Validation of an improved dislocation density based flow stress model for Al-alloys

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ABSTRACT: A microstructure and flow stress model for cell forming metals, 3IVM (3 Internal Variables Model), was developed [1], in which the work hardening and softening effects due to interaction of dislocation densities are taken into account. This model had been applied in through process modelling of sheet production. In the present paper, improvements of 3IVM are introduced. In the new model (3IVM+) the softening effect of recovery by cross slip and by additional dislocation reactions are considered in addition to that of climb. Moreover an improved kinetic equation of state is utilized. For validation, compression tests on a commercial Al-alloy were carried out and the flow curves were determined. The comparison between model predictions and experimental results shows that 3IVM+ can replicate the flow curves much better than the previous model, in particular at low temperatures and in wide temperature range. Since the concept of the model is unchanged, its applicability for through process modelling is not compromised.

Key words: Dislocation density, work hardening model, flow curve, compression test

1 INTRODUCTION

The modelling of forming processes, especially integrative approaches for process chain modelling, requires accurate knowledge on the flow stress of metallic materials. In traditional empirical models the flow stress is mathematically described by the imposed macroscopic forming conditions, such as strain, strain rate and temperature. But beyond the definition range, the model prediction is no more reliable. Moreover, such models provide no information about the microstructure evolution under the forming conditions. So in the recent years, more efforts were put on the development and improvement of physics based flow stress models.

2 3IVM AND ITS IMPROVEMENTS

2.1 Three internal variables model – 3IVM

A microstructure flow stress model 3IVM (3-internal-variable-model) had been developed for the cell building metals, e.g. Al-alloys, to predict the flow stress development [1]. The densities of three types of dislocations, namely mobile dislocation density ρ_m, immobile dislocation density ρ_i in cell interiors, and immobile dislocation density ρ_w in cell walls, are considered as internal state variables. Because of interactions and reactions among dislocations, dislocation densities change during their movements. For each type of dislocation density a rate is used to describe its evolution:

$$\dot{\rho}_{m,i,w} = \dot{\rho}^{+}_{m,i,w} - \dot{\rho}^{-}_{m,i,w} \tag{1}$$

$\dot{\rho}^{+}$ is the production rate and $\dot{\rho}^{-}$ the reduction rate of dislocation densities; they both have several contributions due to dislocation multiplication, spontaneous annihilation, dipole formation, lock formation, and recovery by climb.
The external stress is calculated using the kinetic equation of state

$$\dot{\gamma} = \dot{\varepsilon} \cdot \overline{M} = \rho_m \cdot b \cdot v\left(\tau_{eff}, T\right) \tag{2}$$

resolved to τ_{eff}. Here $\dot{\gamma}$ is the shear rate, $\dot{\varepsilon}$ the imposed strain rate, $\overline{M}$ the average Taylor factor, b the magnitude of the Burgers vector and $v(\tau_{eff},T)$ the average dislocation velocity depending on the effective stress τ_{eff} and the temperature T. To reach the required dislocation velocity, the effective stresses $\tau_{eff\,i,w}$ are needed in the cell interiors and cell walls, respectively. The necessary shear stress for the dislocation slip on a slip plane is the sum of this effective stress and the passing stress of dislocations:

$$\tau_{i,w} = \tau_{eff\,i,w}(v,T) + \alpha \cdot \mu \cdot b \cdot \sqrt{\rho_{i,w}} \tag{3}$$

where μ is the shear modulus and $\alpha \approx 0.5$ is a geometrical constant. The macroscopic flow stress k_f can then be calculated as

$$k_f = \overline{M}\left(f_i \cdot \tau_i + f_w \cdot \tau_w\right) \tag{4}$$

where $f_{i,w}$ are the volume fractions of cell interior and cell walls, respectively. More detailed descriptions of the model 3IVM and its application in the FEM simulations are referred in [1-3].

