

Mesoscopic Model – Simulative Approach to the Scatter of Process Factors in Microforming

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Increasing quantities in the field of microelectronics production as well as continuing miniaturization demand for efficient manufacturing processes. Therefore it is necessary to enhance the understanding of forming processes with smallest dimensions. Forming of micro parts, with dimensions smaller than one millimeter, is associated with a larger scatter of process factors than in common metal forming. The influence of the scatter of the grain size – within a single workpiece as well as within a several workpieces – on the forming process was detected in experiments.

This paper deals with the development of a numerical simulation model for the mesoscopic size, which enables a FE-simulation of the forming process as well as the simulation of the occurring scatter of the process factors. The mesoscopic model considers the influence of different grain structures on the forming process. An individual flow stress is assigned to each grain – modeled as a homogeneous body. It depends on the grain size and its position within the workpiece. The combination of both effects, the dependency of the flow stress on the grain size and on its position, enables an advanced description of the material behavior in FE simulations.

1 Introduction

Continuing miniaturization in many fields of our life results in a steadily increasing amount of industrially manufactured microparts. This demands the investigation of new production technologies. Microforming is such a technology, already established with high production rates and accuracy but also associated with some specifics to be regarded [1, 2]. While miniaturizing workpieces to micro scale, an increasing influence of the microstructure of the workpiece material on the process is detected. Grain interaction affects the integral flow stress as well as the shape and plastic strain. This leads to the fact, that small workpieces can no longer be regarded as homogeneous continuum for simulation purposes. Besides an observed reduction of the flow stress the scatter of the process factors increases. The purpose of the approach presented within this paper is to develop a numerical model that describes the effects detected in the area of micro forming with a minimized computational effort. To reach this goal, the new approach uses a model with simplifications concerning grain boundary conditions and grain orientation. The model is applied in FE-simulations, and the numerical results are compared with those gained in experiments.

2 Fundamentals

Basic research on the topic of simulation in microforming has been done by various authors. Sarma et al. carried out FE simulations discretizing the material in different grains whose forming

behavior depends on the orientation of the crystal lattice associated with each grain and on the critical resolving shear stress parameter of the slip systems. Plastic deformation of the grains is described by modeling grains with different slip plains. Based on Schmid's law, slip starts when the resulting shear stress reaches a critical value. Needed material parameters are obtained by fitting the crystal plasticity model to experimentally verified data [3]. Ku et al. did not model the real shape of each grain, but they also discretized the material in grain elements which are represented by six node elements which consist of two quadrilaterals. Each quadrilateral being built up of two four-node elements. They also introduced a new so-called grain boundary element which is used for the investigation of the sliding and extension between grains [4]. An alternative approach to study the influence of miniaturization on micro-forming processes by means of numerical simulation is shown by Engel et al. [5]. The geometry of the workpiece is divided into two areas: surface area and inner area. Within the simulation model, two different flow curves are assigned to the two areas. Due to the slight grain boundary influence on grains near the surface, the behavior of these grains resembles that of single crystals, while the behavior of grains within the material is equal to polycrystals. The transition between the flow stress $k_{f,i}$ of the inner area and the free surface area $k_{f,FS}$ is described in a discontinuous way. This approach explains the reduction of the integral flow stress with decreasing size of workpieces, but it is not able to show the influence of grain structure on the scatter of the forming factors. Another disadvantage is given by the unsteadiness of the flow stress at the transition from the inner material area to the surface area [6]. Advanced material simulation requires a simulation of grain structure similar to real material. Several techniques for the computational generation of grain structures have been developed. Among these, Monte-Carlo-Potts models, vertex tracking, front tracking, Voroni tessellation, phase field approaches and cellular automata are examples for different grain generation technologies [7]. Cellular automata are algorithms to describe the evolution of complex systems by using transformation rules. They are specified by a set of deterministic or stochastic transformation rules which are applied to the sites of a lattice. The lattice is typically regular and defined by a number of points which carry the actual values of state variables e.g. particle density. Probabilistic cellular automata allow a statistical description of grain growth as well [8].

