Materials Science Forum Vols. 539-543 (2007) pp. 2988-2993
online at http://www.scientific.net

Interaction of Recrystallization and Precipitation during Hot Forming of Alloy 80A

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Keywords: dynamic recrystallization, precipitation, damage, crack initiation, crack growth, EBSD

Abstract. In the high temperature deformation window of the nickel base Alloy 80A the lower temperature region during open die forging was examined with regard to the materials formability. For that purpose, hot compression samples were investigated by means of EBSD and TEM in order to look at recrystallization, precipitations and ductile damage as well as their reciprocal effects. Further a microstructure model was used, which calculates the materials strengthening, softening and the particle kinetics. A micro mechanical damage model of the effective stresses was coupled with the grain structure development in order to describe a retarded damage rate due to the ongoing recrystallization.

Introduction

Severely deformable materials mostly exhibit very narrow deformation windows in terms of temperature and strain rate, which generally can be defined by processing maps. During hot rolling or open die forging for example, thermo-mechanical processing is performed in order to stay within this deformation window over the length and the cross section of the work piece as well as to avoid costly intermediate heat treatments. For a process optimization and the tuning of the specified microstructure, microstructure models can be used that include recrystallization, grain growth and precipitation [1]. Additionally, the materials formability is a function of the local temperature, the strain and the stress state. The resulting damage can be calculated e.g. with the model of effective stresses [2], considering crack closure effects by splitting the Cauchy stress tensor in a compressive and tensile part. Therefore the materials damage state in industrial processes can be simulated by implementing damage models into finite element (FEM) software [3]. If the local hot forming conditions are such that dynamic recrystallization is initiated, deformation energy is reduced by the formation and growth of initially stress free grains. Hence, the damage rate and the probability of crack initiation are reduced.

Microstructure and Damage Models

In semi-empirical models, many materials parameters have to be determined by a comprehensive experimental program for one single alloy [1]. In contrast, more sophisticated physically based models attempt to describe the structural kinetic processes and their interactions. A general formulation allows the simulation of the microstructural evolution for a whole group of materials [4]. This implies the consideration of precipitation processes and their interaction with mobile large angle grain boundaries (recrystallization, grain growth). Additionally the flow stress during a current

deformation results from the corresponding microstructure. The following is a short description of the models developed for the simulation of hot forming processes of alloys with low stacking fault energy; details can be found elsewhere [4,5].

Thermodynamic Model and Multi-Component Diffusion. The precipitation model used accesses the thermo-kinetic program MatCalc [6], which is utilized for the evaluation of the driving forces for precipitation, the equilibrium phase compositions and the multi-component diffusion coefficients. In MatCalc the thermodynamic formalism describing the molar Gibbs free energy of a phase is formed by the sublattice model [6], and the thermodynamic parameters are read from available commercial databases, i.e. the nickel-base database [7]. The chemical diffusion coefficients that are needed to simulate the growth and coarsening kinetics of precipitates are calculated using the model of Andersson and Agren [8]. The required mobility data are specified using the mobility database of the software package DICTRA [9].

Precipitation Model. The precipitation kinetic model [5] is derived from classical nucleation and growth theory. Phase separation in solid alloys often occurs as the thermally activated migration of atoms through a phase boundary. Hence, the free energy changes with the free volume energy (chemical formation energy) because of the formation of new phase volume (energy gain), and the free surface energy because of the formation of new interface area (energy loss). In the case of coherent particles, the elastic strain energy, due to the lattice misfit of the matrix and the particle, additionally has to be considered. For heterogeneous nucleation at dislocations and at interfaces, the phase boundary energy can be set to a smaller value due to the fact that the energy barrier for nucleation at inhomogeneities is lower. In the present model, both the number of potential nucleation sites per unit volume and the rate at which solute atoms from the matrix join the nucleus depend on the nucleation site and are either related to the lattice parameter (homogeneous nucleation), to the grain size (nucleation at grain boundaries) or to the dislocation density (strain induced nucleation) [5].

Grain Structure Model. The grain structure model [4] simulates the grain structure development during and after a hot deformation of alloys with low stacking fault energy and thus treats recrystallization as the predominant softening process. It considers normal grain growth and dynamic, meta-dynamic and static recrystallization.

