tions in single crystals (or individual grains of polycrystalline materials) can be performed by means of dislocation and disclination dynamics. Summaries of the topic can be found in [1,2], for instance. The present paper is restricted to a brief consideration of recent work concerning

- substructure evolution in hot – working and
- generation of lattice rotations by formation of partial disclinatios in cold-working

of f.c.c. metals. The predictions of the modelling are in good agreement with the results of experimental investigations of the microstructure evolution in plastically deformed Cu single crystals oriented for multiple slip.

SOME GENERAL ASPECTS OF MICROSTRUCTURE – RELATED MODELLING OF PLASTIC DEFORMATION

Microstructure–related modelling of global plastic deformation requires the solution of the following tasks:

(1) choice of a problem - relevant microstructure scale and selection of the essential process - variables as, for instance, the deformation temperature T, the strain rate $\dot{\varepsilon}$ and the relevant structural variables (defect populations) S_j,

(2) derivation of a system of evolution equations

$$\frac{\mathrm{d}S_j}{\mathrm{d}t} = E_j\left(\dot{\varepsilon}, T, S_1, S_2, \ldots S_n\right)$$

for the quantities S_j and a kinetic equation for the transition from dS_j/dt to $dS_j/d\varepsilon$

(3) transition to the macroscale by means of a constitutive equation

$$\sigma = \sigma\left(\dot{\varepsilon}, T; S_1 \ldots S_n\right),$$

describing defect-induced changes of the flow stress σ, and

(4) controlling the results of the modelling by comparison with experimentally determined flow curves $\sigma = \sigma(\dot{\varepsilon}, T, \varepsilon)$ and work - hardening plots $d\sigma/d\varepsilon = f(\sigma, \dot{\varepsilon}, T)$ and (if possible) global and/or local substructure characteristics (e.g. mean total dislocation densities ρ, mean cell or subgrain diameters d, cell or subgrain misorientations Θ) estimated after deformation to different strains $\varepsilon = \varepsilon(\dot{\varepsilon}, T)$.

The essential defect populations, which should be taken into account within the framework of global modelling of deformation by means of dislocation - disclination dynamics, are summarised in Table 1. In this connection it seems convenient to remind of Volterra´s conception of elastic distortions [3]. According to this idea, deformation – induced displacement fields in solids can be described in terms of

- dislocations (i.e. translational distortions), the strength of which is characterised by the Burgers vector **b**, and by
- disclinations (i.e. rotational distortions), whose strength is determined by the Frank vector **ω**.

In crystals the strength of elastic distortions must correspond to the lattice geometry. Therefore, slip – induced strain can easily be described in terms of dislocation arrangements with a discrete distribution of Burgers vectors **b**. In contrast, Frank vectors **ω** of complete disclinations, which must be compatible with the rotational symmetry of the lattice, are not realised . However, because disclinations can be interpreted in terms of terminated dislocation walls, the introduction of incomplete disclinations (partial disclination dipoles – PDD´s) with continuously varying Frank vectors **ω** and the quantitative treatment of disclination reactions and dislocation - disclination interactions becomes possible.

Table 1: Essential defect populations in slip-based plastic deformation

Point defects	Dislocations (DL´s)	Disclinations (DDP´s)
• geometrical (g) and thermal (th) vacancies, • intrinsic interstitials (ist) with the concentrations c_g, c_{th}, c_{ist}	• edge (e) and screw (s) DL´s with the total densities ρ_e, ρ_s • mobile (m) and immobile (im) DL´s with the densities $\rho_{e,m}$, $\rho_{s,m}$ $\rho_{e,im}$, $\rho_{s,im}$ • DL´s within walls (w) and within the cell interior (in) of a cell structure with the densities $\rho_{e,w}$, $\rho_{s,w}$ and $\rho_{e,in}$, $\rho_{s,in}$ • excess dislocations (exc) of one sign with the densities $\Delta\rho_{e,exc}$, $\Delta\rho_{s,exc}$	• wedge (wd) and twist (tw) DDP´s with the densities Θ_{wd}, Θ_{tw}, • mobile (m) and immobile (im) DDP´s with the densities $\Theta_{wd,m}$, $\Theta_{tw,m}$ and $\Theta_{wd,im}$, $\Theta_{tw,im}$

The evolution of each structure variable of Table 2 depends on the evolution of all others. That means, in order to model slip–controlled plastic deformation of a single crystal in a general manner, the solution of at least 23 coupled differential equations would be necessary. For this reason it is necessary to reduce the number of structure variables by, for instance,

- specification of the deformation process and/or the problem of modelling,
- suitable collection (e.g. edge and screw dislocations or wedge and twist disclination dipoles) and/or neglection of certain defect populations, or
- adiabatic elimination (e.g. of the mobile dislocations, cp. [4]) of structure variables.

