

NUMERICAL SIMULATION OF MICROLEVEL EXPERIMENTS ON MG ALLOY

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Abstract: *The paper presents a numerical simulation used for design of low level experiments on cantilever micro-beams prepared from magnesium alloy AZ31 by focused ion beam milling. Three dimensional FEM models for un-notched and notched micro-beams characterized with elasto-plastic-fracture behavior were created to compare the deflection of beams at yield strength and at fracture to optimize geometric dimensions of the beams with respect to other experimental techniques used for specimen loading (nanoindentation). Possible collisions with surrounding surface of the milled material are calculated. As the main parameter, the cantilever length was varied in the interval 10 to 20 μm and depth of the notch in 0-50% of the beam depth. Taking into account maximum deflections and possible nanoindenter tip to surface collisions the most reasonable dimensions of cantilevers were selected between length of 12 μm and 14 μm and the notch size of minimum 30 % of the beam depth.*

Keywords: magnesium, AZ31, FEM model, micro-beam

1. Introduction

Magnesium and its alloys are lightweight materials with high specific strength, low density and high damping capacity, see (Krainer, 2003). One of the most common alloys include AZ31 (nominally 3wt.%Al-1wt.%Zn-0.3wt.%Mn-Mg balanced) that is widely used, e.g. in automotive, train and aviation industries. Besides the favourable mechanical properties the alloys suffer from difficult formability mainly at ambient temperatures leading to cracking and brittle failure, which represent one of the primary obstacles to its use. New methods of production have been proposed in order to improve material properties such as dieless drawing, (Huang, 2017; Kustra, 2016). Production parameters of these methods are, however, very sensitive and need to be optimized, (Milenin et al., 2016).

At macroscale, the alloys are characterized with the brittle failure in normal temperatures, (Wu, 2017). The source of the macroscopic brittleness is not obvious but is caused most probably by inter-grain defects that are present at the microstructure. On the other hand, at grain level the material exhibits high ductility as documented by various microscale experiments including micropillars compression or micro-beam bending, (Pozuelo, 2017). These experiments are often performed on samples prepared by advanced microscopic techniques, namely Focused Ion Beam (FIB) milling, (Reyntjens, 2001). Samples are further loaded by in-situ or ex-situ nanoindentors to measure mechanical properties of the samples, (Nemecek, 2018).

The purpose of this contribution is to investigate small-scale plastic-brittle behavior of micro-beams prepared by FIB and tested in bending. Prediction of load-displacement diagrams, onset of plasticity, failure strains and deflections are critical for proper setting of micro-scale experiments (both fabrication of micro-beams and subsequent loading by nanoindenter).

2. Problems connected with micro-beam fabrication and loading

The micro-beams are prepared by FIB where Gallium ions are used to bombard and sputter the material. In this way, various geometries of small scale samples can be prepared. The process is, however, time demanding and thus must be carefully optimized. Creating of a beam takes hours (typically 1 to 8), depending

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on accelerating voltage used. The testing of the beam is done by nanoindentation which is usually used to characterize mechanical properties of the material by penetrating with small diamond tip into the surface. In this case the instrument is used to load the beam by bending. Since high plastic strains are expected at the grain level maximum deflections of the cantilever must not collide with the loading tip and the trench prepared with FIB in the surrounding material. Thus, the tasks are to optimize the trench depth and width to allow high plastic deflections of the beam in bending and limit the time of its production. And secondly, the beam deflection curve should not intersect with the tip geometry which is a relatively flat pyramid with edge to horizontal angle of 13.1° . As a first step in the research solved in this paper, we calculate deflections, strains and stresses of a cantilever micro-beam with triangular cross section characterized with an elasto-plastic-brittle behavior. Two variants of the beams are solved, unnotched and notched. Geometrical interactions with the surrounding material are then calculated to predict optimum experimental setup.

3. Numerical model

The micro-beam bending was modelled as a three dimensional task using Ansys Workbench 17.2 software. Geometry was prepared with CAD software. The initial dimensions of the cantilever were chosen in accordance with previous experimental experience of authors with preparation of micro-beams by FIB and testing with nanoindenter on cementitious materials, see (Nemecek, 2018). The pentagonal cross section with width of $3.5\ \mu\text{m}$, height of $3\ \mu\text{m}$ and side edges $0.2\ \mu\text{m}$ was chosen. FE meshes for cantilever lengths lying in the interval of 10 to $20\ \mu\text{m}$ for either notched or un-notched variant were created. The notch width was $250\ \text{nm}$ for all cases. Since the notch depth greatly influences the beam deformation behavior its depth was varied in the range of 20-50% of the beam depth.

The FE mesh was created for each cantilever with element size of $0.2\ \mu\text{m}$ with further refinement at the cantilever fixed end. Elements SOLID187 were used for body. SOLID187 has a quadratic displacement behavior and is well suited for irregular meshes. The element is defined by 10 nodes with three degrees of freedom at each node. The element has plasticity large strain and deflection capabilities. SURF154 was used for applying the load at free end, see (Ansys, 2017). Micro-beams were loaded on top surface of the free end in central axis. Load was prescribed in time increments and deflections calculated. Several significant parameters were detected: deflection at elastic/plastic transition (onset of plasticity), deflection at reaching tensile strength (deflection at failure) and corresponding vonMises stresses calculated.

