Publishing House
AKAPIT
COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów
Vol. 10, 2010, No. 2

THE EXPERIMENTAL RESEARCH AND THE NUMERICAL MODELING OF THE FRACTURE PHENOMENA IN MICRO SCALE

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Abstract

Magnesium alloys with increased bio-compatibility are applied in medicine for the sake of high compatibility and solubility in human body. Production of surgical threads to integration of tissue can be example of the application of these types of alloys. The MgCa0.8 magnesium alloy has a low plasticity at cold deformation, therefore, the drawing process of thin wire is difficult. Prediction of wire fracture in a drawing process of MgCa0.8 alloy is very important from theoretical and practical point of view. The macro scale fracture models are not capable to predict the important phenomena, such as cracking in grains boundaries, moment of initiation of micro-cracks, stress relaxation in grain after micro-cracking etc. Present work is dedicated to the development of a numerical model of MgCa0.8 fracture phenomena prediction in micro scale. The first part of the work is focused on experimental studies: tensile tests, which are data source for the flow stress model of MgCa0.8 alloy and metallographic analysis of material for micro scale fracture model. To understand fracture mechanism, physical modeling in 10000 N tensile/compression stage for a SEM for MgCa0.8 magnesium alloy was performed. This analysis shows that the material is cracking at the grain boundaries. Experiments in the chamber of SEM allows understanding of the fracture mechanism in special magnesium alloy MgCa0.8 and determining the empiric coefficients of fracture model in micro scale. The limit of deformation before initiations of micro-cracks was obtained. The second part of the work is focused on the development of the micro scale numerical model of fracture. The boundary element method is proposed for micro scale model. The mathematical model of fracture is developed for the two dimensional domain. The elastic-plastic theory of plasticity is used.

Key words: magnesium alloys, MgCa0.8, drawing process, fracture model, boundary element method

1. INTRODUCTION

The MgCa0.8 magnesium alloy can be applied to the production of bone implants and surgical threads (Haferkamp et al., 2001; Thomann et al., 2009). Production of surgical threads for integration of tissue can be an example of the application of these types of alloys. Low plasticity (Yoshida, 2004; Kustra et al., 2009) of Mg alloys causes difficulties at cold forming. In works written by Bach et al. (2005) and Bach et al. (2007) the new manufacture technology for the production of tubes of Mg alloys was developed. In this process metal is heated during the drawing process by heated drawing die. Theoretical description of wire drawing process with heated die is presented by Milenin and Kustra (2008). In this process cold wire drawing is necessary as a final stage after multi-pass drawing to increase the surface quality and mechanical properties of the wire. The studies of mechanism of ductility in

 ISSN 1641-8581

MgCa0.8 alloy (Kustra et al., 2009) showed, that fracture in MgCa0.8 alloy had started in grain boundaries and, in consequence had been propagated along grain boundaries. Therefore, the analysis of fracture phenomena in macro scale is not sufficient and, a micro scale model is necessary. The FEM-based algorithms for simulation of MgCa0.8 fracture in micro-scale have problems in simulation of grain boundaries by thin layers of FE and in modeling of representative numbers of grains (Milenin & Kustra, 2008; Milenin, 1997; Milenin et al., 2010). The purpose of this work is the development of a new mathematical model of MgCa0.8 fracture phenomena in micro scale. For micro scale model the boundary elements method (BEM) was used. The new model can eliminate the problems of FEM – based methods described above.

2. EXPERIMENTAL STUDIES: TENSILE TEST AND DEVELOPMENT OF YIELD STRESS MODEL

The samples with diameter 5 mm and deformable base 20 mm was tested by using Zwick 250 machine in AGH University of Science and Technology. Conditions of experiment were as following: testing temperature 20 °C, tool velocity 0.16 mm/s. During experiment the load and displacement of tools were measured. Experimental results show that stress-strain curve is divided into two zones: non-linear elastic and plastic zones. Transition point between elastic and plastic zones of material model is clearly distinguished ($\varepsilon_p = 0.0076$, $\sigma_p = 173$ MPa) and is shown in figure 1. On the basis of experimental observation the following equation is used for material model of the examined magnesium alloy:

$$\sigma_i = A\varepsilon_i^{n_1} \exp(n_2\varepsilon_i) \qquad (1)$$

with σ_i – equivalent stress, ε_i – equivalent strain, A, n_1, n_2 – empirical coefficients.

The two-zone approximation was used for a model of stress-strain curve, based on equation (1). The coefficients of equation (1) for elastic and plastic zones are presented in table 1. The result of approximation is shown in figure 1.

