# MICROMECHANISMS OF PLASTIC DEFORMATION IN METALS

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The paper reviews the macroscopic work hardening behaviour in the different stages of the deformation curve. While for stages II and III the storage of dislocations caused by multislip and their additional annihilation either via cross slip (low temperatures) or climb (high temperatures) are widely accepted, stages IV and V have found different explanations. These are critically discussed in the light of experimental results presently available. The importance of this discussion is increased since it has become clear that the strengthening behaviour of nanocrystalline metals produced by severe plastic deformation is governed by stage IV – strengthening mechanisms.

## 1. Experimental analysis of deformation stages

In the past, fundamental research of work hardening has been mainly devoted to early deformation stages II and III revealing them as stages of athermal storage and/or thermally activated annihilation of dislocations [1]. Apart from very recent discussion ([2] and below) no doubts have been risen that this annihilation is governed by the mechanisms of cross slip or climb, depending on the ratio of specific activation enthalpies and the deformation temperatures considered [3–6]. For detailed current models the reader is referred to the concepts of Püschl and Schöck [7] for the cross slip mechanisms, and that of Hirth, Lothe, Prinz, Argon, and Moffat [8] for the climb process.

In the last decade, the interests of plasticity science increasingly concentrate on the investigation of strengthening in stages IV and V of plastic deformation. These stages occur irrespectively of the deformation temperature (as an example see paper [9], this colloquium) in fcc [6, 10], bcc [11], hcp pure metals [12], and alloys [13] although on the latter only few studies exist. Following stage III, the features of stages IV and V are: a) a steady (i.e. constant or increasing) hardening in stage IV, and a re-softening in stage V (see Fig. 1, [14]); b) a constant strain rate sensitivity (SRS) in stage IV, a re-increase of SRS in stage V ([9] this colloquium, and [6, 11, 15]); c) the continuous increase of dislocation density in stage IV and its saturation

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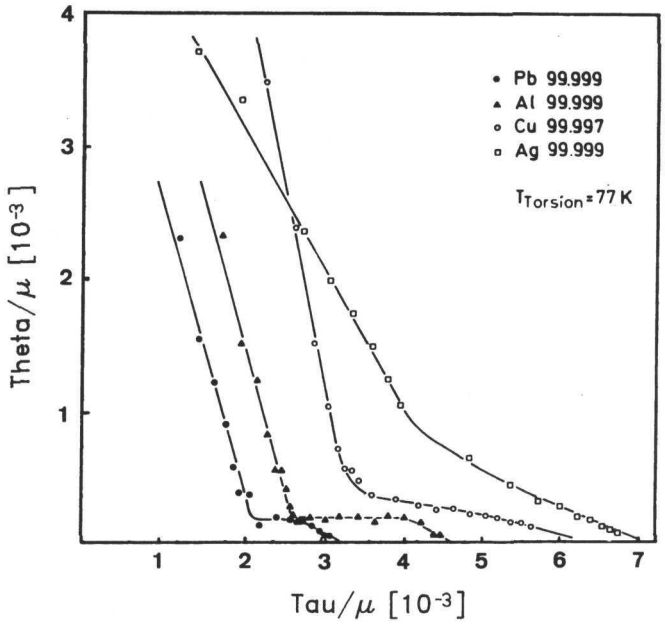


Fig. 1. Normalized work hardening coefficient $\Theta/\mu$ (shear modulus $\mu$) as a function of normalized external shear stress $\tau/\mu$ showing stage IV hardening in four fcc metals (from [14]).