Criteria for the Onset of Dynamic Recrystallization. During hot forming, the time derivative of the dislocation density ρ_0 of the unrecrystallized grains can be described [10] by the equation

$$\frac{d\rho_0}{dt} = \frac{\dot{\varepsilon}}{b\,l_0} - 2M\,\tau\,\rho_0^2 \qquad (1),$$

taking into account the strain hardening and the recovery of dislocations but neglecting recrystallization, where $\dot{\varepsilon}$ is the strain rate, b the Burgers vector, l_0 the mean free path of the dislocations, M the mobility of dislocations and τ the average energy per unit length of a dislocation. A critical dislocation density is necessary in order to initiate dynamic recrystallization (DRX) and is related to the nucleation by the formation of a mobile high angle boundary under deformation conditions, which favour heterogeneity and hence dislocation accumulation. The nucleus usually forms at pre-existing grain boundaries, at least at higher strain rates. Roberts and Ahlblom [11] developed a nucleation criterion, which is based both upon the classical nucleation theory and on the idea that during dynamic recrystallization the concurrent deformation reduces the stored energy difference (i.e. driving force) that effects migration of large angle boundaries.

Nucleation Rate. After reaching a critical dislocation density, new nuclei form with ongoing deformation. Dynamic discontinuous recrystallization can be considered in terms of the rate of

nucleation (formation of interfaces) versus the rate of growth (migration of interfaces) under given boundary conditions [12]. The nucleation consists of the formation of a grain boundary due to dislocation generation and simultaneous recovery and rearrangement. This interface will become a nucleus for dynamic recrystallization if it becomes a large angle grain boundary. The nucleus will grow by the process of grain boundary migration. If nucleation and growth occur simultaneously, the slower of the two will control DRX. In [4] a nucleation rate R_N is derived by the number of dislocations per critical nucleus that recover with time.

Recrystallization Rate. A new model for dynamic recrystallization [4] considers two recrystallization cycles. It is assumed that during recrystallization for each time step a grain class is formed, consisting of nuclei with critical radius. Nuclei grow by the movement of large angle grain boundaries with a boundary velocity that depends on time due to the precipitation of particles, changing temperature and strain rate. Hence the velocity of a high angle boundary during recrystallization is the product of the boundary mobility and the sum of the driving and dragging forces. The recrystallized fraction f at the time t is given by the sum over all nucleation times t_g, starting at the time t_{cr}, where the dislocation density reaches a critical value for the onset of DRX [4]

$$f = \frac{\pi}{6}\int_{t_{cr}}^{t} s^3(t_g)\, R_N(t_g)\left(1 - f(t_g)\right)dt_g \qquad (2),$$

where $s(t_g)$ is the size of a grain class corresponding to its time of generation $t_g > t_{cr}$.

Damage Model. Since the introduction of the finite elements method in the hot bulk forming different damage criteria were defined. The model of effective stresses [2] divides the material into representative volume elements. With the occurrence of a damage D it is assumed that by formation of pores or cracks only the fraction $(1-D)$ of the section of a volume element carries the applied loads. All parameters affected by ductile damage are accordingly treated as effective values. This is valid for tensile and also for compressive stresses, if the micro cracks and micro cavities remain open, which is often the case for very brittle materials. If the defects close completely in compression, the area which effectively carries the load equals the initial undamaged area. To define an effective area in compression, a crack closure parameter was defined [3] that depends a priori upon the material and the loading. The law of evolution of damage derives from the potential of dissipation Ψ, which is a scalar convex function of the state variables in case of isotropic plasticity and isotropic damage

$$\dot{D} = -\frac{\partial \Psi}{\partial Y} = \left(\frac{Y}{S_0}\right)^{s_0} \dot{\varepsilon}_{eq} \qquad (3),$$

where S_0 and s_0 are material and temperature dependent and $\dot{\varepsilon}_{eq}$ is the equivalent true strain rate. The damage strain energy release rate Y corresponds to the variation of internal energy density due to damage growth at constant stress. For the implementation of a crack closure parameter, a distinction between tensile and compressive stresses in a multi-axially stressed state has to be made, thus to split the stress tensor in a positive and a negative part, related to the signs of the principal stresses. For the prediction of the material parameter, tensile tests of Alloy 80A were carried out at different temperatures in the range of 900°C-1000°C [3].