Table 1. *Coefficients of the stress function (1).*

Plastic zone		Elastic zone	
A	400.2311	A	12039.68
n_1	0.168096	n_1	0.776996
n_2	-0.83199	n_2	-57.7732

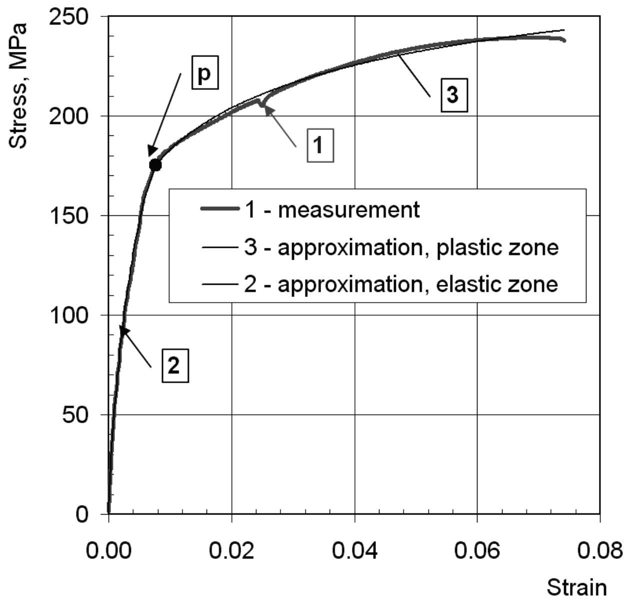


Fig. 1. *Experimental dependence of stress on strain (1) and approximation for elastic (2) and plastic (3) zones, p – transition point between elastic and plastic zones.*

3. EXPERIMENTAL STUDIES: METALLOGRAPHIC ANALYSIS OF FRACTURE IN MICRO SCALE

To understand fracture mechanism, physical modeling in micro scale was performed. Metallographic analysis of fracture in micro scale was performed at room temperature using testing machine 10000 N tensile/compression stage for Scanning Electron Microscope (figure 2) at the Institute of Materials Science, Leibniz Universität Hannover. During tensile testing the stretching load and displacement of tools were measured. A sample after tensile test is shown in figure 3. Three variants of the experiment were executed (table 2). In variant 1 the tension of the sample was carried out at a rate of 0.005 mm/s till the break. In variants 2 and 3 two-stage deformation was carried out. The annealing was achieved between the stages of deformation. The temperature of annealing was 300 °C, the time of holding was 6 minutes. The varied parameter was the value of deformation in first stage. This value was selected on the basis of the analysis of the microstructure of model during the testing in accordance with variant 1. In variant 1 the sample cracked at 1.49 mm tool displacement. Microstructures in the center of the sample in different stages of this test are shown in figure 4. The experiment showed that fracture in MgCa0.8 alloy had started in grain boundaries and, in consequence had been propagated along the grain boundaries.

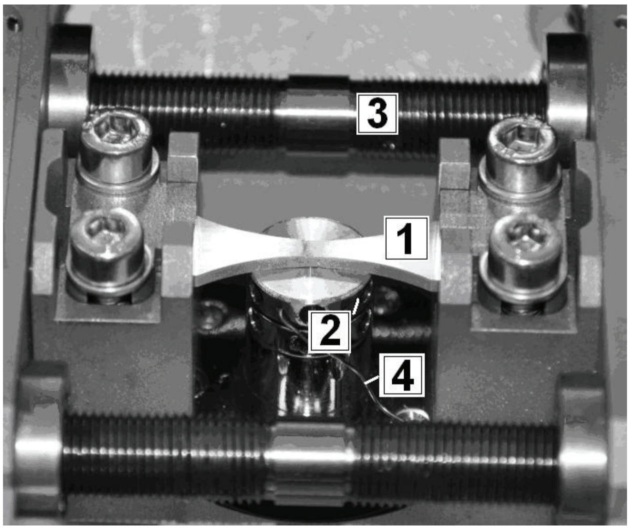


Fig. 2. Testing device – micro tensile/compression stage for SEM, 1 – sample, 2 – heating plate, 3 – deformation module, 4 – thermocouple.

Table 2. Conditions and results of tensile tests in micro-chamber of SEM.

Nr	Deformation between annealing, mm	Total deformation, mm
1	-	1.49
2	0.8	1.52
3	0.4	1.80

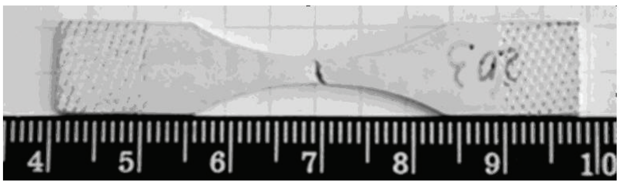


Fig. 3. Sample after tensile test in micro chamber.

The photos of microstructure were data source to obtain the longitudinal strain of RVE during the tensile test in micro scale. The strain is calculated by the natural logarithm of the ratio of longitudinal dimensions of grains before and after deformation. Values of calculated strain are shown in table 3.

Table 3. The longitudinal strain during the tensile test in micro scale.