3 Procedure of FE Simulation Applying a Mesoscopic Model

To get significant information about the scatter of process factors like forming limit and development of shape, a new simulation procedure is developed. It combines the advantages of grain modeling e.g. description of strain distribution and strain rate distribution close to real distributions with a more realistic material behavior e.g. description of the influence of the free surface on the flow stress of a single grain. The basic approach used in the mesoscopic simulation is shown in Fig. 1. The material is subdivided into grains. The grain structure is created by the approach of a cellular automata. Each single grain is modeled as a homogeneous area. The behavior of each grain is characterized by its size by means of the Hall-Petch equation, and by its position within the workpiece. In both, simulations and experiments, a cylindrical flat upsetting test is carried out. To get information concerning the scatter of the forming process the detected correlation between mean grain size, grain size distribution and the resulting scatter of the process parameters detected by experiments is used.

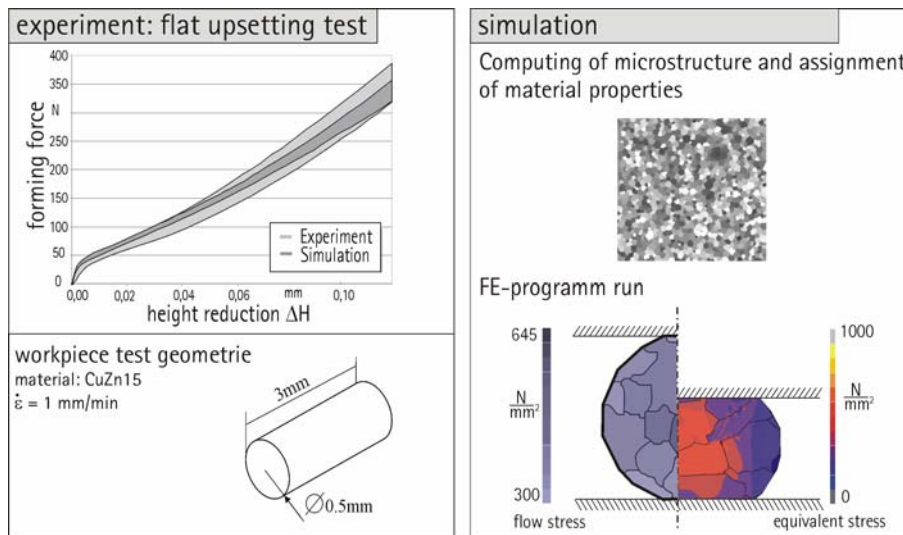


Fig. 1: Proceeding to simulate distribution and size effects

For the experimental cylindrical flat upsetting test, workpieces made of CuZn15 with different microstructures are used. The process factors of interest are the forming force and its scatter, respectively. The comparison of the results of experiments and simulation makes it possible to verify the chosen parameters of the simulation.

4 Experimental Setup

Cylindrical flat upsetting tests are carried out applying an UTS 5K testing machine with a Walter & Bai AG controller. The machine is equipped with a HBM 5kN load cell. The dimensions of the workpiece - as shown in Fig. 2 - are 0.5 mm in diameter and 3 mm in length.

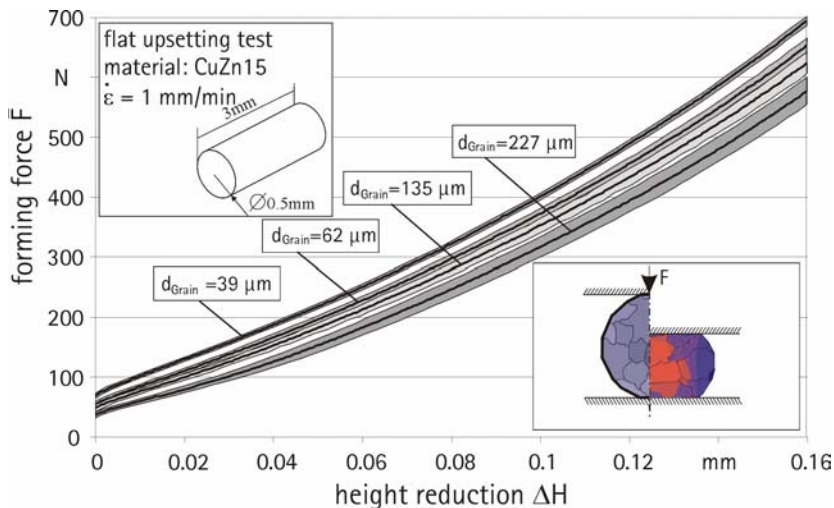


Fig. 2: Mean upsetting forces and their standard deviation obtained by experiments

