambda^2}{s^2} (q_0 - s_u) \]  

(A-20)

\[ \frac{\partial H_i}{\partial q_i} = \frac{\partial H_i}{\partial g_0} g_0 = \frac{\rho_i b \Lambda v_i}{m \bar{\Sigma}_{\text{ref}}} \frac{\Lambda^2}{g^2} g_0 \]  

(A-21)

where \( \frac{\partial \Lambda}{\partial s^2} \) and \( \frac{\partial \Lambda}{\partial g^2} \).

Mobile dislocation velocity relation

\[ H_5 = \frac{\bar{\Sigma}_f}{\bar{\Sigma}_i} \rho_{\text{ref}} \frac{v}{v_{\text{ref}}} = 0 \]  

[ Eq. (82) ]

with

\[ \frac{b \rho_{\text{ref}} v_{\text{ref}}}{m} = \bar{\Sigma}_i = 1 \text{s}^{-1} \]  

[ Eq. (81) ]

which gives

\[ \frac{\partial H_5}{\partial q_5} = \frac{\partial H_5}{\partial \rho_{\text{ref}}} \rho_{\text{ref}} = -\frac{v}{v_{\text{ref}}} \]  

(A-22)

\[ \frac{\partial H_5}{\partial q_5} = \frac{\partial H_5}{\partial v_{\text{ref}}} = -\frac{\partial H_5}{\partial \rho_{\text{ref}}} \rho_{\text{ref}} \]  

(A-23)

\[ \frac{\partial H_5}{\partial \bar{\Sigma}^p} = \frac{1}{\Delta t} \frac{\partial H_5}{\partial \bar{\Sigma}^p} = \frac{1}{\Delta t} \frac{\partial H_5}{\partial \bar{\Sigma}^p} = \frac{1}{\Delta t} \]  

(A-24)

Solute fraction in mobile dislocation

\[ H_k = (c^0 - c_0^0) - (c^\alpha - c_0^\alpha) \left( 1 - \exp \left[ -\lambda^t \right] \right) = 0 \]  

[ Eq. (83) ]

where

\[ \lambda = h \frac{D_i^\alpha t_v}{b^2}, \]  

(A-25)

\[ D_i^\alpha \frac{c_v}{c_v^0} D_i^\alpha = \frac{c_v}{c_v^0} D_i^\alpha \left( c_v/c_v^0 \right) \]  

[ Eq. (84) ]

\[ t_v = \frac{\dot{c}_\text{ref}}{E^v v_i}, \]  

[ Eq. (56) ]

We will use
\[
\frac{\partial H_{6}}{\partial \lambda} = \left( c_{r}^* - c_{o}^* \right) \exp(-\xi) \left[ -\xi \cdot \lambda^{-1} \right] \tag{A-26}
\]

which gives
\[
\frac{\partial H_{6}}{\partial q_{2}} = \frac{\partial H_{6}}{\partial c_{r}} c_{r}^* = \frac{\partial H_{6}}{\partial \lambda} \frac{\partial D_{6}^{c_r}}{\partial c_{r}} c_{r}^*
\]
\[
= \frac{\partial H_{6}}{\partial \lambda} \frac{ht_{r} D_{6}^{c_r}}{b^2} c_{r}^* = \frac{\partial H_{6}}{\partial \lambda} \frac{ht_{r} D_{6}^{c_r}}{b^2} c_{r}^*
\tag{A-27}
\]

where we used
\[
\frac{\partial \lambda}{\partial D_{6}^{c_r}} = \frac{ht_{r}}{b^2} \tag{A-28}
\]

and
\[
\frac{\partial D_{6}^{c_r}}{\partial c_{r}} = D_{6}^{c_r} \tag{A-29}
\]

Furthermore,
\[
\frac{\partial H_{6}}{\partial q_{6}} = \frac{\partial H_{6}}{\partial c_{r}} = 1, \tag{A-30}
\]
\[
\frac{\partial H_{6}}{\partial \bar{\varphi}^p} = \frac{1}{\Delta t} \frac{\partial H_{6}}{\partial \bar{\varphi}^p} \frac{1}{\Delta t} = \frac{\partial H_{6}}{\partial \lambda} D_{6}^{c_r} \frac{t_{r}}{b^2} D_{6}^{c_r} \frac{1}{\Delta t} \tag{A-31}
\]

Grain size model
\[
H_{g} = \frac{g}{g_{0}} - 1 = 0 \quad \text{[ Eq. (85) ]}
\]

where all derivatives are zero except \( \frac{\partial H_{6}}{\partial q_{7}} = \frac{\partial H_{6}}{\partial g_{0}} = 1 \), as the grain size is constant.