Numerical Model. Both microstructure and damage models, described above, were implemented into the FE program DEFORM 2D® with Lagrange code. The flow potential after von Mises was modified in order to describe the damaged material behaviour, i.e. to reduce the flow stress

$k_f = \sigma_{eq}/(1-D)$, where σ_{eq} is the equivalent von Mises stress. The evolution of damage as a function of the dynamically recrystallized fraction was calculated by

$$D_i = D_{i-1} + \frac{\dot{D}\,\Delta t}{D_c}(1-f) \quad (4),$$

where i demarks the time step, Δt the time increment and D_c is the rupture criterion. Therefore rupture is assumed if D_i equals *1*. If we reach a fully recrystallized structure during steady state, i.e. $f=1$, the progress of materials damage stops.

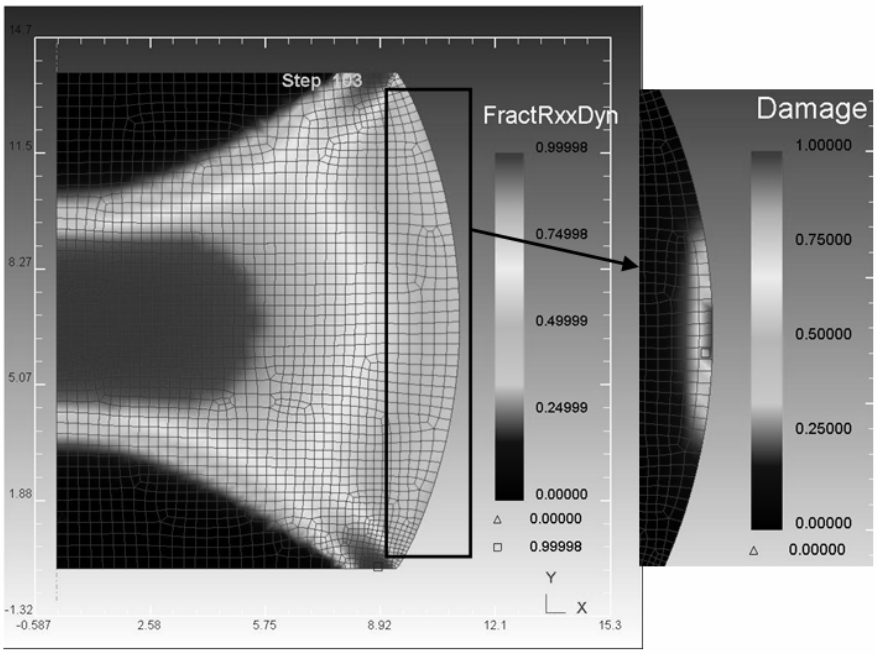

Fig. 1: Simulation of the dynamically recrystallized fraction f at 1000°C at the first appearance of macro cracks (left). The true accumulated strain in the centre is approx. 1.0 and at the edge at half the specimen height it is approx. 0.4. The accumulated damage D (i.e. lifetime consumption) in the barrelling zone where the first macro cracks appear is zoomed out.

Experiments and Simulations. To assesses the effectiveness and applicability of fracture criteria at elevated temperatures, compression tests with different starting temperatures (900°C, 950°C, 1000°C) for Alloy 80A were performed [3]. Because of the friction between the specimen and the tools a barrelling effect occurs during the experiments at the surface near the horizontal symmetry section of the sample. The resulting circumferential stresses cause specimens to fracture. During hot compression maximum strain typically accumulates in the centre of the specimen as well as in the 45° direction related to the global load. Therefore, the deformation heat that develops during the deformation leads to a temperature gradient between the centre and the edge of the specimen. Hence the highest DRX fractions can be found in the areas of both maximum strain rate and temperature (Fig. 1). The calculated damage starts as a function of the combination of the equivalent strain rate and the stress state (Eq. 3). The crack closure parameter has to be chosen very small (close to zero) in order to let damage initiate at the equatorial surface. Hence only tensile (here circumferential) stresses have a significant influence on the lifetime consumption. With the onset of DRX the deformation strain is reduced and the grain triple points, critical for crack initiation, are removed by the progress of new DRX grains. Thus at steady state DRX, damage diminishes, even to zero. This is typically found for industrial hot forming applications at approx. 1050-1200°C, moderate strain rates and compressive stresses (<10/s) for the investigated Alloy 80A [4].