This ensures plain strain condition in the center of the workpiece. A reason for the chosen material CuZn15 is the single phase material structure which simplifies the grain structure generation in simulation and reduces effects typical for multiphase materials. For each batch of 25 workpieces, heat treatments at different temperatures and tempering delays are done which results in mean grain sizes of $d_{\text{Grain}} = 39, 104, 193$ and $227 \mu\text{m}$ and a corresponding standard deviations of 20,7,

42.5, 100.3 and 113.6 μm [9]. High temperature oxidation is avoided by evacuating the heat chamber to a pressure of 10^{-5} bar. In order to get comparable measurements, friction is minimized by using MoS_2 -paste. The deflection of the testing machine is considered for the evaluation of the experiments. The number of 25 upsetting tests per batch is chosen to make a reliable statistical analysis of the experiments possible. The resulting runs of the mean upsetting forces obtained by the tests as well as their standard deviation are shown in Fig. 2. It is obvious that the scatter of the forming force depends on the mean grain size and thus on the chosen heat treatment. The distribution is identified by a Kolmogorov-Smirnov-Test as normal distributed at a confidence level of 99%.

5 Simulation setup

The material properties modeled in the FE-simulation should depict the behavior of real material at microscale, in order to get simulation results as close to experimentally obtained ones as possible. In conventional simulations, the material is assumed to be homogenous. Applying the mesoscopic model, each grain has different properties, depending on its size and position within the material. To automatize the procedure of FE-modeling, a simulation tool has been developed which generates grain structures with grain size and its distribution as input parameters and transfers the grain structure to the FE simulation program (MSC Superform 2002). The workpiece is modeled by 4890 quad elements. Depending on the grain a single element is attached, a certain flow curve is assigned to it. The approach of grain structure generation is based on the method of probabilistic cellular automata and enables a grain structure generation with predefined parameters. At first, a calculated number of start cells – depending on the mean grain size and the material volume – are positioned in a virtual area that will represent the material to be modeled. This area is divided into discrete lattice points, where some lattice points are occupied by start cells. To each start cell a maximum grain size is attached, calculated by means of a logarithmic normal distribution. The distance between two adjoining start cells is defined by half of the sum of their previously calculated maximum grain size. Several experiments show a significant interrelation between tempering delay, temperature and grain size distribution [10]. This statistical distribution is approximated by the density function of a logarithmic normal distribution, eq. (1).

$$f(d_{\text{Grain}}) = \frac{1}{d_{\text{Grain}} \cdot s_{d_{\text{Grain}}} \cdot \sqrt{2\pi}} \cdot e^{-\frac{(\log d_{\text{Grain}} - \bar{d}_{\text{Grain}})^2}{2s_{d_{\text{Grain}}}^2}} \quad (1)$$

The computed grain size distributions coincide very well with the experimentally determined ones. To describe grain structure generation, a statistical transformation rule is applied which consists of two parts, on the one hand the statistical selection of one cell to grow and on the other hand the statistical growing law. For grain selection, a normally distributed algorithm is used where each grain has the same probability to be selected for grain growth. Grain growth itself is characterized by an algorithm to minimize grain boundary energy. This is achieved by selecting the growing part x_i of the grain boundary by a statistically calculated frequency $p(x_i)$ which is affected by a frequency $p(x)$ equal for each part of the grain surface, the distance between the selected part of the grain surface and the center of gravity of the grain r_i as well as of the mean actual radius of the grain \bar{r} according to eq. (2).

