A constitutive model for texture dependent deformation hardening and pressure dependent initiation of ductile failure in metallic materials

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Abstract

In this report a phenomenological constitutive model is presented and applied to the copper material used for the SKB canisters. The model takes into account change of micro texture and is able to capture the difference in deformation hardening between uniaxial loading and shear loading. The model has been validated against test data and parameter values for the copper material are given.

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Notations

Physical quantity	Description	Unit (SI)
σ_{eq}	Von Mises equivalent stress	Pa
σ_{tex}	Texture equivalent stress	Pa
s_{ij}	Deviatoric stress tensor	Pa
$\hat{s}_{ij}$	Rotated deviatoric stress tensor	Pa
R_{ij}	Rotation tensor	-
β	Texture function	-
α	Texture parameter	-
a	Failure strain parameter (linear)	-
b	Failure strain parameter (exponential)	-
ε_{p}	Plastic strain	-
ε_{f}	Failure strain	-
D	Damage	-
p	Hydrostatic pressure	Pa
H	Deformation hardening modulus from uniaxial tensile test	Pa
H^*	Texture deformation hardening modulus	Pa
T	Stress triaxility	-
σ_{ij}	Stress tensor	Pa
$\boldsymbol{\delta}_{\mathbf{ij}}$	$\boldsymbol{\delta_{ij}} = \begin{cases} 0, for \text{ i}\neq\text{j} \\ 1, for \text{ i=j} \end{cases}$	-

1 Introduction

Here a plasticity model for texture dependent deformation hardening and initiation of ductile failure in metallic materials is presented. The model was originally developed for copper material used by the Swedish Nuclear Fuel and Waste Management Company (SKB) for nuclear fuel canisters, cf. "Intryck i kopparmaterial" (SKBdoc 1205273). The constitutive model has since been developed further and an implementation is currently available in the finite element code Impetus Afea Solver, cf. Olovsson (2013). The original version of the model has also been implemented as a user routine in the finite element code Abaqus, version 6.12.

For crystalline metals the deformation hardening is lower, the material is softer, when subjected to shear loading compared to uniaxial loading if the Von Mises equivalent stress measure is used to evaluate tests. The explanation for this difference lies on the microstructural level, how the texture of the material rotates during loading and thus the rotation of slip planes, see for example Jonas et al. (1982) and Tome et al. (1984).

The Von Mises equivalent stress σ_{eq} is a scalar valued function of the deviatoric stress tensor and defined as

$$\sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2} s_{ij} s_{ij}} = \sqrt{\frac{3}{2}\left(s_{11}^2 + s_{22}^2 + s_{33}^2 + 2(s_{12}^2 + s_{13}^2 + s_{23}^2)\right)} \qquad \textit{Equation 1-1}$$

Here s_{ij} denotes the components of the deviatoric stress tensor in index notation. The Von Mises equivalent stress is an invariant, i.e. it is independent of transformations. The Von Mises yield criteria corresponds to the theory of maximum distortion energy and is the most commonly used yield theory in engineering computations. However, it does not take into account any difference in deformation hardening for different loading paths, ie. changes in the microstructural texture.

The presented model encompasses a modified equivalent stress measure and was developed to capture this difference in deformation hardening due to different loading paths.

2 Model

2.1 Texture dependent deformation hardening

First, it is here assumed that the rotation of slip planes follows the rotation of the principal strain directions. So, we transform the deviatoric stress tensor s_{ij} to a co-ordinate system defined by the principal strain directions.

$$\hat{s}_{ij} = R_{ik} s_{kl} R_{jl} \qquad \textit{Equation 2-1}$$

where $\hat{s}_{ij}$ is the components of the rotated deviatoric stress tensor and R_{ij} is a tensor that rotates the stresses to the principal strain directions. This of course requires a spatial strain tensor, or a push-forward operation on a material strain tensor. The original implementation of the model is based on the integral of the rate of deformation, i.e. an approximation to the logarithmic strain. If another strain measure is used, the optimization of the texture parameter might have to be adapted. In this rotated configuration a modified version of the equivalent stress measure, σ_{tex}, is introduced.

$$\sigma_{\mathbf{tex}} = \sqrt{\frac{3}{2}\left(\hat{s}_{11}^2 + \hat{s}_{22}^2 + \hat{s}_{33}^2 + \beta(\hat{s}_{12}^2 + \hat{s}_{13}^2 + \hat{s}_{23}^2)\right)} \qquad \textit{Equation 2-2}$$

Apart from replacing the un-rotated stresses with rotated stresses, the constant 2 in the original expression is replaced by a function β that depends on the plastic strain ε_{p} according to

$$\beta = 2\left(1 + \alpha\varepsilon_p\right)^2 \qquad \textit{Equation 2-3}$$

where α is a scalar valued material parameter. When there are no plastic strains the expression evaluates to 2, but as plastic strain increases the shear stresses in the rotated configuration is increasingly weighted. This can also be viewed as a reduction of the yield stress for shear dominant loading.