2.2 Improvements in 3IVM: 3IVM+

3IVM+ comprises a number of changes, they are compiled in [4]. In respect of dislocation density evolution, three additional effects are considered in equation (1): (i) immobilisation, for instance caused by the collinear reaction [5]; (ii) the clearing effect [4]; (iii) cross slip. Effects (i) and (ii) are reactions between mobile dislocations on the one hand (ρ_m) and immobile ones on the other (both ρ_i and ρ_w). They had not been considered in 3IVM. In (i), mobile dislocations are turned into immobile ones by the presence of other immobile dislocations. In (ii), mobile dislocations interact with immobile ones with the net effect of a reduction of ρ_i and ρ_w, whereas ρ_m is left unchanged. Finally in (iii), it is assumed that recovery can take place not only by annihilation after climb, which requires edge dislocations, but also by annihilation after cross slip, which requires screw dislocations. Still, no distinction is made between edge and screw dislocation densities because the cellular structure with its strongly bent single dislocations suggests that edge and screw contributions always remain essentially the same.

Another improvement from 3IVM to 3IVM+ lies in the function $v(\tau_{eff},T)$ of the kinetic equation of state (2). In 3IVM, the activation volume of thermally activated dislocation glide had been used as a fitting parameter (among others) [1]. The new model 3IVM+ makes use of a function $v(\tau_{eff},T)$ that had been derived from dislocation dynamics simulations of thermally activated dislocation glide [6]:

$$v(\tau_{eff},T) = \lambda v_0 \exp\left(-\frac{\Delta G(\tau_{eff})}{k \cdot T}\right) \tag{5a}$$

where $v_0 = 3 \cdot 10^{10}\,Hz$ is the attack frequency [6] and $\lambda = b / c^{1/2}$ is taken as the distance between activation events. c is the atomic concentration of solved atoms. The activation enthalpy ΔG is given by [6]:

$$\Delta G(\tau_{eff}) = \beta\sqrt{b^3 d_0{}^3 \mu \tau_{0K}}\,\frac{\tau_{0K}}{\tau_{eff}}\left(1-\frac{\tau_{eff}}{\tau_{0K}}\right)^{5/4} \tag{5b}$$

where β is a geometrical constant in the range 1.3 to 1.7 (fixed to $\sqrt{2}$), d_0 is the diameter of a foreign atom (fixed to $d_0 = b$), and τ_{0K} means the mechanical stress required to overcome the solved atoms at the temperature $T = 0K$. This stress depends on the solute concentration: $\tau_{0K} = c^{1/2}\tau_{0K,ref}$, where $\tau_{0K,ref}$ is a chemical fit parameter that only depends on the solved element. In 3IVM+, like in 3IVM, the inverted function $\tau_{eff}(T,v)$ is required. In order to get an analytical expression for $\tau_{eff}(T,v)$, the exponent $5/4$ in equation (5b) is altered slightly to unity before inversion of the function.

3 EXPERIMENTS

To validate the 3IVM+, uniaxial compression tests were carried out on the commercial aluminium alloy 8079-L delivered by Hydro Aluminium Deutschland GmbH. The chemical composition is listed in Table 1. Cylindrical samples (diameter = 18mm, height = 27mm) were taken from a partially recrystallised transfer-slab with a thickness of about 30mm and the cylinder axis parallel to the slab's normal direction.

All combinations of the temperatures 25, 100, 150, 200, 300, 400, 500, 550°C and the strain rates

$\dot{\varepsilon} = 0.1$, 1, 10, 100/s were applied. These test conditions comply with the industrial process conditions for both hot rolling and cold rolling. From 25°C to 200°C boron nitride and Teflon were used as lubrication, otherwise no lubrication was used. The experimental flow curves were temperature compensated [7], so that they can be considered as isothermal. The flow curves were used to setup the model parameters in 3IVM+ on the basis of experimental data. By the subsequent comparisons of experimental and calculated curves, the quality of 3IVM+ is examined.

Table 1. Chemical composition (in wt%) of the test material

Element	Si	Fe	Cu	Zn
Content	0.05	0.8	0.05	0.1

4 DISCUSSION

In materials modelling, an ideal physics based model would be able to predict the material property with one set of constant parameters for the whole process window. But it is often impossible to get such a suitable parameter set due to model assumptions. So in the following the performance of 3IVM+ will be discussed under two conditions, namely at low temperatures and with high strain rates.