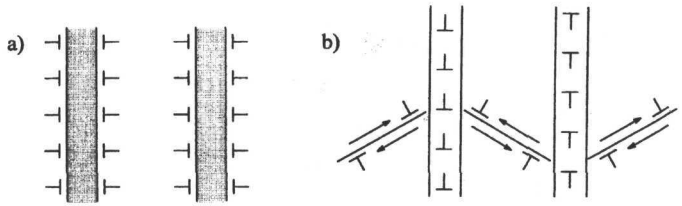


Fig. 2. Sketches of (a) polarized dipolar walls ("PDWs"), and of (b) polarized tilt walls ("PTWs") [17].

in stage V while the rate of subgrain shrinking compared to stage III is slowing down [6], and d) the transformation of dipolar dislocation cell walls into tilted subgrain--type walls (Fig. 2) as being indicated by the breakdown of internal stresses at stage IV onset which were measured by X-ray Bragg profile analysis (XPA) ([16–19],

Fig. 3a). Original dipolar cell separating areas with the same lattice orientation will change into tilt walls initiating lattice misorientation in stage IV. In recent XPA measurements with synchrotron radiation [19], a spatial resolution of 10 $\mu$m allowed for identifying local fluctuations of dislocation density and internal stresses (Fig. 4a), and their gradual spreading with increasing deformation (Fig. 4b). This confirms previous TEM findings [20, 21] that at the onset of stage IV, large lattice areas with several equally oriented cells ("cell blocks") start to disintegrate into smaller misoriented cell blocks finally reaching the minimum subgrain size at largest strains (called "*fragmentation*" in what follows).

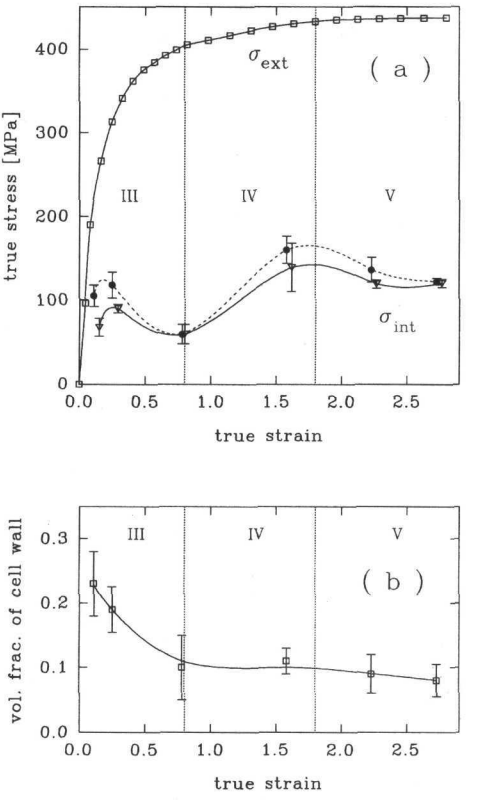


Fig. 3. Features of late stage deformation in cold rolled Cu: (a) □ – external stress-strain relationships [6], •, ▽ – internal stresses from XPA method [16, 19]: • in grain boundary, ▽ in grain interior; (b) volume fraction of cell wall material as a function of deformation [16].

## 2. Models for stage IV hardening

Although the statistical model of Kocks [22] appeared as fascinating in its elegant description of work hardening, it could not describe the work hardening at large strains. However, since Mughrabi made clear that a heterogeneous ("cell") dislocation structure can be described as a composite of soft and hard regions [23], the concept of Kocks proved its abilities by applying separately to hard and soft lattice areas. Several models have been designed by this principle [2, 15, 24–28], the most important being (in chronological order) these by *Zehetbauer* and *Les* (ZL) [15, 26], *Argon* and *Haasen* (AH) [27], and recently, by *Marthinsen* and *Nes* (MN) [2] and *Estrin, Toth* and co-workers (ET) [28]. The *ZL-model* formulates the hardening (athermal dislocation storage) and softening (thermally activated dislocation annihilation) for areas of screw and edge dislocations separately, without any interaction between inequal dislocations. This is derived from the idea that each of the dislocation type has a specific interaction