Nr	Tool displacement, [mm]	Longitudinal strain of RVE, [-]
1	0.5	0.08
2	0.7	0.10
3	1.0	0.13
4	1.2	0.18
5	1.4	0.27

The dependence of the porosity of sample on the value of deformation is established on the basis of the obtained microstructures. Extremely significant result is the value of deformation, to which the sample is deformed without the appearance of porosity. This value is equal to 0.4 mm (figure 5). Another characteristic point on the curve in figure 5 corresponds to a displacement of 1 mm. From this value an increase of the porosity becomes intensive. On the basis of the obtained data, the value of displacement

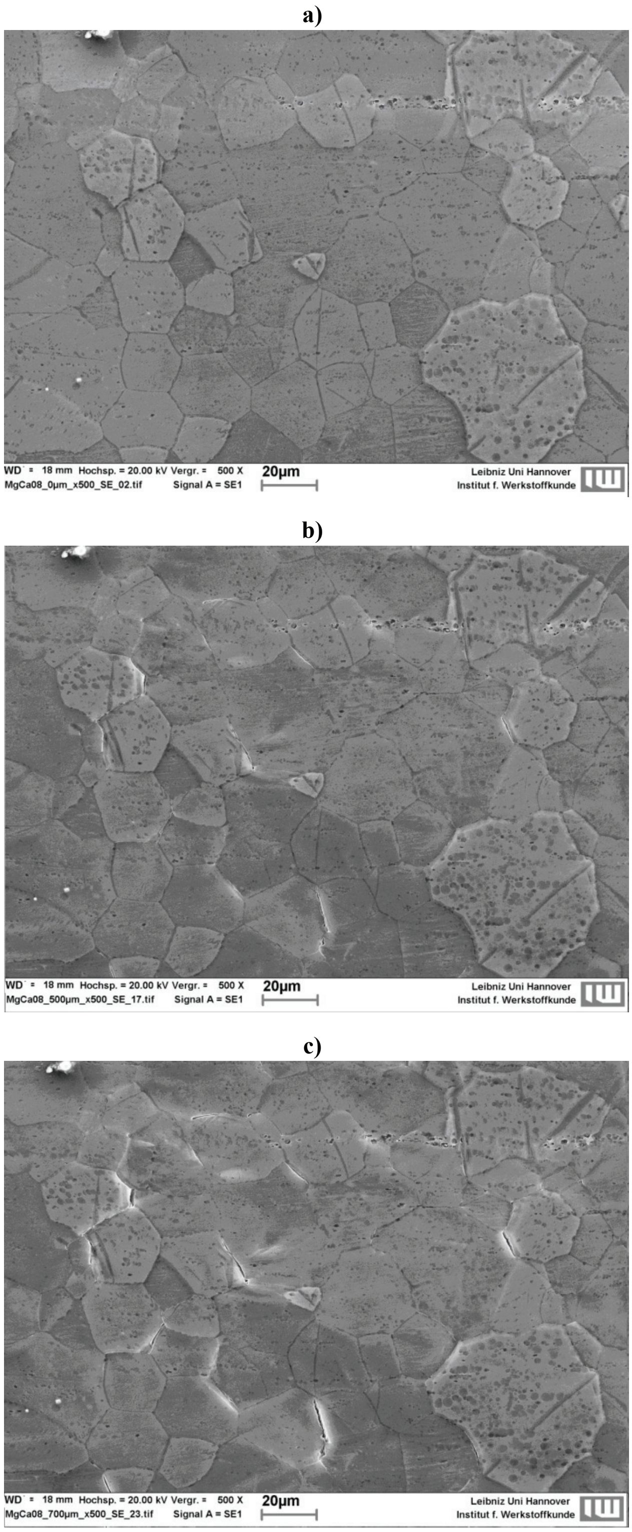
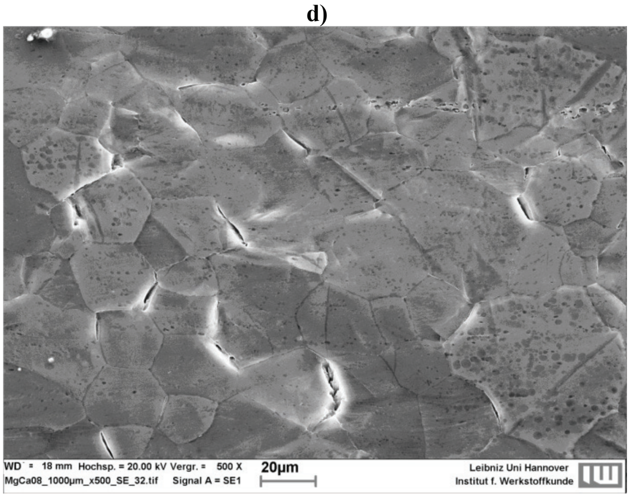


Fig. 4a. Fracture mechanism in micro scale for MgCa0.8, central point of sample; (a) before tensile test, (b)-(f) during tensile test, tool displacement is 0.5 mm (b), 0.7 mm (c), 1.0 mm (d), 1.2 mm (e) and 1.4 mm (f).