EBSD and TEM Investigations. The OIM-maps show that with decreasing temperature the fraction of recrystallized grains also strongly decreases. At a temperature of 1000°C it changes from approximately 40% at 2/3 of the radius (56% in the simulation) to 25% at the edge of the specimen (21% in the simulation). The measured DRX grain size was approx. 12µm (calculations: 9µm) at 2/3 of the radius and approx. 11µm at the edge of the specimen (7µm in the simulations). For 900°C only a few recrystallized grains can be observed (compare Fig. 2). The grain orientation spread was used to discriminate between the original and the recrystallized grains [13]. For the unrecrystallized grains a texture can be observed, which increases with increasing strain. This corresponds with investigations of dynamic recrystallization in Alloy 80A at a temperature of 1120°C [14]. But contrary to the latter case at temperatures of 1000°C DRX also inside the grains is taking place, not only at grain boundaries. Possibly this is linked with the formation of carbides at temperatures below approx. 1020°C.

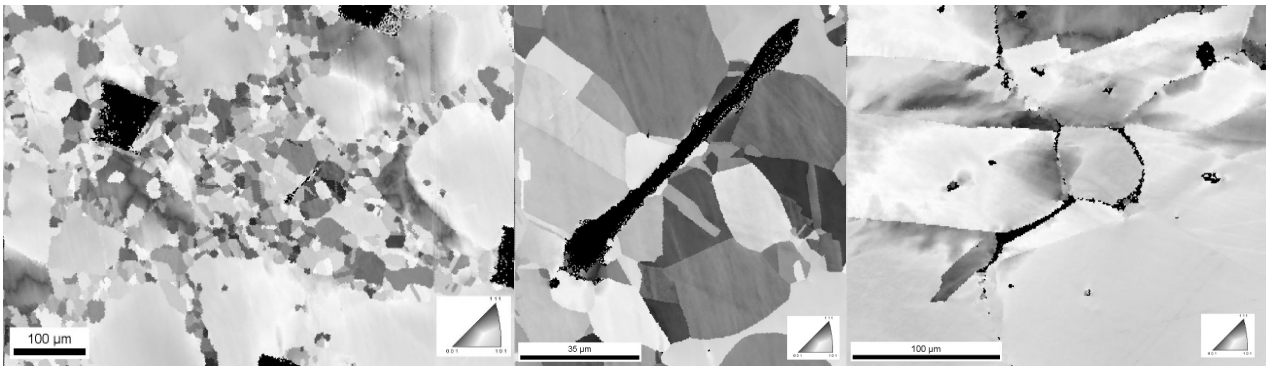

Fig. 2: Inverse pole figure at a transversal cross section of a compression specimen at 2/3 of the radius: T=1000°C (left, bar length: 100µm); Zoom from the left image with crack (centre, bar length: 35µm); T=900°C (right, bar length: 100µm); inset: grey code for crystal orientations; the black regions in the left image result from micro-indentations made after the compression test.

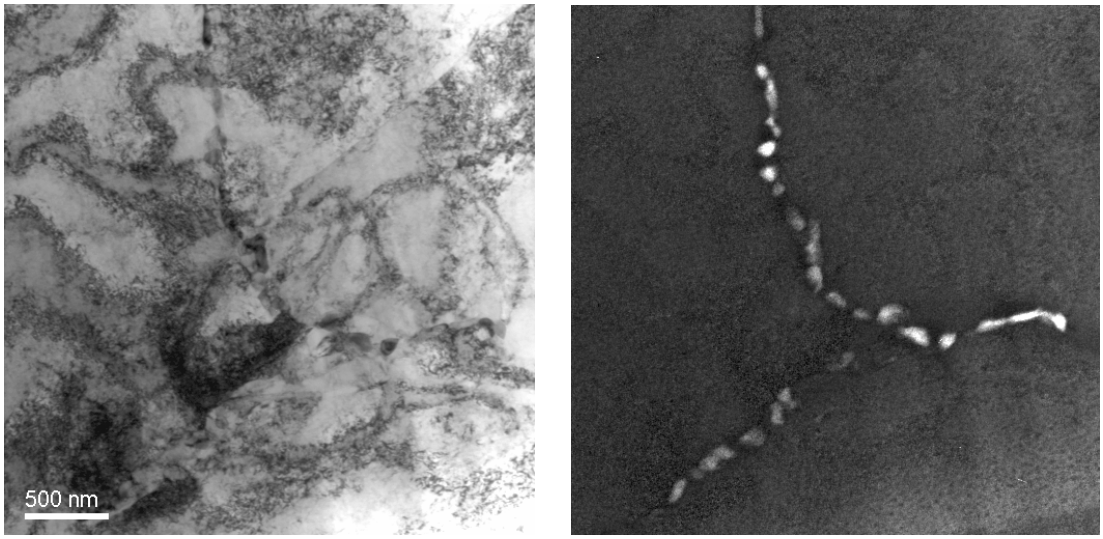

Fig. 3: TEM investigations clearly indicate chromium carbides (Cr_7C_3 according to [15]) at the grain boundaries (T=900°C). Bright field image (left) and corresponding Cr L ratio image (right).