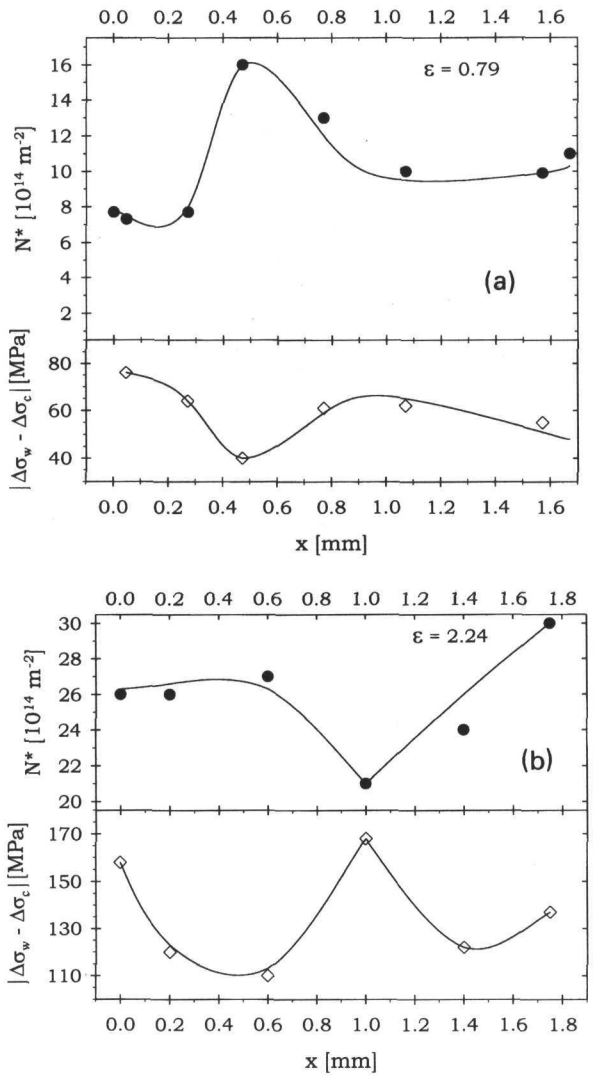


Fig. 4. Local fluctuations of dislocation density $N^*$ and long range internal stresses $|\Delta\sigma_w - \Delta\sigma_c|$ observed by synchrotron XPA-scans from grain boundary to grain boundary ($x$ = site of measurement, $\varepsilon$ = true strain, same samples as Fig. 3). (a) in transition range between stages III and IV, (b) well in stage IV (from [19]).

as well as annihilation behaviour which simply results in four different deformation stages. Stage IV hardening arises from the steady increase of one type of

dislocation density while the other is constant (for more details, see section 4). The *AH-model* [27] also starts from a composite ansatz but derives the stage IV hardening from long range internal stresses which evolve because of increasing misorientation between the subgrains. The *MN-model* [2] is also a "composite" model, and like in the ZL-model, the hardening of stage IV arises from storage of dislocations in cell walls while the dislocation density in cell interior is in steady state. However, the model distinguishes between different dislocation *structures* in cell interior (Frank network) and walls (subgrain dislocations). Stage IV hardening is related to the production of new cell/subgrain walls, corresponding to a decrease of cell/subgrain size which fits to the well known but only empirical relation [29] $\tau_w \equiv (\tau - \tau^*) = \alpha\mu b d^{-1}$ for the stress contribution from walls of cells *or* subgrains with size $d$ to total stress $\tau$, with shear modulus $\mu$, Burgers vector $b$, and constant $\alpha \approx 3$. The most recent *ET-model* [28] builds upon a careful mechanical treatment of a two phase stress composite. It considers not only the evolution of dislocation densities in each of the phases but also takes into account exchanges of dislocations between them. Essentially, stage IV hardening turns out to arise from a continuous decrease of the volume fraction of cell walls.