$$p(x_i) = p(x) \cdot \left(1 - \frac{r_i}{r}\right) \quad (2)$$

If the growing part of the surface is selected, the grain size is enlarged by the lattice cell positioned next to the selected boundary element. The growth of each grain stops, if the maximum grain size is reached. The deviation between the predetermined mean grain size and the generated is less than 0.6 %. When the grain structure is defined, the individual flow stress for each grain has to be assigned. As mentioned above, the individual flow stress of each grain depends on its size and its position within the material. The reduction of the flow stress with the increase of the grain size is calculated by the well known Hall-Petch equation. As long as the grain structure is not at nanoscale, this model is well suited to describe the reduction of the flow stress. The dependency on the position in the material is based on Ashby [6] – where grains at the surface have less constraint than grains within the material – and on the surface layer model [5] – which deals with the reduction of the flow stress at a distinct surface area. To combine this influence of the free surface with the Hall-Petch equation, eq. (3), a pile-up Factor ξ is introduced which describes the amount of dislocation pile-up at the grain boundary at a single grain, eq. (4).

$$\tau = \tau_0 + \frac{m_{1,2} \cdot \tau_1 \cdot \sqrt{\lambda}}{\sqrt{d_{Grain}}} \quad (3)$$

$$\xi = \frac{1}{l_{Boundary}} \sum_{Boundary} \frac{l_{contact} \cdot k_{f,neighbor}}{k_{f,Grain}} = \frac{\bar{k}_{f,neighbor}}{k_{f,Grain}} \quad (4)$$

Dislocations are assumed to pile up until the stress concentration exceeds the stress τ_1 at which dislocation sources will be activated in neighboring grains. The factor λ represents the distance between the pile-up source from the dislocation, τ_0 is the critical shear stress in the considered grain and $m_{1,2}$ a matrix to transform the shear stress from the first sliding system into the next one. In eq. (4) $k_{f,neighbor}$ represents the flow stress of the neighboring grain, $k_{f,Grain}$ is the flow stress of the selected grain, $l_{Boundary}$ the total boundary length of the considered grain and $l_{contact}$ the length of the grain boundary between two adjoining grains. With the assumptions of homogeneous material behavior within each grain, the negligibility of grain orientation and a stress required to activate gliding systems in neighboring grains equal to its flow stress, the critical shear stress can be formulated as eq. (5).

$$\tau = \tau_0 + \frac{1}{l_{Boundary}} \cdot \sum_{Boundary} \left(\frac{m_{1,2} \cdot l_{contact} \cdot k_{f,neighbor} \cdot \sqrt{\lambda}}{\sqrt{d_{Grain}}} \right) \quad (5)$$

Combining eqs (5) and (4) leads to eq. (6)

$$\tau = \tau_0 + \frac{m_{1,2} \cdot k_{f,Grain} \cdot \xi \cdot \sqrt{\lambda}}{\sqrt{d_{Grain}}} \quad (6)$$

Eq. (6) could be simplified to eq. (7).

$$\tau = \tau_0 + \frac{k \cdot \xi}{\sqrt{d_{Grain}}} \quad (7)$$

In equation (7), k is the Hall-Petch material parameter which can be determined by upsetting tests using material with different grain size as shown in Fig. 3a. The introduced pile-up factor is defined for each part of the volume as the ratio of yield stresses between two adjoining grains, which are calculated by the Hall-Petch equation. The pile-up factor, attached to the free surface of the workpiece is set to zero because of the missing ability for dislocations to pile up. The distribution of the pile-up factor in a two dimensional section of the workpiece is shown in Fig. 3b.