MODELLING OF HOT – WORKING OF F.C.C. METALS

Phenomena and problems

Hot - working of metallic materials ($T/T_m > 0.5$) is characterised by the competition of

- work - hardening due to the storage of immobile dislocations and
- mechanical softening due to dynamic recovery (i.e. dislocation annihilation and rearrangement) and, especially in f.c.c. and h.c.p. materials, also dynamic recrystallisation (DRX), i.e. generation and migration of high-angle boundaries.

Because DRX is experimentally observed even in uniaxial deformation of single crystals [5], its onset must be connected directly with the evolution of the dislocation structure and its nucleation stage should, therefore, be explicable theoretically within the framework of dislocation dynamics. However, in this connection it has to be taken into account that dynamic recovery and DRX are related to different length scales and modelling of hot – working requires two steps:

- consideration of the evolution and the stability of the dislocation arrangement (*microscale*) in dependence on the deformation temperature T, the strain rate $\dot{\varepsilon}$, and the stacking-fault energy Γ, and
- explanation of the occurrence of large lattice misorientations (high - angle grain boundaries; *mesoscale*) by dislocation reactions.

Modelling

Detailed information about the model presented here can be found in [1, 6 – 10]. It is based on the assumption of uniaxial deformation on multislip conditions (e.g. by compression of [001]-oriented single crystals) and the existence of an initial dislocation – cell structure [11] with prismatic dislocation–cells parallel and cell–wall orientations [110], [110] perpendicular to the operating stress σ, which has the following features:

- dislocation density ρ_w and flow resistance $\tau_w = \alpha G b \sqrt{\rho_w}$ [11]
- mean cell diameter : $d_w = K_w / \sqrt{\rho_w}$ with $K_w = 16$ [12]
- volume fraction of cell walls: $\xi = 2w_w/d_w = 0.45 = \text{const.}$ [13]
- mean dislocation path: $\lambda = 3d_w$ [14]

The evolution of the deformation-induced microstructure can then be described in terms of fluxes of mobile dislocations penetrating cell walls. In this connection the following defect reactions are taken into account:

- accumulation (immobilisation) of dislocations within the cell walls with the probability P = 1/3
- annihilation of screw dislocations via cross - slip events at distances $y_s = y_s(\rho_w, \dot{\gamma}, T, \Gamma)$ depending on the dislocation density ρ_w, the strain rate $\dot{\gamma}$, the temperature T [15,7], the stacking fault energy Γ, and
- annihilation of edge dislocations by spontaneous disintegration of dipoles at distances $y_e \approx 2 \times 10^{-9}\,\text{m} \approx 6b$ [16] or annihilation via vacancy – assisted climb.

Consequently, the essential structural variables of the deformation process are screw dislocations (s), edge dislocations (e), and geometrical (g) vacancies, and the global evolution of the defect populations is described by the equations (D – coefficient of self – diffusion)

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} c_g &= \frac{2\dot{\gamma}}{b}\frac{b^2}{3P} w_w \rho_s - \frac{24D}{d^2}\frac{c_g}{c_{th}} \\
\frac{d}{dt}\rho_s &= \frac{2\dot{\gamma}}{b}\frac{P}{w_w} - \frac{2\dot{\gamma}}{b} y_s\left(\rho_w, \dot{\gamma}, T, \Gamma\right)\rho_s \\
\frac{\mathrm{d}}{\mathrm{d}t}\rho_e &= \frac{2\dot{\gamma}}{b}\frac{P}{w_w} - \frac{2\dot{\gamma}}{b} y_e \rho_e - \frac{24Dd}{\sqrt{2}.bd^2}\frac{c_g}{c_{th}}\rho_e
\end{aligned} \tag{1}$$

Eliminating here the ratio c_g/c_{th} of the vacancy concentrations and introducing the dislocation content $N_w = w_w \rho_{w,\infty}$ of a cell wall and the fraction $\eta = \rho_{s,\infty}/\rho_{w,\infty}$ of the screw dislocations, the following expressions are obtained for the stationary state of the deformation process (ℓ_{SF} - stacking - fault width):

$$\frac{P}{N_{w,\infty}} = y_s\left(N_{w,\infty}, \dot{\gamma}, \ell_{SF}\right)\eta_\infty ; \quad \frac{P}{N_{w,\infty}} = \left[y_e + \frac{\sqrt{8bK^2}}{24P}\eta_\infty \right]\left(1 - \eta_\infty\right) \tag{2}$$

Numerical solution of the equations (2) with the material parameters of Cu leads to the following result [1,6,7,9]:

- Above a critical strain rate $\dot{\gamma}_{cr}$ only one stable value $N_{w,\infty}$ characterised by a high fraction η_∞ of screw dislocations occurs, while below $\dot{\gamma}_{cr}$ and above a critical value $N_{w,cr}$ three so-

lutions $N_{w,\infty}$ related to different fractions η_∞ are obtained. Two of them are stable, but one is instable. This indicates that spatial fluctuations of the initial dislocation structure give rise to the evolution of regions with different dislocation content $N_{w,\infty}$, the transition between them must be connected with remarkable lattice misorientations due to excess dislocations of one sign.
- The occurrence of a bistable deformation regime, which is considered as a criterion for the onset of DRX, depends on the strain rate $\dot{\gamma}$ and the stacking - fault energy Γ in satisfactory agreement with the experimental observations of DRX in pure f.c.c. metals.