### 3. Discussion of models in the light of experimental results

The *AH-model* for the first time stresses the importance of the developing misorientation on a substructural level. Although the development of misorientation indeed seems to be intimately connected with stage IV hardening, and although an increase of internal stresses has been measured in stage IV [16, 18, 19], it is clearly seen in Fig. 3b that basically the internal stresses are a *consequence* of structural evolution rather than a *cause* of external strengthening. Moreover, the dislocation density in the walls is described to remain constant in stage IV, in contrast to the experimental evidence mentioned above. Without giving a theoretical basis, the *MN-model* provides the law $\tau_w \propto d^{-1}$ as the reason for stage IV and V hardening with a continuously shrinking cell/subgrain size $d$ because of new wall creation. However, most available experiments [19–21] favour the substructural fragmentation to occur where more and more cell walls within a cell block (CB) transform into tilt walls, finally reducing the size of this misoriented lattice area to a single cell which remains constant in stage V of the steady state deformation. Moreover, according to estimations by one of the authors [17] the hardening typical of stage IV, $\Theta_{IV} \approx 7$ MPa [6, 24] only results if one inserts the experimental sizes of *cell blocks* [6, 21] for $d$ instead of the cell/subgrain size. The *MN-model* also states two different climb mechanisms to operate which are specific to the networks of the cell walls and interiors. In the light of model calculations done in [26], however, it seems questionable how self-diffusion mechanisms and thermal vacancies could launch dislocation annihilation at such low deformation temperatures. In the *ET-model*, the crucial feature for stage IV hardening is the variation of volume

fraction occupied by cell walls with deformation. In contrast to TEM, the XPA method is capable to measure this quantity in representative sample volume at an enhanced accuracy (Fig. 2b): At first sight, the slope of $f$ in stage IV seems to be too small to satisfy the ET-model but, in view of the measuring error as well as of the somewhat uncertain limits of stage IV in a cold rolled sample, this question must be left to further experiments.

## 4. The model of Zehetbauer and Les

### 4.1 Model equations for low temperature

The theoretical composite model of Zehetbauer [26] is based on the assumption that the screw and edge dislocations do not interact and thus are placed in separate regions, screws in cell interiors, edges in cell walls. Then the macroscopic hardening $\Theta = \mathrm{d}\tau/\mathrm{d}\gamma$ is described in terms of hardening contributions $\Theta_1 = \mathrm{d}\tau_1/\mathrm{d}\gamma$ of screw regions with width $L_1$ (corresponding to the cell interiors) and $\Theta_2 = \mathrm{d}\tau_2/\mathrm{d}\gamma$ of the edge regions with width $L_2$ (corresponding to the cell walls). $\tau_1$ and $\tau_2$ are the plastic resistances of screw and edge regions, respectively. Using volume fractions $f_1 = [L_1/(L_1 + L_2)]^3$ for screws and $f_2 = 1 - f_1$ for edges* one can write the macroscopic hardening as $\Theta = f_1\Theta_1 + f_2\Theta_2$ and derive for the respective hardening contributions the equations: $\Theta_1 = C_1 - C_2\tau_1$, and $\Theta_2 = C_3 - C_4[\tau_2 - \tau_2(\gamma = 0)] \cdot \tau_2^5$ where the $\{C_i\}$ are the fitting constants of the model which describe storage and annihilation of dislocations. Using $\{C_i\}$ and material constants: Burgers vector $b$, Debye's frequency $\omega_\mathrm{D}$, Poisson's ratio $\nu$, atomic volume $\Omega$, core diffusion coefficient $D_{c0}$, enthalpy of vacancy migration $H_c^m$, dislocation interaction parameter of screws $\alpha_1$, and edges $\alpha_2$, and shear modulus $\mu$ one can calculate following physical parameters as output values of the model [26, 30]:

1. dislocation density $N = (f_1\tau_1^2/\alpha_1^2 + f_2\tau_2^2/\alpha_2^2)/b^2\mu^2$,
2. vacancy concentration $c = \sqrt{\pi/2}(1 - \nu)\exp(-H_c^m/\mathrm{k}T)\ C_4[\tau_2 - \tau_2(\gamma = 0)]\ \mathrm{d}\gamma/\mathrm{d}t\ \mathrm{k}T\alpha_2^4 b^2\mu^3/(\Omega D_{c0})$,
3. cell size $L = \alpha_1^2\mu^2 b/(2C_1\tau_1)$,
4. activation enthalpy of annihilation of screw dislocations $\delta G = -\mathrm{k}T\ln(C_2/\omega_D \cdot \mathrm{d}\gamma/\mathrm{d}t)$.

### 4.2 Model equations for high temperature

Modifying the model for high deformation temperatures ($T > 0.5T_m$) it is necessary to replace the mechanism of core diffusion by bulk one ($D_{v0}$) and the concentration of deformation induced vacancies by that of thermal ones. Edges are now in the cell interiors, screws in the cell walls [15]. Then, one arrives at new

* These equations for the $f_i$ are valid for $L_1 > L_2$. In the other case one has to use $f_2 = [L_2/(L_1 + L_2)]^3$ and $f_1 = 1 - f_2$.

equations for edge dislocation hardening contribution [15]: $\Theta_2 = C_3 - C_4\tau_2^3$ and for vacancy concentration $c = \exp(-H_c^m/kT)C_4\ d\gamma/dt\ kT\alpha_2^2 b^2\mu(1-\nu)/(2\Omega D_{v0})$. As a difference to low temperature, climb instead of cross slip governs stage III.

### 4.3 Consistency of the ZL-Model with experiments

In several publications [9, 15, 26, 30] the relevancy of the ZL-model to experimental findings has been demonstrated by revealing all the physical parameters to be realistic. We now examine whether the model also accounts for the structural fragmentation mentioned. In order to give an explanation for the $\tau_w \propto D^{-1}$ law ($D$ is cell block size) we assume that before they are incorporated into the walls, the edge dislocations have been piled up in front of a tilt wall, by a stress $\tau_p = \alpha_{\text{pile}} \cdot n \cdot \mu b/D$ for edge dislocations ($n$ is number of the piled-up dislocations [8]). By taking into account that wall strength $\tau_w$ only contributes by $f_w\tau_w$ to the total strength, one arrives at the empirical description of stage IV strengthening mentioned before (for Cu: $\alpha_{\text{pile}} = 0.5$, $n = 20$, $f_w = 0.3$). Since this stress must be equal to the local edge area stress in the ZL-model, one can derive $\alpha_2 = \alpha_{\text{pile}} \cdot n \cdot l_2/D$ ($l_2$ is the average dislocation distance in the edge area). After inserting the experimental values $l_2/D \approx 1/100$ and the other constants given above, $\alpha_2 = 0.1$ results which fairly coincides with the value obtained from fitting the strengthening data by the ZL-model. Therefore the above relation for $\alpha_2$ still reflects the fragmentation of cell blocks within the ZL model, although the relation has to be checked by further experiments, especially in the high temperature range.

## 5. Practical applications of stage IV

Comparison of the large-strain microstructures from the various deformation modes shows differences in the final subgrain size [29]. These probably arise from the different number and nature of slip systems activated in a given deformation mode. This idea may have motivated several workers [31–33] to use *a combination of deformation modes* in order to reach a very small cell, and in consequence, subgrain size being connected with a very high strength, according to the $\tau \sim D^{-1}$ law. It has been shown by the group of Valiev [33] that this could be used to produce even nanocrystalline metals and alloys which have a lot of attractive properties, in a commercial way and without harmful voids in the grain boundary produced by Gleiter's method of inert gas condensation [34]. Careful inspection of the literature shows that stage IV is extended by combination of different deformation modes. Therefore, a thorough knowledge on the strengthening processes of stage IV should enormously help in ruling the final grain size and/or in optimizing in the production procedure of this new important material.

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