Crack initiation will necessarily take place at the triple points of the unrecrystallized grains because of the high stresses present there, especially near the edge of the sample with circumferential tensile stress components. But crack propagation itself seems to be dependent on the degree of recrystallization. In samples with a rather high fraction of recrystallized grains the crack preferentially propagates in the recrystallized region, not only along grain boundaries, but also

across the recrystallized grains themselves (Fig. 2 centre). This is an indication that at least part of the dynamic recrystallization has taken place before cracking started. The propagation proceeds very often roughly parallel to the <100> direction of the cubic grains. Unfortunately in a two dimensional cross section the actual start and end point of the crack are generally not in the same plane, thus it is difficult to determine the direction of the crack propagation. Additional investigations demonstrated that at a temperature of 1000°C parts of the crack appear rather ductile. Even if only small clusters of recrystallized grains are present, the crack seems to be connected to these clusters, which often also confine the crack to a part of an unrecrystallized grain boundary. Only in case of samples with negligible recrystallization during the compression, the crack propagates along the whole grain boundaries of the deformed grains, tearing apart the grains, often singling out individual grains (Fig. 2 right). This brittle fracture may be caused by grain boundary embrittlement entailed by the precipitation of grain boundary carbides taking place at the respective temperatures [15] (Fig. 3). Thus a clear transition in the fracture behaviour can be found when lowering the temperature during deformation from 1000°C to 900°C.

Summary

A physically based microstructure model was linked to the damage model of effective stresses in order to consider the influence of dynamic recrystallization on the life time consumption during hot forming. Hot compression tests and FEM simulations were performed and results were compared related to DRX and lifetime consumption. Both the simulations and the experiments showed that the critical area for crack initiation is the barreling zone with its circumferential stresses. Additionally the coupled damage-microstructure model led to retarded lifetime consumption. For temperatures above the solution temperature of precipitations further ductile crack growth seems to take place in the DRX grains in a specific direction. Thus, crack initiation and growth have to be treated separately. At lower temperatures damage is caused by brittle grain boundary fracture.

References

[1] C. Sommitsch and V. Wieser: *Microstructural Simulation of Hot Forming Processes* (Proc. EUROMAT 2001, Associazione Italiana di Metallurgia, Rimini 2001).
[2] J. Lemaitre: *A Course on Damage Mechanics* (Springer Verlag, Berlin 1996).
[3] C. Sommitsch and G. Rüf: *Ductile fracture analysis with damage models of effective stresses at high temperatures* (Proc. ICTP ’05, Verona 2005).
[4] C. Sommitsch and W. Mitter: Acta Mater. 54 (2006), p. 357
[5] C. Sommitsch, E. Kozeschnik, G. Wasle and B. Buchmayr: *A precipitation model for multi-component multi-phase systems in nickel-base superalloys* (Proc. THERMEC´2000, Elsevier, Las Vegas 2000).
[6] E. Kozeschnik: Calphad 24/3 (2000), p. 24
[7] N. Saunders: Phil. Trans. 351A (1995), p.543
[8] J.-O. Andersson and J. Agren: J. Appl. Phys. 72 (1992), p.1350
[9] J.O. Andersson, L. Hoeglund, B. Joensson and J. Agren: *Fundamentals and Applications of Ternary Diffusion* (Pergamon Press, New York 1990).
[10] R. Sandström and R. Lagneborg: Acta Metall. 23 (1975), p. 387
[11] W. Roberts and B. Ahlblom: Acta Metall. 26 (1978) p. 801
[12] N. Srinivasan and Y. Prasad: Mater. Sci. Techn. 8 (1992), p. 206
[13] C. Sommitsch, M. Walter, S. Kleber, P. Pölt and S. Mitsche: STEEL GRIPS 3 (2005) 4, p. 287
[14] P. Pölt, C. Sommitsch, S. Mitsche and M. Walter: Mater. Sci. Eng. A (2006) in press.
[15] B.Tian, G.Zickler, C.Lind and O.Paris: Acta Mater. 51 (2003), p. 4149