d)



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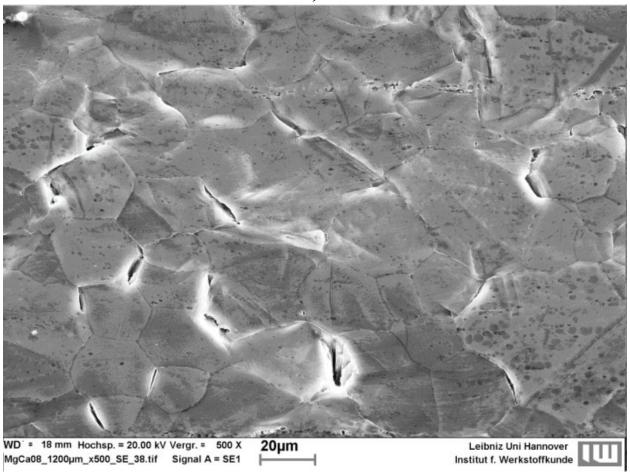

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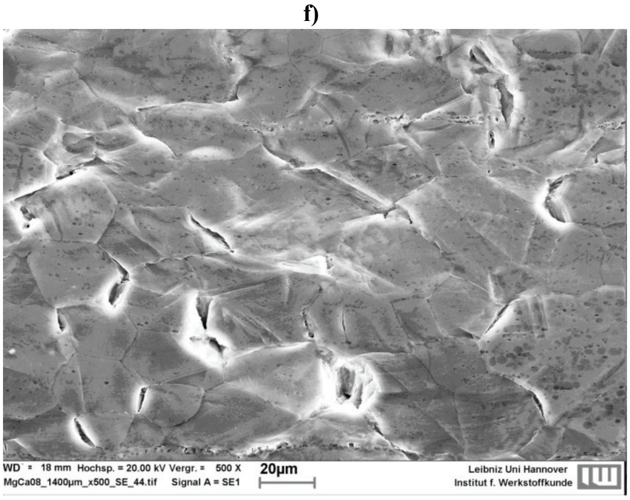


Fig. 4b. *Fracture mechanism in micro scale for MgCa0.8, central point of sample; (a) before tensile test, (b)-(f) during tensile test, tool displacement is 0.5 mm (b), 0.7 mm (c), 1.0 mm (d), 1.2 mm (e) and 1.4 mm (f).*

in first stage was selected as 0.8 mm (variant 2) and 0.4 mm (variant 3). The summary deformation of the model before the destruction was the goal function in the executed experiment. The maximum value of summary displacement is obtained for experiment 3 (1.8 mm). This allows to assert when to most effectively carry out annealing before the appearance of microscopic cracks on the grain boundaries. Consequently, the prediction of this phenomenon for different conditions of the deformation (for example, during drawing) of MgCa0.8 alloy is a very important task. Solution of this problem requires the development of the mathematical model of destruction on the grain boundaries. The mechanism of fracture described above was modeled by BEM in a micro-scale model.

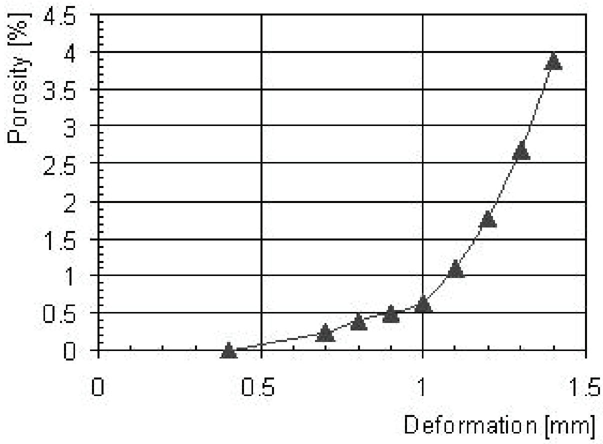


Fig. 5. *Dependence of porosity on deformation of sample.*

4. BEM MODEL OF MICROSTRUCTURE DEFORMATION AND FRACTURE PHENOMENA IN MICRO SCALE

The selection of BEM in development of micro-scale model gives significant advantages (in comparison with existing FEM models) in precision of the calculations at boundaries, because normal and shear stresses and displacements are calculated directly on boundaries. This approach significantly reduces also the number of variables, providing the ability to attach to a large number of RVE grain models.

The proposed BEM algorithm is based on idea, which is described by Milenin (1997, 1995). The Representative Volume Element (RVE) is divided into elements with linear mechanical properties (figure 6, 7). The new model in micro scale includes stages of generation of the BEM mesh (for example, shown in figure 7) for digital fragment of microstructure and numeric solutions in micro scale. Boundary conditions for micro-scale model were obtained from solution of boundary problem in macro-scale or directly from experiment.

