

Modeling approach regarding surface functionalization by force-controlled micro and nano forming

E. Uhlmann^{1,2}, S. Kühne¹, M. Jagodzinski¹, M. Malcher¹, R. Trevino¹

¹Institute for Machine Tools and Factory Management IWF, Technische Universität Berlin, Germany

²Fraunhofer Institute for Production Systems and Design Technology IPK, Germany

kuehne@mfg.tu-berlin.de

Abstract

Surface functionalization allows the control of fluidic, tribological, biological or optical properties. Suitable processes are interference lithography (IL), ultra-precision machining and micro and nano forming. The force-controlled forming process enables a reproducible production of structures with an absolute height in the double-digit nanometer range. The deformation is a complex process consisting of controlled and uncontrolled material deposition. Knowledge about the uncontrolled behaviour, however, allows a reproducible production of defined structures. A model approach with regard to machining parameter prediction is presented here. The tool shape is transferred into the surface by plastic penetration of a faceted diamond tool. By means of a superimposed tool movement, linear structures can be generated. Larger areas can be structured by repeating this process. The advantage of the force control in comparison to the displacement control is a defined penetration depth relative to the surface with reproducibility in the single-digit nanometer range. The force-control is carried out gravimetrically ($0.05 \text{ N} < F < 0.15 \text{ N}$). Therefore the tool and additional precision weights are suspended on low stiffness ($C = 0.0007 \text{ N}/\mu\text{m}$) flexures. The structuring of free formed surfaces can be realized by adapted tool manipulation. For this purpose, the tool needs to be guided along the corresponding surface. Depending on the structure, suspension of the tool can tolerate shape deviations of the substrate. This process can be adapted to different materials and applications. The development of the model is based on the example of diffractive optical structures ($1000 \text{ mm}^{-1} < g < 500 \text{ mm}^{-1}$, $30 \text{ nm} < h < 300 \text{ nm}$) and statistical experimentation. The deviation of the ideal profile from the cross-sectional area measured via AFM was used as control variable. A surface deviation that approaches nearly zero ($10 \text{ nm}^2 < A_{\text{neg}} < 100 \text{ nm}^2$) is considered as ideal load. As additional result of these experiments, physical approaches are available, which can later form the basis of a physical model.

Keywords: DOE, micro forming, surface functionalization, micro optics, nano forming

1. Introduction

Micro forming includes a variety of technologies. A comprehensive summary is given by VOLLERTSEN [1]. The processes are divided into bulk metal forming and sheet metal forming. The process presented below describes a deformation of a thin surface layer of bulk material. A tool shape is transferred into a surface by plastic penetration. By means of a superimposed tool movement, linear structures are generated. Larger areas are structured by repeating this process. The forming process enables a reproducible production of structures with a height of $h = 30 \text{ nm}$. The origins of this technology, carried out on special machines, are attributable to ROWLAND [2]. They can be replaced with ultra-precision machines [3] to enable increased degrees of freedom in production. The deformation is a complex process which cannot be completely described physically yet. The process consists of controlled interactions, which are determined by the tool geometry, and uncontrolled behaviour, which leads to interactions of the structural features. Knowledge about the uncontrolled behaviour allows a reproducible production of defined structures. The process is very sensitive to the feature geometry and material properties. If the feature dimensions are in the range of the material grain size, the material loses the isotropic behaviour of the bulk material and local anisotropic behaviour occurs [4]. For this reason, fine-grained or amorphous materials were used. The following

investigations address saw tooth (blaze) structures for the production of diffraction gratings.

2. Experimental setup

2.1. Machine and measurement

The machine used for the basic research is a modified 3-axis ultra-precision machining center LT-ULTRA Mmc1100. To enable 5-axis machining a tilt and turn module with two additional rotational hydrostatic axes (A and C) is mounted to the machine. The positional reproducibility of all linear axes is $< 40 \text{ nm}$, the angular resolutions of the rotatory axis is $< 5''$. All structures are produced on a 300 nm layer of finely grained Au on a polished silicon substrate. To enable the required measurement accuracy in the nanometer range a BRUKER NEOS N8 AFM has been used. The lateral and vertical resolution is $< 1 \text{ nm}$.

2.2. Micro forming module

A specially developed tool module (Figure 1) enables the force-controlled forming. The module is based on a flexure parallel kinematic, which allows a soft suspension (stiffness $C = 0.0007 \text{ N}/\mu\text{m}$) in the Z-direction and offers a high stiffness in the lateral directions. On the moving parts of the module there is a squeeze-film damping to reduce vibrations. The adjustment of the process force is carried out gravitationally, by applying precision weights. This weight control has absolutely no fluctuations, which is an advantage compared to

closed loop systems. The force is measured on a high-precision scale within the machine. The tool is positioned on the scale by means of the machine axes. The fine adjustment can be made by deflecting the flexure. The deflection of the movable part of the module is detected by means of a chromatic sensor. The operating point determined in this way is adjusted when the work piece is being touched. The tool holder offers the possibility to adjust the tool in three degrees of freedom (Figure 1).

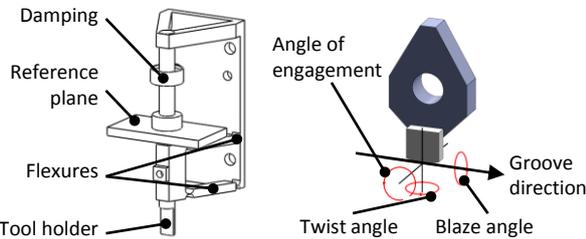


Figure 1. Micro and nano forming module

3. Procedure

3.1. Micro forming

The saw tooth geometry is defined by the line spacing b and the angle of the individual features (blaze angle) α . Additional parameters are feed rate f , angle of the substrate β , twist angle γ , and weight force F or weight m . In order to understand the structure formation, the profiles of three grooves for different weight forces are shown in figure 2. It is characteristic that the structure is not completely filled at small weights. By discrete increase of the weight, the filling rises to the point of completeness. By further increases, deformations occur in the adjacent lines. In addition, it can be seen that there is a lateral displacement as well as a changed penetration depth of the single lines. The consideration of different structural parameters shows that the filling is influenced by the weight which relates to b and α as well as by the shear of the material which relates to α .