3.1. Material parameters

Uniaxial behavior of the AZ31 magnesium alloy was defined with an elasto-plastic constitutive law with linear isotropic hardening and ultimate tensile strength. Young's modulus of the material was determined by quasi-static indentation from several tens of indents as $42\ \text{GPa}$, (Jäger, 2018). Plasticity parameters were taken from the literature. Since there is a plenty of alloy manufacturing ways, the characteristics without any manufacturing improvement were taken into account. The values of yield and tensile strengths of extruded AZ31 were taken as $257\ \text{MPa}$ and $289\ \text{MPa}$, respectively, (Park, 2013). The hardening tangent modulus was taken as $188.35\ \text{MPa}$. The uniaxial stress-strain diagram of the material is shown in Fig. 1.

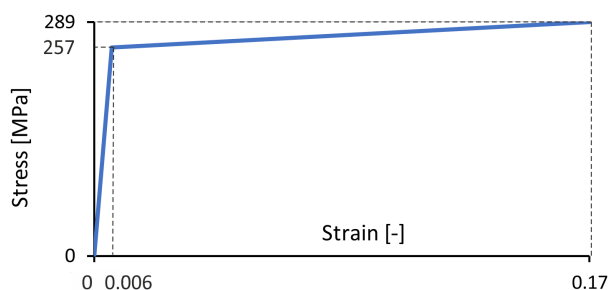


Fig. 1: The uniaxial stress-strain diagram.

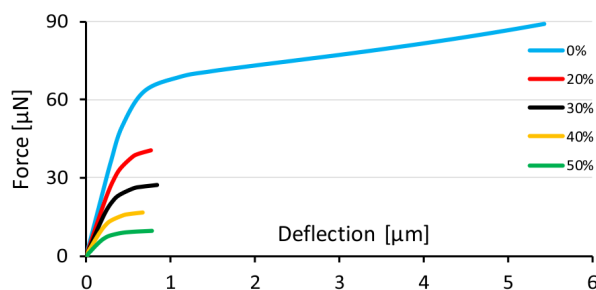


Fig. 2: Force-deflection diagrams - $14\ \mu\text{m}$ beams.

Thirty geometrical variants of the model have been calculated. The calculated deflections are summarized in Tab. 1. An example of distribution of equivalent (vonMises) stresses at failure load are shown in Fig. 3. An example of load-deflection diagram is shown in Fig. 2.

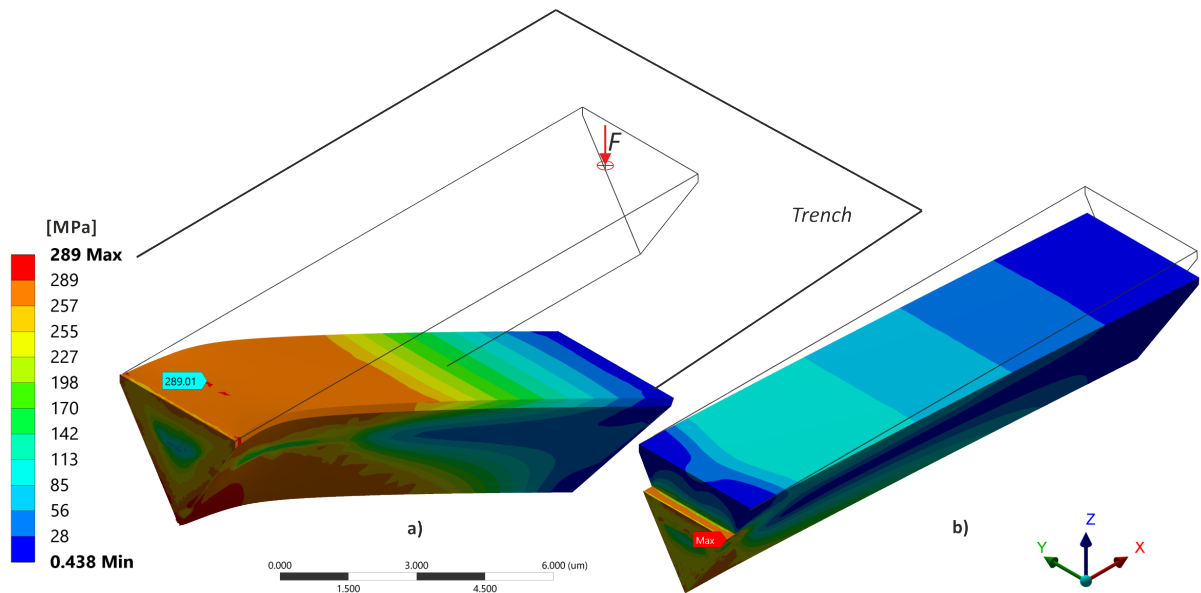


Fig. 3: Deformed shape and Equivalent von-Mises stress in FEM model 14 μm length cantilever at failure load a) un-notched b) notched.