Standard isotropic associated plastic flow is used. For the implementation, scaling of the deformation hardening *H* from a uniaxial tensile test is used to get the texture dependent plastic behaviour. The scaled, or adjusted, hardening can be deduced by combining the equations for standard plasticity and Eq. 2-2. The resulting expression is

$$H^* = H\frac{\sigma_{\mathbf{eq}}}{\sigma_{\mathbf{tex}}} - \sigma_{\mathbf{y}}\frac{\sigma_{\mathbf{eq}}}{\sigma_{\mathbf{tex}}^3} 3\alpha\left(1 + \alpha\varepsilon_p\right)\left(\hat{s}_{12}^2 + \hat{s}_{13}^2 + \hat{s}_{23}^2\right) \qquad \textit{Equation 2-4}$$

That is, the deformation hardening for uniaxial tension (*H*) for the current material is here modified, or tweaked, with respect to the stress state. This means that the plastic behaviour of the material becomes different for in for example tension, compression and shearing. Which is in accordance with test data.

2.2 Pressure dependent failure

The failure strain ε_{p} depends on the stress state, cf. for example Xue and Wierzbicki (2008). An often-made simplification is that only the ratio between the invariant hydrostatic pressure and the equivalent Von Mises stress governs the failure strain. This is the approach used here. Also, it is assumed that damage D is accumulated according to

$$D = \int \frac{\dot{\varepsilon}_\mathrm{p}}{\varepsilon_\mathrm{f}} dt$$

Equation 2-5

Here $\dot{\varepsilon}_\mathrm{p}$ is the plastic strain rate and the failure strain ε_f is assumed to be

$$\varepsilon_\mathrm{f} = ae^{-bT}$$

Equation 2-6

where a and b are material parameters and T is a measure of the stress triaxiality, ie.

$$T = -\frac{p}{\sigma_\mathrm{eq}}$$

Equation 2-7

where

$$p = -\frac{1}{3}\sigma_{ii}$$

Equation 2-8

$$\sigma_\mathrm{eq} = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$$

Equation 2-9

$$s_{ij} = \sigma_{ii} + p\delta_{ij}$$

Equation 2-10

When implementing in a finite element code, the expression for the damage accumulation above is replaced by its incremental counterpart.

$$D = \sum \frac{\Delta\varepsilon_\mathrm{p}}{\varepsilon_\mathrm{f}}$$

Equation 2-11

For undamaged material $D = 0$ and at failure $D = 1$.

3 Optimization of parameter values for Cu-OFP

Numerical simulations of tensile testing and torsion testing were utilized to optimize the values of the parameters in the model against average test data from several tests on phosphorus-alloyed oxygen-free copper (Cu—OFP). All tests were carried out at room temperature and quasi-static loading conditions with nominal strain rates less than 0.01 s^{-1}. However, the strain rate increases as deformation is localized, i.e. necking in the case of a tensile test.

3.1 Tensile testing – Experimental set-up and results

See Appendix A for the complete test report on the tensile tests. The tensile specimens were not deformation hardened during manufacturing and not subjected to heat treatment afterwards. This can be seen from the rather low values on the yield strength and hardness in the test report.

In Figure 3-1 the geometry and dimensions of the test specimens are shown.

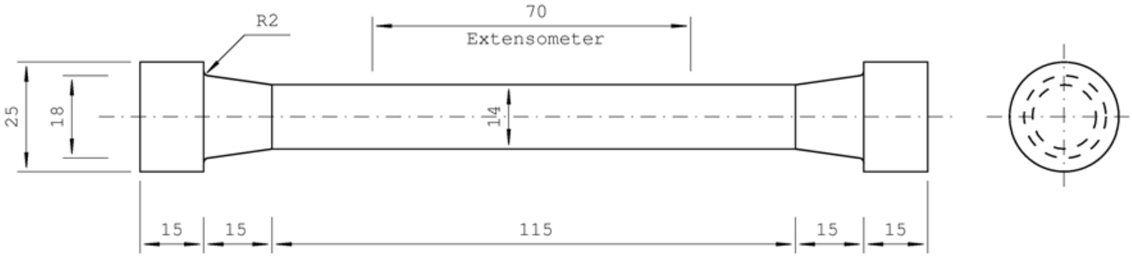

Figure 3-1: Specimen geometry for the tensile testing.