4.1 Model prediction for low temperatures

A set of model parameters was firstly determined on the basis of flow curves at low temperatures (from 25°C to 200°C) with all tested strain rates. Fig. 1. shows the comparison of the experimental and the flow curves calculated with this parameter set at 150°C. Good agreement is found for the curves including their strain rate dependence. Similarly, Fig. 2. shows a good agreement of temperature dependence at the example strain rate of 10/s. The quality of agreement is similar in the whole range of flow curves with $T \leq 200°C$.

In order to demonstrate the improvement over the previous model 3IVM, a corresponding fitting attempt with 3IVM is plotted in Fig. 3. It must be stated that the agreement between calculations with the original 3IVM and the experiments is rather poor. In particular, 3IVM simulations always tend to have a constant work hardening rate at low temperatures, as can be seen from the constant slope for $\varepsilon = 0.2$ at $T = 25°C$ in Fig. 3. Since 3IVM had been developed for hot rolling, using climb as the only recovery process, it is not surprising that the ability of 3IVM to cover deformation at low temperatures is rather limited. At high temperatures however ($T > 200°C$), and for alloys with much higher alloying contents, 3IVM had been proven to be more successful [1-3].

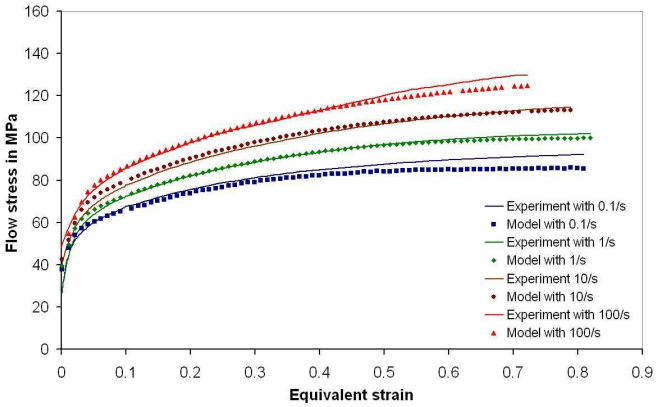

Fig. 1. Experimental and with 3IVM+ calculated flow curves of the alloy 8079-L at the temperature of 150°C

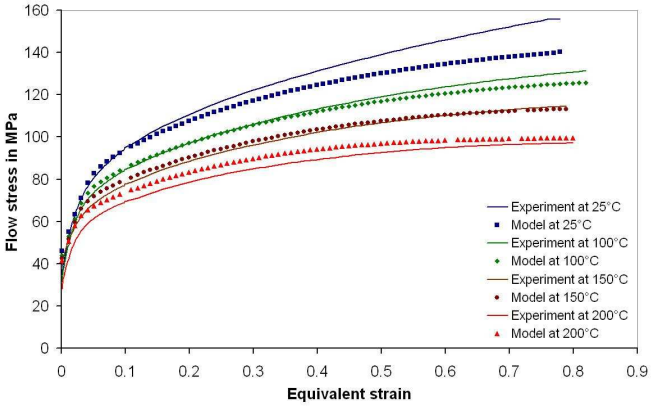

Fig. 2. Experimental and with 3IVM+ calculated flow curves of the alloy 8079-L with the strain rate of 10/s, using the same parameter set as in Fig. 1

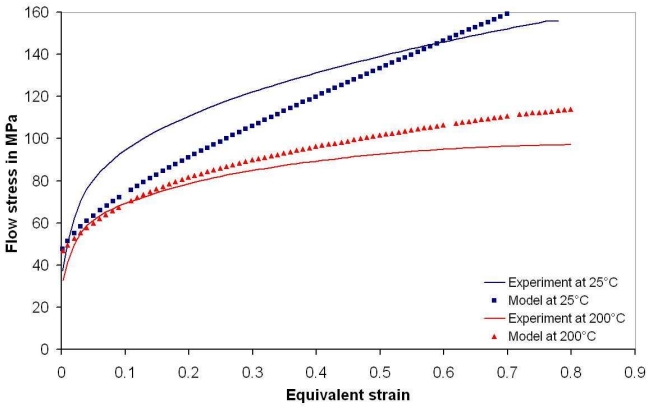

Fig. 3. With the previous model 3IVM calculated low temperature flow curves with the strain rate of 10/s

4.2 Model prediction for high strain rates

To validate the new model 3IVM+ even further for the demands of industrial applicability, another set of model parameters was fitted for a wide range of temperatures ($25°C \le T \le 550°C$). The strain rates were restricted to an industrially relevant range: $10/s \le \dot{\varepsilon} \le 100/s$. Fig. 4. shows the experimental and modelled flow curves with the strain rate of 10/s for all test temperatures. Again, a good agreement is found between model and experiment.