In order to describe the development and the magnitude of local misorientations during the deformation, a linear chain of equidistant cell walls was considered, which is passed by dislocation fluxes $j^{\rightarrow} \neq j^{\leftarrow}$ of mobile dislocations of opposite direction with an immobilisa- tion probability $P = 1/3$ [1,5 - 7]. The accumulation of dislocations within the walls can be described in terms of the fluxes $j^{\rightarrow} \neq j^{\leftarrow}$ of mobile dislocations passing the cell walls in opposite direction with an immobilisation probability $P = 1/3$. Accordingly, introducing the flux $j = j^{\rightarrow} + j^{\leftarrow} = \dot{\gamma}/b$ of redundant (i.e. not contributing to the misorientations) dislocations and the excess flux $\Delta j = j^{\rightarrow} - j^{\leftarrow}$ responsible for the lattice rotations, evolution equations for both the total dislocation density $\rho_{w,i}$ and the excess $\Delta\rho_{exc,i}$ of a dislocation wall i can be derived. The misorientation α_i caused by $\Delta\rho_{exc,i}$ is estimated via the well-known Read-Shockley relationship $\alpha_i = b\, w\, \Delta\rho_i$.
The treatment shows that an evolution of the disorientations α_i takes place only if the strain rates $\dot{\gamma}_k$ (or the densities of mobile dislocations, respectively) within the cell walls $k \neq i$ are different. This requires the existence of significant local fluctuations of the dislocation content $N_{w,i} = w_{w,i}\, \rho_{w,i}$ and is in agreement with the conclusions drawn from the equations (2). Moreover, the model is able to predict misorientations corresponding to those of high-angle boundaries [1,5 - 7].

MODELLING OF COLD –WORKING UP TO LARGE STRAINS

Phenomena
Cold-working of metallic materials up to large strains ($T/T_m << 1$; negligible mobility of point defects) is characterised by
- dominating work-hardening due to dislocation accumulation in cell walls (*microscale* corresponding to stage III of single - crystal deformation) and in cell blocks or deformation bands (*mesoscale* related to stage IV of single-crystal deformation), whose generation is accompanied by considerable lattice rotations, and
- weak dynamic recovery induced by cross-slip of screw dislocations and spontaneous disintegration of edge-dislocation dipoles.

In this connection the following problems are of actual interest:
- description of cell-block formation and generation of long-range stresses in terms of disclinations
- usefulness of a dislocation - disclination reaction kinetics for modelling the transition from stage III to stage IV of flow curves (*micro- to mesoscale* transition)
- interrelations between lattice rotations and flow stress and work hardening.

Modelling

Detailed information about the model presented here is given in [2, 17 - 20]. As in the treatment of hot - working it is assumed that the plastic deformation takes place on multislip conditions and is accompanied by the development of a dislocation – cell structure with the density $\rho_r = \rho_w = \rho_M + \rho_\upsilon$ of redundant dislocations and the flow resistance $\Delta\sigma_r = \alpha MGb\xi\sqrt{\rho}$ [11], but in addition the formation of mobile and immobile partial disclination dipoles with densities Θ_m, Θ_{im} by consumption of sessile dislocations and capture of mobile dislocations [21] is supposed. In order to describe the substructure evolution, the following defect reac-tions are taken into account:

- generation of mobile dislocations by double cross slip (D)
- immobilisation (I) of mobile dislocation by storage within the cell walls (redundant dislocations)
- pairwise annihilation of mobile (A) or mobile and redundant (R) dislocations,
- formation of mobile disclination dipoles (F) via cracking and subsequent incorporation of arrangements of sessile dislocations by propagating microbands or capture of mobile dislocations by existing disclination dipoles, and
- immobilisation of mobile disclinations (J) by disclination reactions as e.g. the formation of triple junctions of cell blocks.