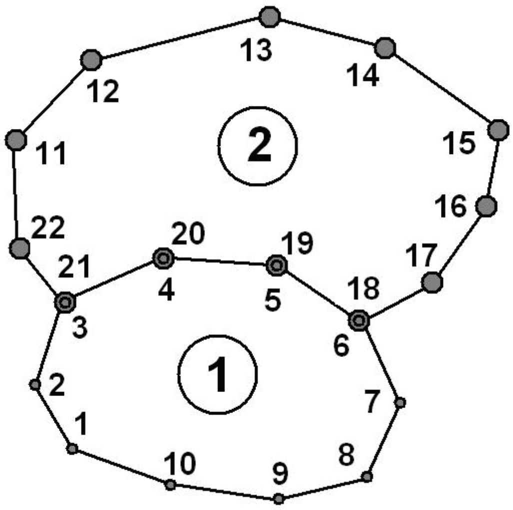


Fig. 6. The example of BEM grid for contact of two grains. The nodes 3-6 of grain 1 are contacted with nodes 18-21 of grain 2.

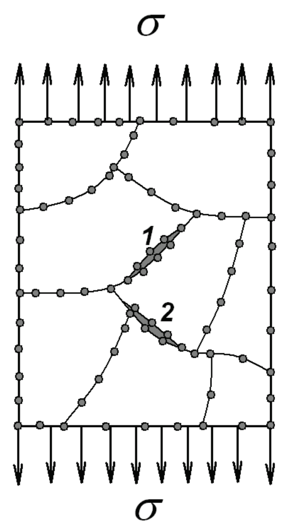


Fig. 7. The scheme of model of ductility process in RVE: 1 and 2 – examples of cracks on grain boundary, σ – boundary conditions.

Solution of boundary problems in micro-scale can be based on a fundamental solution of Kelvin, which is obtained in theory of elasticity. The formulas of Kelvin may be written as follows:

$$u_{ij}(p,q)=\frac{(1+\nu)}{8\pi rE(1-\nu)}\left((3-4\nu)\delta_{ij}+\frac{\partial r}{\partial x_i}\frac{\partial r}{\partial x_j}\right) \quad (2)$$

$$T_{ij}(p,q,n)=-\frac{1}{8\pi(1-\nu)r^2}\left(\left((1-2\nu)\delta_{ij}+3\frac{\partial r}{\partial x_i}\frac{\partial r}{\partial x_j}\right)\frac{\partial r}{\partial n}+\right.$$

$$\left.(1-2\nu)\left(\frac{\partial r}{\partial x_i}n_j-\frac{\partial r}{\partial x_j}n_i\right)\right) \quad (3)$$

with x_i – axis of coordinate system (x_1, x_2, x_3); $u_{ij}(p, q)$ – displacement of point p along the axis x_j from the action of the unit load, applied at point q in direction x_i; $T_{ij}(p, q, n)$ – internal components of the vector of force in point p on surface with direction of normal n is along of axis x_j from the action of the unit load, applied at the point q in direction x_i, E – Young's modulus; ν – Poisson ratio; r – vector of distance between points p and q; δ_{ij} – Kronecker delta.

Transformation of formulas (2) and (3) for plane strain state gives the following equations (Crouch & Starfield, 1983):

$$u_1=\frac{F_1(1+\nu)}{E}\left(g(3-4\nu)-x_1\frac{\partial g}{\partial x_1}\right)-\frac{F_2x_2(1+\nu)}{E}\frac{\partial g}{\partial x_1}, \quad (4)$$

$$u_2=\frac{F_2(1+\nu)}{E}\left(g(3-4\nu)-x_2\frac{\partial g}{\partial x_2}\right)-\frac{F_1x_1(1+\nu)}{E}\frac{\partial g}{\partial x_2}, \quad (5)$$

$$\sigma_1=F_1\left(2(1-\nu)\frac{\partial g}{\partial x_1}-x_1\frac{\partial^2 g}{\partial x_1^2}\right)+F_2\left(2\nu\frac{\partial g}{\partial x_2}-x_2\frac{\partial^2 g}{\partial x_1^2}\right), \quad (6)$$

$$\sigma_2=F_2\left(2(1-\nu)\frac{\partial g}{\partial x_2}-x_2\frac{\partial^2 g}{\partial x_2^2}\right)+F_1\left(2\nu\frac{\partial g}{\partial x_1}-x_1\frac{\partial^2 g}{\partial x_2^2}\right), \quad (7)$$

$$\sigma_{12}=F_1\left((1-2\nu)\frac{\partial g}{\partial x_2}-x_1\frac{\partial^2 g}{\partial x_1^2}\right)-$$

$$F_2\left((1-2\nu)\frac{\partial g}{\partial x_1}-x_2\frac{\partial^2 g}{\partial x_1\partial x_2}\right), \quad (8)$$

$$g(x_1,x_2)=-\frac{1}{4\pi(1-\nu)}\ln\sqrt{\left(x_1^2+x_2^2\right)}, \quad (9)$$

with F_1 and F_2 – components of load which impact in linear elasticity material; u_1, u_2, σ_1, σ_2, σ_{12} – displacements in directions x_1 and x_2 and stresses due to the load F; E – elastic - plasticity modulus of material.