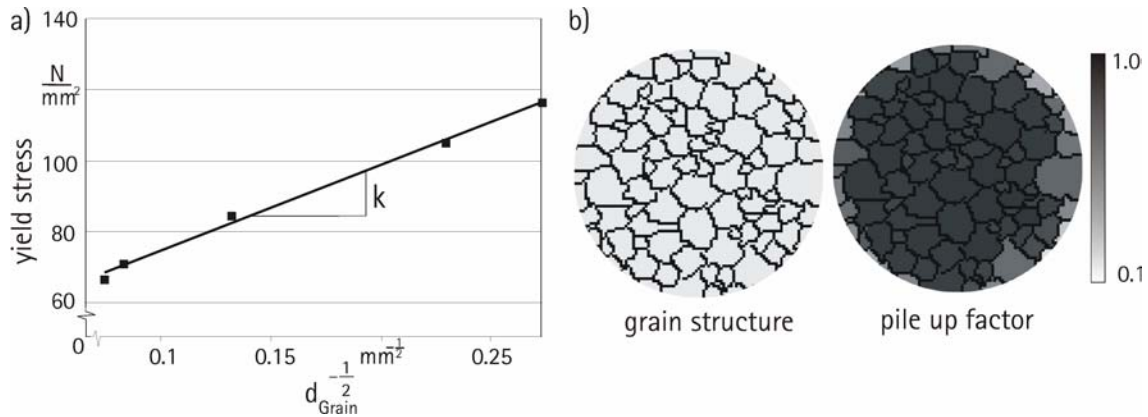


Fig 3: a) Hall-Petch relation for the material CuZn15
 b) Distribution of the pile up factor on the cross section of the specimen

6 Determination of the scatter of process factors

Various flat upsetting tests at microscale with different mean grain size show a significant correlation between the standard deviation of the grain size s_{Grain} , the diameter of the workpiece $d_{workpiece}$ and the mean standard deviation of the forming force \bar{s}_F related to the mean forming force \bar{F} as can be seen in Fig 4.

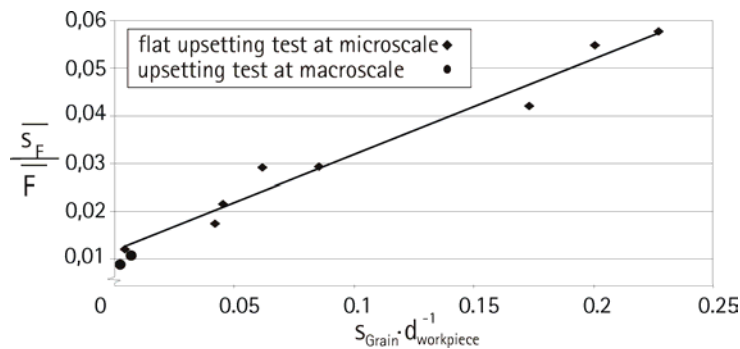


Fig. 4: Correlation between the variation coefficient of forming force and scatter of grain size

It is obvious that the increasing scatter of the grain size is the reason for the increasing scatter of the forming force. At a level of high scatter of the grain size, the individual grain structure of each sample is more different from the others than at a level of small grain size scatter.

7 Comparison of Simulation and Experimental Results

In order to compare simulation results with experiments, simulation is carried out with parameters equivalent to experimental determined grain structure attributes. The input data for the grain generation in simulation is the mean grain size and its distribution. The friction coefficient for simulation is set to $\mu = 0.2$. A variation of the friction coefficient shows only small influence on the simulation results. As shown in Fig. 5 a linearly decreasing offset depending on the grain size could be observed.

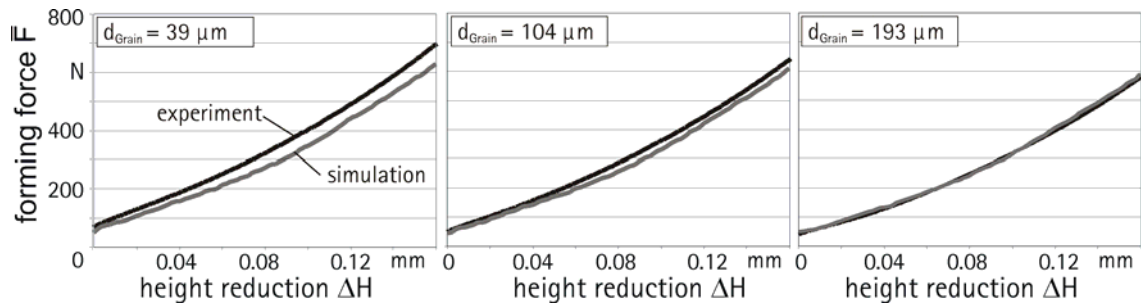


Fig. 5: Comparison between simulation and experimental results concerning flat upsetting test