Short range flow stress contribution
\[
H_{s} = \left( \frac{\sigma^*}{\tau_{0} G} \right)^p \left[ \frac{c_{o}}{c_{o}^*} \right] \left( \frac{c_{o}}{c_{o}^*} \right)^{\frac{n}{2}} \left( \frac{kT}{\Delta s G h^3 \ln(\frac{\delta_{ref}}{\bar{\varphi}^p})} \right)^{\frac{1}{p}} = 0 \quad \text{[ Eq. (86) ]}
\]

If the above expression yields \( \sigma^* < 0 \), a cut-off is introduced,
\[
H_{s} = \frac{\sigma^*}{\tau_{0} G} = 0, \tag{A-32}
\]

and the only non-zero derivative in this case is
\[
\frac{\partial H_{s}}{\partial q_{8}} = \frac{\partial H_{s}}{\partial \sigma^*} \tau_{0} G = 1. \tag{A-33}
\]

Otherwise the first expression of \( H_{s} \) is used, which gives remaining derivatives:
\[
\frac{\partial H_s}{\partial q_{eq}} = \frac{\partial H_s}{\partial \sigma^*} = -\frac{p}{2c_v^0} \left( \frac{c_v^0}{c_v^0} \right)^{\frac{1}{m}} + \frac{1}{c_v^0} \left( \frac{p}{2} - \frac{1}{2q} \right) \left( \frac{c_v^0}{c_v^0} \right)^{\frac{1}{m} \frac{1}{2}} \left( \frac{kT}{\Delta f_Gb} \ln \left( \frac{\bar{\sigma}_{eq}}{\bar{\sigma}} \right) \right)^{\frac{1}{m}}
\] (A-34)

\[
\frac{\partial H_s}{\partial q_{eq}} = \frac{\partial H_s}{\partial \sigma^*} \bar{T}_G = p \left( \frac{\sigma^*}{\bar{T}_G} \right)^{p-1}
\] (A-35)

\[
\frac{\partial H_s}{\partial \bar{T}} = \frac{1}{\Delta T} \frac{\partial H_s}{\partial \bar{T}} = \frac{1}{q} \left( \frac{c_v^0}{c_v^0} \right)^{\frac{1}{m} \frac{1}{2}} \left( \frac{kT}{\Delta f_Gb} \ln \left( \frac{\bar{\sigma}_{eq}}{\bar{\sigma}} \right) \right)^{\frac{1}{m}} - \frac{kT}{\Delta f_Gb} \left( \frac{1}{\bar{\sigma}} \right)\Delta T
\] (A-36)

The equation for the long-range stress contribution is written in non-dimensional form as

\[
H_s = \frac{\sigma_{eq}}{\sigma_{eq,0}} - \frac{m\alpha Gb}{\sqrt{\rho_i}}
\] [ Eq. (87) ]

which gives

\[
\frac{\partial H_s}{\partial q_{eq}} = \frac{\partial H_s}{\partial \rho_i}, \rho_{eq} = -\rho_i \frac{m\alpha Gb}{2\sigma_{eq,0}} \frac{1}{\rho_i}
\] (A-37)

\[
\frac{\partial H_s}{\partial \sigma^*} = \frac{\partial H_s}{\partial \sigma^*} \sigma_{eq,0} = 1
\] (A-38)
Paper C
A three-dimensional finite element simulation of stainless steel tube extrusion using a physically based material model

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ABSTRACT: Extrusion of stainless steel tubes is associated with large deformations, high strain rates and high temperatures, which results in computationally challenging problems in process simulation. In the present study, a three-dimensional, thermo-mechanically coupled finite element analysis of tube extrusion was carried out using a dislocation density-based model for the austenitic stainless steel AISI 316L. The model was rotational symmetric and built up by four-node tetrahedrons. The numerical prediction of the extrusion force was compared to experimental measurements and force predictions from two-dimensional axisymmetric simulations. The results showed that a fine mesh would be required to accurately simulate three-dimensional tube extrusion using four-node tetrahedrons.

Key words: finite element, extrusion, physically based material model, stainless steel, dislocation density

1 INTRODUCTION

Stainless steel tubes are extruded at high temperature with molten glass as lubrication. The process is associated with large deformations and high strain rates [1]. The main goal in tube extrusion is to manufacture consistent products with minimal dimensional variation. One particular dimensional problem is referred to as eccentricity, i.e. the hole in the extrudate is not centred along the centreline of the billet outer diameter. The major causes of eccentricity are expected to be billet temperature gradients, billet preparation, equipment misalignment and improper lubrication [2], but not much work has been reported in this field. The present study is part of a project aiming at investigating dimensional control in stainless steel tube extrusion using finite element (FE) simulations. Though recent advances in FE software and computer development, extrusion simulation in three dimensions is still a challenging task. This is mainly due to the large deformations. If a Lagrangian approach is used, the elements get heavily distorted and remeshing is needed frequently during the analysis.