In the plastic deformation the material is considered incompressible: $\nu = 0.5$. To calculate the coefficients of system of equations the Castigliano's theorem is used:

$$\int_S(t_1\upsilon_1+t_2\upsilon_2)dS=\int_S(\tau_1u_1+\tau_2u_2)dS, \quad (10)$$

with S – surface of contact; t_1, t_2, u_1, u_2 – real stresses and displacements on boundary (in boundary elements); τ_1, τ_2, ν_1, ν_2 – control solutions in boundary with determination on basis of equations (4)-(9).

In order to take into account the connection between grains and probability of cracking at grain boundaries the following boundary conditions are introduced:

$$\sigma_s^{[1]}(x_{1q}, x_{2q}) = \sigma_s^{[2]}(x_{1q}, x_{2q}), \tag{11}$$

$$\sigma_n^{[1]}(x_{1q}, x_{2q}) = \sigma_n^{[2]}(x_{1q}, x_{2q}), \tag{12}$$

$$u_s^{[1]}(x_{1q}, x_{2q}) = -u_s^{[2]}(x_{1q}, x_{2q}), \tag{13}$$

$$u_n^{[1]}(x_{1q}, x_{2q}) = -u_n^{[2]}(x_{1q}, x_{2q}), \tag{14}$$

where $\sigma_s^{[1]}(x_{1q}, x_{2q})$, $\sigma_n^{[1]}(x_{1q}, x_{2q})$ – shear and normal stresses in boundary elements of first grain in point q; $\sigma_s^{[2]}(x_{1q}, x_{2q})$, $\sigma_n^{[2]}(x_{1q}, x_{2q})$ – shear and normal stresses in boundary elements of second grain in point x_q, y_q. Similarly notation was used for displacements.

For simulation of cracking on boundary between elements [1] and [2], the equations (11)-(14) are excluded from system of algebraic equations (10).

The elastic - plasticity modulus of material for each grain can be determinate according to the following equation:

$$E = \frac{\sigma_i(\bar{\varepsilon}_i)}{\bar{\varepsilon}_i}. \tag{15}$$

with $\bar{\varepsilon}_i$ – mean equivalent strain in grain; $\sigma_i(\bar{\varepsilon}_i)$ – stress-strain curve of material (formula 1).

The proposed criteria of crack based on theory of L.M.Kaczanov and Y.N.Rabotnov, which was successfully used in modeling of grain boundary cracking in work written by Diard et al. (2002). The following modified model of criteria of crack in grain boundary was proposed:

$$D = \int_0^{\tau} \dot{D} d\tau = 1, \tag{16}$$

$$\dot{D} = b_1 \left(\frac{\sigma_{eq}}{E} \right)^{b_2} (1 - D)^{b_3}, \tag{17}$$

$$\sigma_{eq} = \sqrt{\sigma_n^2 + b_0 \sigma_S^2}, \tag{18}$$

where: σ_n – positive component of normal stress on boundary between two grains; σ_s – shear stress on boundary between two grains; b_0-b_3 – empirical coefficients. In work written by Diard et al. (2002) the value 0.4 was proposed for b_0.

5. MODELING OF DISCONTINUITY IN GRAINS BOUNDARIES DURING TENSILE TEST

Stress-strain curve of material were implemented as model (1). The local displacements of fragment of microstructure were used as boundary conditions in micro-scale model. The BEM model included 167 nodes and 256 boundary elements. The shape of model is shown in figure 8.