Consequently, the essential defect populations of the model are mobile dislocations ρ_m, redundant dislocations ρ_r stored within the dislocation walls (*microscale* substructure), and mobile and immobile partial disclination dipoles Θ_m, Θ_{im} (*mesoscale* substructure). The evolution equations of these structure variables are

$$\begin{aligned}
\frac{1}{\bar{v}}\frac{\mathrm{d}\rho_m}{\mathrm{d}t} &= D\rho_m - A\rho_m^2 - I\sqrt{\rho_m}.\rho_r - R\rho_m\rho_r - E\rho_m\Theta_m - K\sqrt{\Theta_{im}}.\rho_m \\
\frac{1}{\bar{v}}\frac{\mathrm{d}\rho_r}{\mathrm{d}t} &= I\sqrt{\rho_m}.\rho_r - R\rho_m\rho_r \\
\frac{1}{\bar{V}}\frac{\mathrm{d}\Theta_m}{\mathrm{d}t} &= F\Theta_m + \frac{K\bar{v}}{n\bar{V}}\sqrt{\Theta_{im}}.\rho_m - J\sqrt{\Theta_{im}}.\Theta_m \\
\frac{1}{\bar{V}}\frac{\mathrm{d}\Theta_m}{\mathrm{d}t} &= J\sqrt{\Theta_{im}}.\Theta_m
\end{aligned} \qquad (3)$$

In contrast to [21] the present model assumes that the propagation of PDD`s is caused by the consumption of a homogeneous current of mobile dislocations passing through the area $\Delta A = w_{PDD} \times y_c$ (w_{PDD} – dipole width) in front of the PDD. This results in a reaction term (E)

$$\left(\frac{\mathrm{d}\rho_m}{\mathrm{d}t}\right)_F = -j_v^{\rightarrow} y_c\Theta_m \approx -\frac{a\omega}{2\pi(1-\nu)}\frac{G}{\tau_{eff}}\bar{v}\rho_m\Theta_m$$

proportional to the dislocation flux $j_V^{\rightarrow}$ and to the capturing length y_c, which can be estimated by comparison of the stress due to the PDD´s with an effective slip resistance τ_{eff} caused by an irregular dislocation distribution [21], and allows the connection of the mean velocity $\bar{V}$ of the disclinations with the mean velocity $\bar{v}$ of the dislocation motion, $\bar{V} = (Gba/2\pi(1-\nu)) \cdot \bar{v}$ and via Orowan´s law the transition to the strain ε which is needed for the prediction of flow curves.

CHOICE OF CONSTITUTIVE LAWS FOR THE PREDICTION OF FLOW CURVES

The solutions of the equation systems (1) and (3) were used for the prediction of flow curves. In the first case the procedure is based in usual manner on the Taylor relationship (α interaction constant, M – Taylor factor, G – shear modulus, b – module of the Burgers vector, ξ - volume fraction of the cell walls, ρ - mean total dislocation density, cp. [11])

$$\Delta\sigma = \alpha(\dot{\gamma},T)\mathrm{MGb}\xi\sqrt{\rho} \tag{4}$$

and the calculated flow stresses are in satisfactory agreement with experimental data [1].
In the second case the formula (4) gives only the contribution of the redundant dislocations to the flow stress. In order to take into account the effect of disclinations, two additional equations are introduced:

- a Hall – Petch type relationship

$$\Delta\sigma_{CB} = K_{CB} / \sqrt{d_{CB}} \approx 0.776 k_{CB} \Theta_{im}^{1/4}, \tag{5}$$

  which assumes that the cell-block structure formed by the network of immobile DDP´s with the density Θ_{im} can be described in terms of a Poisson-Voronoi mosaic [22] and
- the relationship [3]

$$\Delta\sigma_{\omega} = \beta G\omega \approx 0.83\beta Gb(\Delta\rho_{exc} / \sqrt{\Theta_{im}}), \tag{6}$$

which takes into account the flow resistance due to the long range stresses of the disclinations
As shown in [1,19,20], solution of the equations (3) with interaction constants and material parameter for Cu and application of the relationships (4) – (6) leads to a flow-curve, whose course corresponds well to that experimentally obtained for a cold – rolled Cu single crystal with multislip orientation. Moreover, the deformation stage IV in the Kocks – Mecking plot $d\sigma/d\varepsilon = f(\sigma)$ of the calculated flow curve is obtained without special assumptions.

CONCLUSIONS

From the substructure models presented here the following conclusion can be drawn:

- Considering geometrical vacancies, screw and edge dislocations as the essential structure variables of hot – working and the deformation process as penetration of chains of cell walls, both the evolution of the global dislocation content and the formation of significant lattice rotations are predicted in a physically realistic manner and the onset of DRX can be interpreted as an instability of the dislocation structure.
- Schematisation of the substructure of cold –worked metals at larger strain in terms of disclinations offers an explanation for occurrence of long-range stresses and is able to describe the transition from stage III to stage IV of plasticity. The predicted values of the disclination strengths are in agreement with those determined recently by TEM [23].

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