To obtain reliable simulation results a good constitutive model is an absolute necessity. Physically based material models [3,4] are models which are based on the underlying physical processes that cause the deformation. These models are therefore expected to have a larger range of usability and validity than more commonly used empirical models. This is interesting for applications associated with high strain rates, such as extrusion, where extrapolation of existing material data often is necessary. With the physically based models it is also possible to utilize information from other sources than mechanical tests to determine the model parameters.

In this study, a dislocation density-based material model for the AISI type 316L stainless steel was used in FE simulations of tube extrusion in three dimensions. The problem that was considered was rotational symmetric and therefore only a quarter of the process was modelled. Axisymmetric analyses in two dimensions have earlier been carried out successfully [5] and the model presented here is a further development in the work towards a fully three dimensional extrusion model.

2 METHODS AND MODELS

2.1 Material model

The yield stress was predicted by a dislocation density-based material model. In this model the
yield stress is assumed to consist of two components
\[ \sigma_\gamma = \sigma_0 + \sigma^*, \] (1)
where \( \sigma_0 \) is an athermal stress contribution due to the long-range interactions with the dislocation substructure. \( \sigma^* \) is a friction stress that is needed to move dislocations through the lattice and to pass short range obstacles. This process is thermally activated.

The long range term in equation 1 can be written as
\[ \sigma_0 = m\alpha Gb\rho, \]
where \( m \) is the Taylor orientation factor, \( \alpha \) is a proportionality factor, \( G \) is the shear modulus, \( b \) is Burger’s vector and \( \rho \) is the density of immobile dislocations [6]. The evolution of the dislocation density is given by
\[ \dot{\rho} = U\dot{\sigma}^* - \Omega \rho^*, \]
where \( U \) is the dislocation multiplication parameter, related to the mean free path, \( \Lambda \), by
\[ U = \frac{m}{b\Lambda}, \]
\( \Omega \) is the remobilization parameter that accounts for the static and dynamic recovery controlled by diffusional climb and interactions with vacancies [8]. The model has earlier been calibrated by comparison with a set of compression tests performed at different temperatures and strain rates for the austenitic stainless steel AISI 316L [5]. Five model parameters were found by curve fitting and all values were physically reasonable when compared to those found in literature. Experimental yield stress curves and corresponding curves predicted by the model at 1100 °C and 1300 °C are shown in figure 1 and figure 2, respectively.

2.2 Finite element models
Thermo-dynamically coupled finite element simulations were carried out in two and three dimensions using the Lagrangian finite element code MSC.Marc. The extrusion model in three dimensions is shown in figure 3. The process parameters for the extrusion are given in table 1. In order to reduce the computational time, only part of the total billet length was considered in the numerical model. The billet length was chosen long enough to correctly simulate the transient start-up phase of extrusion until steady-state was obtained. Only a quarter of the geometry was modelled due to rotational symmetry in loading and workpiece.

Fig.1. Experimental (solid line) and predicted (circle) flow stress at 1100 °C.

Fig.2. Experimental (solid line) and predicted (circle) flow stress at 1300 °C.

Fig.3. Finite element model of tube extrusion.
Table 1. Extrusion process parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Billet material</td>
<td>AISI 316L</td>
</tr>
<tr>
<td>Tool material</td>
<td>AISI H13</td>
</tr>
<tr>
<td>Ram speed</td>
<td>125 mm/s</td>
</tr>
<tr>
<td>Container diameter</td>
<td>125.3 mm</td>
</tr>
<tr>
<td>Billet inner diameter</td>
<td>33 mm</td>
</tr>
<tr>
<td>Billet outer diameter</td>
<td>121 mm</td>
</tr>
<tr>
<td>Billet length</td>
<td>374 mm</td>
</tr>
<tr>
<td>Billet initial temperature</td>
<td>1170 ºC</td>
</tr>
<tr>
<td>Tube outer diameter</td>
<td>33.2 mm</td>
</tr>
<tr>
<td>Tube wall thickness</td>
<td>6.35 mm</td>
</tr>
</tbody>
</table>

The material was assumed to be elastic-plastic with isotropic hardening, and the von Mises yield criterion was used together with the flow stress prediction introduced in the previous section. Linear isoparametric tetrahedrons were used in three dimensions, while two different element types were tested in the two dimensional case. First, four-node, isoparametric, arbitrary quadrilateral elements, especially written for axisymmetric applications. Three-node, isoparametric, triangular elements were also tested. The deformation behaviour of the triangular axisymmetric elements is comparable to the tetrahedrons used in three dimensions. Remeshing during the analyses was controlled by automatic remeshing schemes available in MSC.Marc.