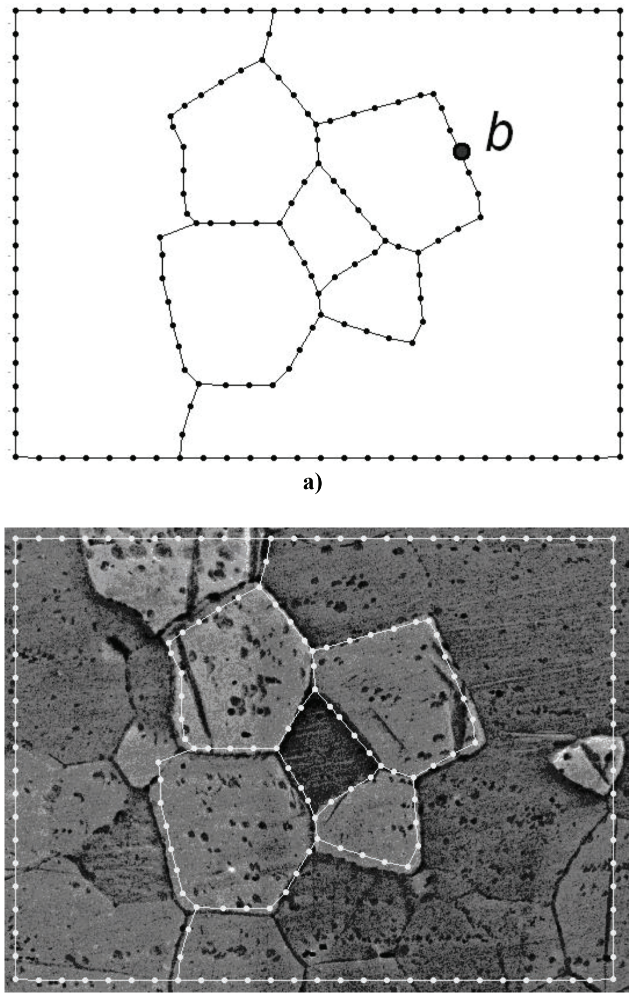


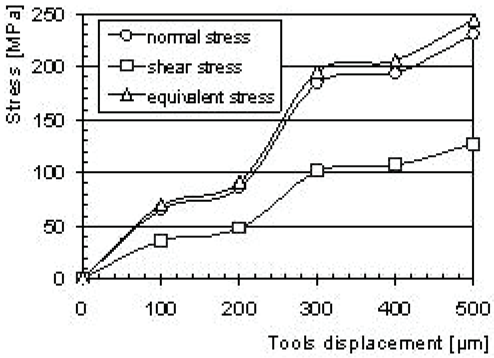
Fig. 8. The BEM model (a) of a fragment of the initial microstructure (b).

The microstructure after the tensile test (figure 4) shows that in selected fragment of microstructure the fracture begins in the grain boundary marked in figure 8a. Distribution of normal, shear and equivalent stress in point b is shown in figure 9a. The ductility function D for each point was calculated on the basis of formulas (16) - (18) and calculated values of stresses. The numerical integration for equation (16) was used. Square of the difference between the experimental and computed (D_{calc}) value of D at the moment of the fracture in point b is used as the objective function:

$$\delta = \left(D_{calc} - 1\right)^2 . \qquad (19)$$

The minimum of the objective function is reached by a variation of the coefficients b_1-b_3. The following values of coefficients were obtained: $b_1 = 170$; $b_2 = 0.11$; $b_3 = 2.0$.

The distribution of ductility function D in point b is shown in figure 9b.



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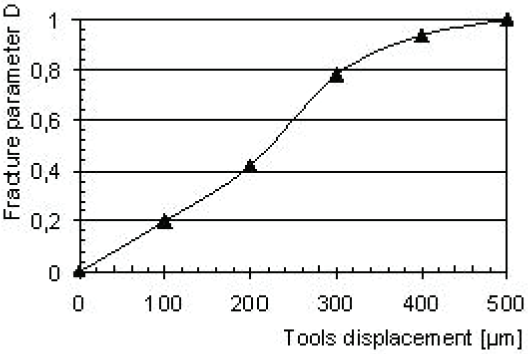
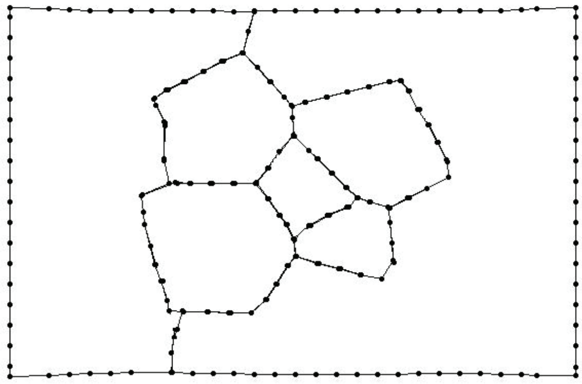


b)

Fig. 9. *Distribution of normal, shear, equivalent stress (a) and fracture parameter D in point b during deformation of sample from 0 to 0.5 mm.*

The simulation of further development of the crack is executed on the basis of the obtained values of coefficients b_0-b_3. An example of calculation in micro-scale and comparison with the experimental data (microstructure) is shown in the figure 10-11.

The time of step-by-step simulation of the task on the personal computer of middle class composes several minutes.



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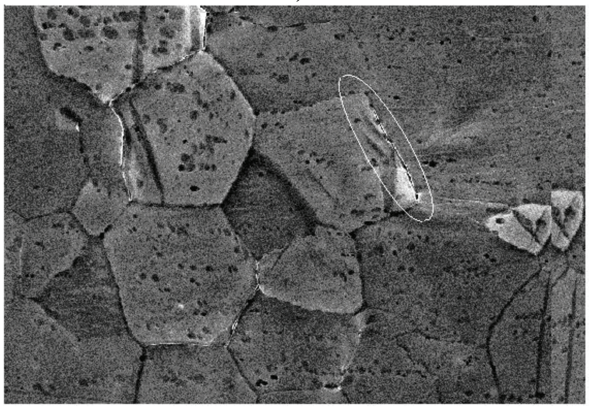
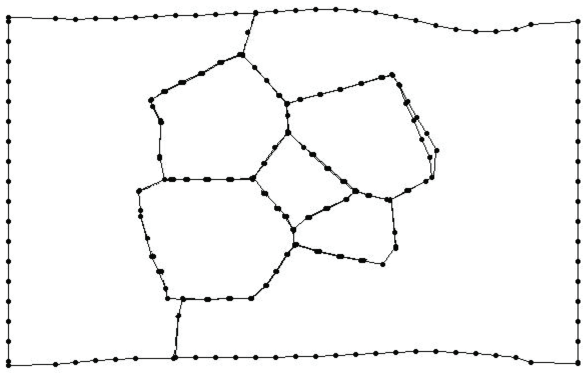