The production process of workpieces at microscale – which are drawn from a wire with a high forming degree – causes additional pile-ups and distortions of the grain lattice. A heat treatment reduces, depending on the annealing duration, the amount of these additional pile-ups as well as the distortions. Therefore the influence of the production process on the flow stress is reduced by a heat treatment down to no influence determined at a mean grain size larger than $193 \mu\text{m}$. Fig. 6 shows experimentally determined flow curves, both done with the same material but at different scales and production processes. As expected, the experiment with macroscopic specimen ($d = 5 \text{ mm}$, $l = 5 \text{ mm}$) manufactured by turning shows a significantly lower flow stress than the microscopic experiment ($d = 0.5 \text{ mm}$, $l = 3 \text{ mm}$) whose billets are drawn from wire. To take into account the work hardening effects, the mean flow stress of the simulation has been raised from 15 % (mean grain size $d_{\text{Grain}} = 4 \mu\text{m}$) down to 0 % ($d_{\text{Grain}} > 193 \mu\text{m}$). As shown in Fig. 7, simulation considering the work hardening fits the experimentally determined process forces with a mean deviation of 3.47 %.

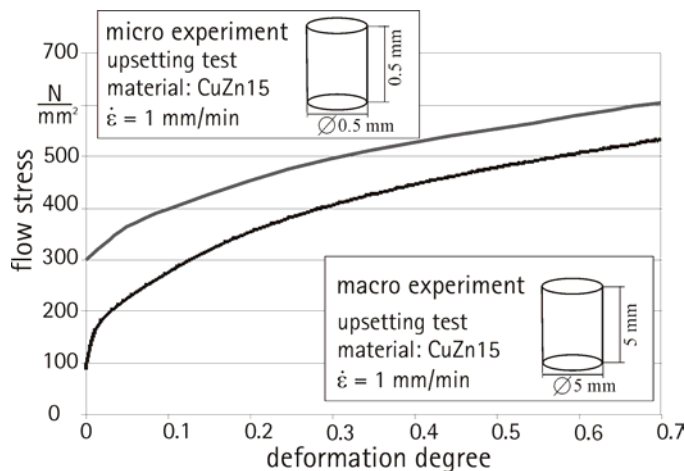


Fig.6: Comparison of the flow stress gained with experiments at microscale and at macroscale

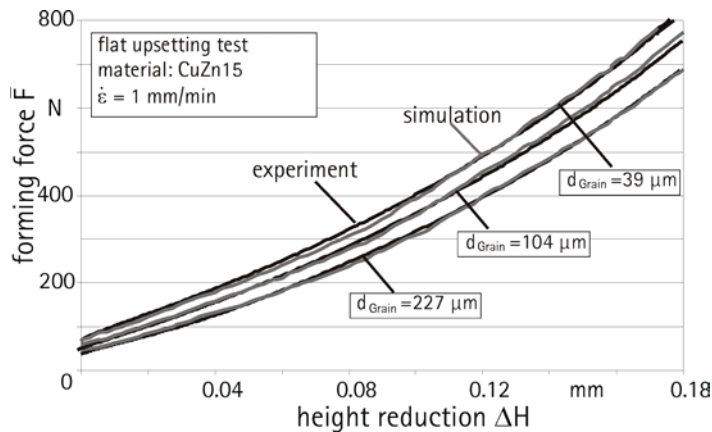


Fig. 7: Comparison between simulation and experiment considering the work hardening effect

8 Conclusion and Outlook

The presented results show that the mesoscopic model developed so far turns out to be a promising and simply applicable basis for the size dependent process simulation yielding not only discrete information about the process but also about its scatter. Thus, it is in particular suited to be applied for microforming. Compared to conventional process simulation the only input parameters additionally required are the mean grain size, its standard deviation and the Hall Petch coefficient for the material in consideration. Actually the model is confined to single phase material and grain orientation is not considered. Future investigations are targeted to make the model applicable for other microforming processes finding out which improvements (e.g. consideration of grain boundary behavior) are necessary and in which way they can be realized.

9 References

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