In tube extrusion, lubrication through the die is provided by a disc of compacted glass, the glass pad, which is placed between the billet and the die. This pad deforms and melts progressively during extrusion to assure good lubrication through the whole process. The die profile with the metal is therefore difficult to predict. In this study, the path of the metal flow was determined by examining cross sections of stickers, i.e. extrudates that for some reason were stuck during extrusion. No heat transfer was considered between the billet and the glass-pad in the models. All tools were assumed to be rigid bodies with constant temperature. The tool temperatures and other parameters that were used in the models are summarized in table 2. When glass is used as lubrication, the metal flow is almost frictionless and the isolating properties of the glass film leads to low contact heat transfer.

Table 2. Parameters used in the FE models.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mandrel temperature</td>
<td>350 ºC</td>
</tr>
<tr>
<td>Ram temperature</td>
<td>800 ºC</td>
</tr>
<tr>
<td>Die temperature</td>
<td>900 ºC</td>
</tr>
<tr>
<td>Container temperature</td>
<td>500 ºC</td>
</tr>
<tr>
<td>Friction coefficient, glass-lubricated contact</td>
<td>0.02 (Coulomb)</td>
</tr>
<tr>
<td>Friction coefficient, billet-ram</td>
<td>0.35 (Coulomb)</td>
</tr>
<tr>
<td>Billet length</td>
<td>374 mm</td>
</tr>
<tr>
<td>Contact heat transfer coefficient</td>
<td>5 kW/m²/K</td>
</tr>
<tr>
<td>Surface heat transfer coefficient</td>
<td>0.66 kW/m²/K</td>
</tr>
</tbody>
</table>

To verify the models, ten tubes were extruded in a 1450 MN production press. The extrusion force was recorded during the process.

3 RESULTS AND DISCUSSION

The maximal extrusion force was found to be 10.4 MN from the experimental data recording. After the transient start-up of extrusion, the force stabilized at a level of approximately 9.0 MN. Figure 4 shows the numerical predictions of the extrusion force.

![Fig. 4. Numerical predictions of extrusion force.](image)

As can be seen in figure 2, the axisymmetric finite element simulation performed with quadrilateral elements is in agreement with the experimental results. The maximum extrusion force and the steady-state force are 10.0 MN and 9.5 MN, respectively. Main sources of errors are the thermal conditions and heat transfer, together with the coefficient of friction. The strain rate distribution in the extrusion simulation is given in figure 5.

![Fig. 5. Strain rate distribution in extrusion simulation.](image)

The three dimensional simulation overestimated the extrusion force, which could be expected by the four-node tetrahedrons. Hexahedral elements would perform much better for large strain plasticity, but...
these elements are not yet available with remeshing in MSC.Marc. The jerky flow of the extrusion force curve is due to the remeshing. If the number of elements were increased in the three-dimensional model, the results would undoubtedly be much better. This can be concluded from the axisymmetrical simulations using triangular elements with different mesh densities. The results from these simulations are included in figure 2. 1000 triangular elements in two dimensions are approximately comparable to the mesh density used in the three-dimensional simulation and the extrusion force curves are also similar. If the triangular mesh is refined, the force approaches the experimental results. 6000 axisymmetrical elements provide an acceptable solution regarding the extrusion force. The same mesh refinement in three dimensions would, however, result in very long CPU time to carry out the simulation. The three-dimensional simulation presented here consisted of about 35000 elements. Generally, the simulation time for the axisymmetric analysis is an hour or less, whereas a typical simulation time in the three-dimensional case could be a couple of days. A drawback in the three-dimensional case is that global adaptive remeshing is not yet supported in parallel mode in MSC.Marc. This means that multiple processors cannot be used in the simulations.

For tube analyses with rotational symmetry there is really no point in using three-dimensional simulations. The axisymmetric analyses in two dimensions provide good and fast solutions to these problems. In this study, however, the quarter symmetry model is just a first step towards a fully three-dimensional extrusion model, which is a must for eccentricity studies.

4 CONCLUSIONS

The axisymmetric model with quadrilateral elements could successfully predict the extrusion force, which indicates that the extrusion model is essentially correct. Four-node tetrahedrons could be used in three-dimensional simulations but a very fine mesh would be needed to get good results, and this in turn means long computational times. The required mesh refinement can perhaps be carried out with a symmetric quarter model, but would almost be impossible if the model would be extended to fully three-dimensional. Other element types must then be considered. Today, there are not many elements that can be used together with remeshing and there is a great demand for good remeshing routines for hexahedral elements. Another development that would improve three-dimensional extrusion simulation would be the possibility to run these simulations on parallel processors.

ACKNOWLEDGEMENTS

The author wishes to thank the Swedish Knowledge Foundation (KK-stiftelsen) and the Swedish Steel Producers’ Association (Jernkontoret) for their financial support.

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