4. Practical implications

It can be seen in Tab. 1 that the notch depth has almost no effect on the results when it is between 30 % and 50 % and only the beam length plays the role. However un-notched and 20 % notched beams show significantly higher deflections compared to other variants. The deflection for the un-notched cantilever is from 2.9 μm to 10.1 μm which is significantly higher than for the notched micro-beams, see Fig. 3. From the practical point of view, it is therefore beneficial to prepare notched variants in experiments to limit deflections at failure loads. The deflection at failure is then dependent mainly on the cantilever length. In order to load cantilever predominantly in bending the length to depth ratio should be high enough (approximately more than 4) which yields optimum cantilever length 12 to 14 μm .

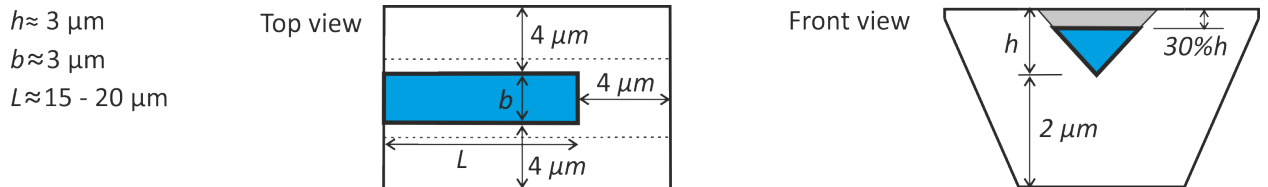


Fig. 4: Minimal dimensions of the trench in vicinity of cantilever.

Tab. 1: Deflection of cantilever at yield strength / tensile strength in nanometres [nm] for different beam lengths and depths of notch.

Notch depth \ Length	10 μm	12 μm	14 μm	16 μm	18 μm	20 μm
0 %	262/2899	344/3784	275/5580	661/6921	793/ 8388	917/10166
20 %	50/409	115/530	233/670	661/811	793/970	917/1144
30 %	49/421	71/530	185/669	170/805	125/928	154/1061
40 %	49/456	71/575	139/686	146/808	114/939	148/977
50 %	48/530	70/652	138/762	94/881	111/1021	144/1148

Another aspect given by the tip geometry used for loading must be taken into account. The tip (called Berkovich) has a pyramidal shape with surface-edge angle of 13.1°. The beam tilt shown in Tab. 2, must be less than the angle to avoid beam-tip collision.

This condition is fulfilled for all notched beams whereas it is not for the un-notched. Taking into account maximum beam deflection at failure and geometry of the indenter tip the size of FIB milled trenches must be as follows: minimum trench depth to avoid cantilever/trench contact ... cantilever depth plus 500-900 nm; minimum trench width to avoid cantilever/tip contact ... beam width plus 4 - 6 μm ; maximum cantilever length to avoid tip/beam contact at tilt ... satisfied for all notched beams, see Fig. 4.

Tab. 2: Force at failure and beam tilt for different micro-beam models.

	10 μm		12 μm		14 μm		16 μm		18 μm		20 μm	
	$F[\mu\text{N}]$	$\alpha[^\circ]$	$F[\mu\text{N}]$	$\alpha[^\circ]$	$F[\mu\text{N}]$	$\alpha[^\circ]$	$F[\mu\text{N}]$	$\alpha[^\circ]$	$F[\mu\text{N}]$	$\alpha[^\circ]$	$F[\mu\text{N}]$	$\alpha[^\circ]$
0 %	120.8	16.17	100.0	17.50	90.0	21.73	79.6	23.39	71.6	24.99	66.0	26.94
20 %	55.3	2.34	46.2	2.53	39.7	2.74	34.6	2.90	30.8	3.08	27.8	3.27
30 %	37.1	2.41	31.0	2.53	26.7	2.74	23.4	2.88	20.7	2.95	18.6	3.04
40 %	23.2	2.61	19.4	2.74	16.7	2.81	14.6	2.89	13.0	2.99	11.4	2.51
50 %	13.3	3.03	11.1	3.11	9.5	3.12	8.4	3.15	7.5	3.25	6.7	3.29

5. Conclusions

FEM numerical simulations have been used to design experiments on cantilever micro-beams from magnesium alloy AZ31 with different lengths varying from 10 to 20 μm and different depth of the notch up to 50 % of the beam depth. Yield and failure points have been detected and corresponding deflections calculated. In the designed experiment, FIB milling is used for preparation of micro-beams and nanoindenter is used for beam loading. Maximum beam deflections at failure load and some geometrical restrictions of the loading device were taken into account in the design. The beams without the notch are not usable for the testing because of their high deflections which would lead to necessity of very deep trenches and increase in milling times. Also, nanoindenter tip to beam collisions can occur on unnotched beams. ON the other hand, notched beams are practical to be used. Optimum length and notch depths lie in the interval of 12 to 24 μm and 30-50 % of the beam depth, respectively.

Acknowledgments

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