b)

Fig. 10. *Results of simulations after a tool displacement of 400 µm (a) and real microstructure before crack in grain boundary.*



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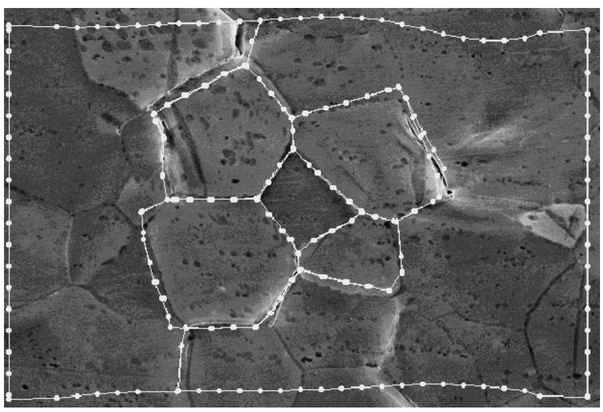

b)

Fig. 11. *Results of simulations (a) after a tool displacement of 700 µm and real microstructure (b) after crack in grain boundary.*

6. CONCLUSIONS

A new model of MgCa0.8 alloy fracture phenomena is proposed. The conception of simulation of the fracture phenomena is based on the boundary elements method and on the results of physical modeling in micro-scale. The selection of BEM in development of micro-scale model gives significant advantages (in comparison with existing FEM models) in precision of the calculations at boundaries, because normal and shear stress and displacements are calculated directly. The presented approach also significantly reduces the number of variables, providing the ability to attach to a large number of grains in RVE model.

The following phenomena are predicted by the mathematical model of fracture in micro-scale: stresses and strains in grains before grain boundary cracking, shape and moment of initiation of micro-cracks, fracture phenomena in macro-scale.

ACKNOWLEDGMENTS

Financial assistance of the Ministry of Science and high Education of Poland, project no. 4131/B/T02/2009/37, is acknowledged.

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BADANIA EKSPERYMENTALNE I NUMERYCZNE MODELOWANIE ZJAWISKA PĘKANIA W SKALI MIKRO

Streszczenie

Stopy magnezu o podwyższonej biozgodności znajdują zastosowanie w medycynie dzięki ich wysokiej zgodności z organizmem człowieka i odpowiedniej resorbowalności. Przykładem może być produkcja resorbowalnych nici chirurgicznych z tego typu stopów. Jednak wytwarzanie tak cienkich drutów ze stopu MgCa0.8 stwarza wiele trudności ze względu na ich niską plastyczność w temperaturze pokojowej, dlatego przewidywanie powstających pęknięć w trakcie ciągnienia ma duże znaczenie praktyczne i teoretyczne. Modelowanie w skali makro zjawiska pękania nie jest wystarczające do opisu takich zjawisk jak powstawanie mikropęknięć na granicach ziaren, czy relaksacja naprężeń na granicach ziaren po pojawieniu się mikropęknięć. Niniejsza praca poświęcona jest numerycznemu modelowaniu powstawania pęknięć na poziomie mikrostruktury. Pierwsza część pracy opisuje przebieg eksperymentu, z którego otrzymano dane do wyznaczenia naprężenia uplastyczniającego stopu MgCa0.8. W celu przeanalizowania mechanizmu pękania stopu magnezu MgCa0.8 na poziomie mikro wykonano test rozciągania w specjalnej mikrokomorze 10000 N tensile/compression stage for a SEM. Test ten pozwolił stwierdzić, że stop MgCa0.8 charakteryzuje się mechanizmem pękania tylko na granicach ziaren. Na podstawie opisanej próby rozciągania wyznaczono eksperymentalne współczynniki dla modelu pękania w skali mikro. Określono również graniczne odkształcenie przed powstaniem mikropęknięcia. Druga część pracy dotyczy matematycznego modelu pękania w skali mikro. Zaproponowano rozwiązanie tego problemu metodą elementów brzegowych. Zadanie rozpatrywane jest jako dwuwymiarowe zagadnienie sprężysto–plastyczne.

Received: March 31, 2010
Received in a revised form: May 2, 2010
Accepted: May 7, 2010