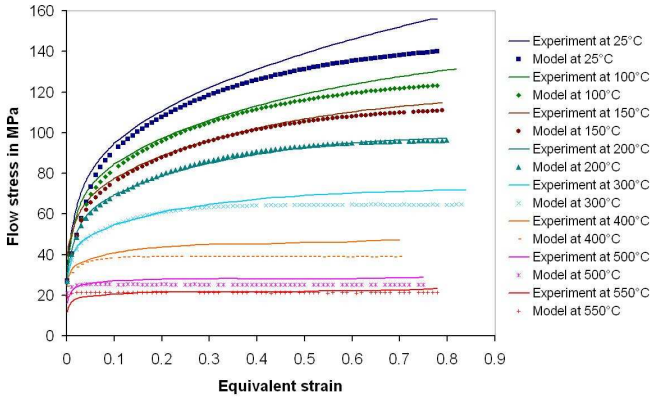

Fig. 4. Experimental and with 3IVM+ calculated flow curves of the alloy 8079-L with the strain rate of 10/s, using a single parameter set

It can be concluded, that 3IVM+ is able to describe the flow curves during the forming process at low temperatures much more accurately than the previous model 3IVM. Actually, it seems that no other physics based work hardening model in literature so far was able to cover such a wide range of temperatures with a single parameter set. The improvement of 3IVM+ is to be attributed to the new kinetic equation of state and to the dislocation interaction mechanisms newly introduced into the dislocation density evolution, namely dislocation cross slip, the clearing and the immobilisation effect.

5 CONCLUSION AND OUTLOOK

The dislocation density based microstructure flow stress model 3IVM is upgraded to 3IVM+. In 3IVM+, new aspects of interactions among dislocations are considered: immobilisation, clearing and cross slip. As the comparison between experimental and calculated flow curves from compression tests show, good agreements are achieved. Especially at low temperatures and for alloys with low alloying content, the flow curve description is improved.

After the integration of 3IVM+ into FEM, it is possible to carry out the through-process modelling in a refined way. For instance, recovery during the interpass time between rolling steps can be simulated with 3IVM+ using the strain rate $\dot{\varepsilon} = 0$. Subsequent recrystallisation modelling should be more accurate than before. For further validation of 3IVM+, double compression tests and the corresponding simulations will be performed, in which one compression test is interrupted, the sample is unloaded for the interpass period, and then reloaded. This procedure will offer a means for validation and hints for further improvements.

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REFERENCES

1. F. Roters, D. Raabe and G. Gottstein, Work Hardening in heterogeneous alloys – a microstructural approach based on three internal variables, *Acta Materialia* 48 (2000) 4184-4189.
2. R. Luce, M. Wolske, R. Kopp, F. Roters and G. Gottstein, Application of a dislocation Model for FE-process simulation, *Comp. Mat. Sci.* 21 (2001) 1-8.
3. M. Goerdeler, M. Crumbach, M. Schneider, G. Gottstein, L. Neumann, H. Aretz and R. Kopp, Dislocation density based modelling of work hardening in the context of integrative modelling of aluminium processing, *Mat. Sci. Eng.* A 387-389 (2004) 266-271.
4. G. S. S. V. Prasad, *An improved dislocation density based work hardening model for Al-Alloys*, PhD thesis, 2007, RWTH Aachen University.
5. B. Devincre, T. Hoc, L. P. Kubin, Collinear interactions of dislocations and slip systems, *Mat. Sci. Eng.* A 400-401 (2005) 182-185.
6. V. Mohles. *Thermisch aktivierte Versetzungsbewegung in Kristallen auf der Grundlage von Simulations-rechnungen*, Shaker Verlag, Aachen, 1997.
7. R. Kopp, R. Luce, B. Leisten, M. Wolske, M. Tschirnisch, T. Rehrmann and R. Volles, Flow stress measuring by use of cylindrical compression test and special application to metal forming processes, In: *Steel Research* 72 (2001), No. 10, 394-401.