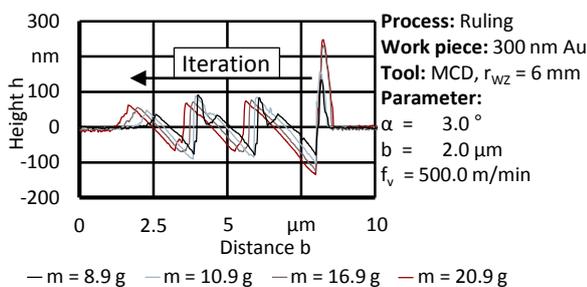


Figure 2. Measurements of the structure formation

3.2. Modeling

The described parameters are used for the modeling. The twist angle has a fixed setting $\gamma = 0^\circ$ due to the method. The influence of the variables f and β is present but determined as not significant in the first model and excluded. As the command variable for the modelling, the surface deviation at underload A_{neg} is used (Figure 3). The optimum is achieved when $A_{neg} \approx 0 \text{ nm}^2$. The determination is automated with using MATLAB®. The complex program essentially compares the structure with the targeted structure by means of discrete integration. Therefore, the structure is determined by discrete derivation of the measured profile and determination of the saw tooth flanks with threshold filters. The automation allows a large number of samples to be analysed. Using the design of experiment (DOE) method of circumscribed central composite design (CCCD) on the basis of statistical experimentation, the obtained data is used to set up and validate a multi-regression model. The modeling space is selected in the application-oriented range $1 \mu\text{m} < b < 3 \mu\text{m}$, $2^\circ < \alpha < 5^\circ$ and

$30 \text{ nm} < h < 300 \text{ nm}$. In preparatory one factor at a time trials, it has been shown that a logarithmic fit promises a realistic approach. Nevertheless, various model approaches were investigated.

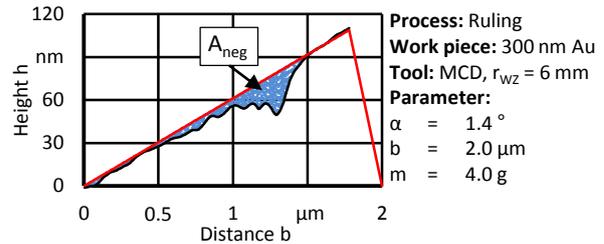


Figure 3. Schematic representation of the command variable A_{neg}

4. Results

The statistical evaluation has shown that a model with the approach of formula 1 ($A \rightarrow m$, $B \rightarrow b$, $C \rightarrow \alpha$) considering the interactions $m b$ and $b \alpha$ allows the best approximation $R^2 = 0.9814$ with the least error probability $p = 0.02976 \%$.

$$A_{dom} = \exp(a_0 + a_1 A + a_2 B + a_3 C + a_4 AB + a_5 BC) 10^{12} \quad (1)$$

$$a_0 = -34.57, a_1 = -1.12, a_2 = 2.86, a_3 = 0.58, a_4 = 0.37, a_5 = 0.86$$

Particularly conspicuous on the model is the very small influence of α . Especially because it has a larger contribution to the cross-sectional area of the saw tooth profile a high influence was expected. This is also justified due to material shearing. The model allows the determination of the optimum weight at A_{neg} near zero. Of course, the logarithmic function will never reach zero. However, depending on the structure in the region $10 \text{ nm}^2 < A_{neg} < 100 \text{ nm}^2$, the surface deviation is reduced to the noise level of the surface roughness. On this assumption, a direct mathematical relation between b and m can be established, which permits the determination of an ideal weight force. The previously iterative determination of this force is thus simplified. Due to process noise, only a fine adjustment may be necessary. Figure 4 represents the model and validation attempts.

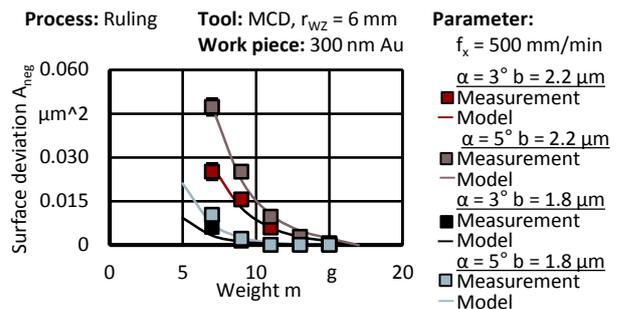


Figure 4. Exemplary comparison of model and validation data

5. Summary

The structuring by means of micro and nano forming was modeled by the DOE method CCCD based on an introduced command variable A_{neg} . In particular, the high influence of shear is a basis for a physical modeling, taking into account the previously neglected friction effects.

References

- [1] Vollertsen F 2013 Micro Metal Forming Springer
- [2] Rowland H.A. 1882. Preliminary notice of the results accomplished in the manufacture and theory of gratings for optical purposes. The Observatory 5, 224–228.
- [3] Kühne S., Haskic K., Lemke S., Schmidt M., 2014. Fabrication and characterization of machined 3D diffractive optical elements. Microsyst Technol 20 (10-11), 2103–2107.
- [4] Rosochowski A, et al 2007 Micro-extrusion of Ultra-fine Grained Aluminium. The International Journal of Advanced Manufacturing Technology 33:137–146.