Results (mean values) from the tensile tests used for the optimization were

- Global force vs. extensometer displacement
- Local reduction of area at material failure

In Figure 3-2 the finite element version of the specimen geometry is shown.

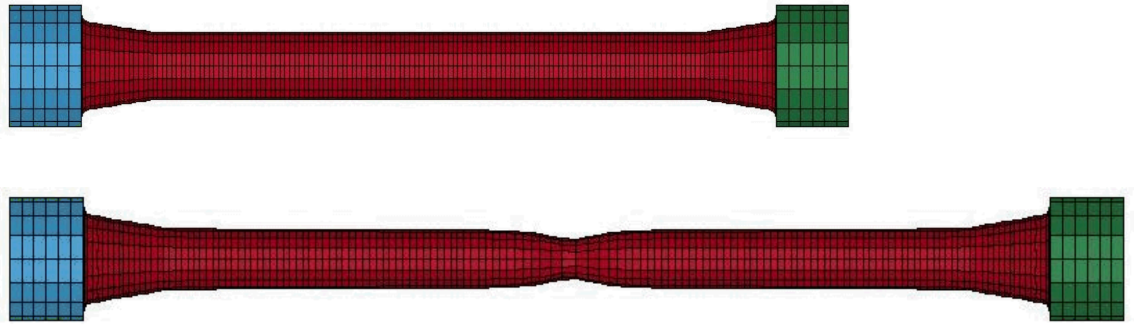

Figure 3-2: Finite element representation of the tensile test specimen.

An iterative simulation procedure was adopted to optimize the deformation hardening curve for the copper material, where the deformation hardening was changed until a good fit between experiment and model was achieved. In Figure 3-3 results from the tensile test (experimental) are compared to results from the numerical model for the optimized deformation hardening, see Figure 3-4 and Appendix B.

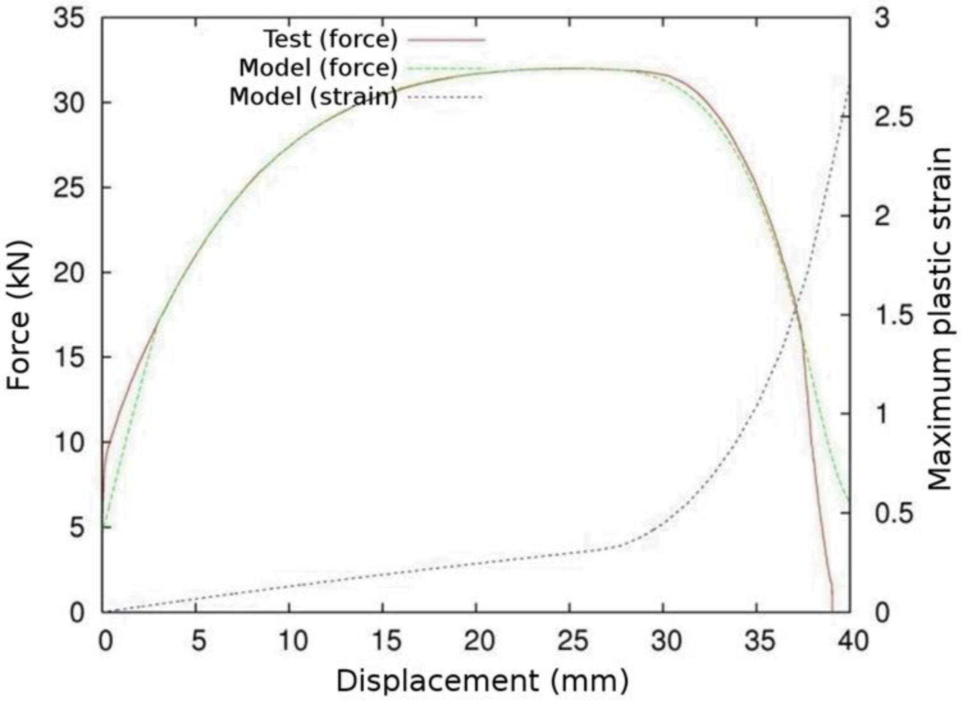

Figure 3-3:Comparison of results from tensile test and numerical model with optimized deformation hardening. Test data is represented by a mean value curve corresponding to five tensile tests, see Appendix A.

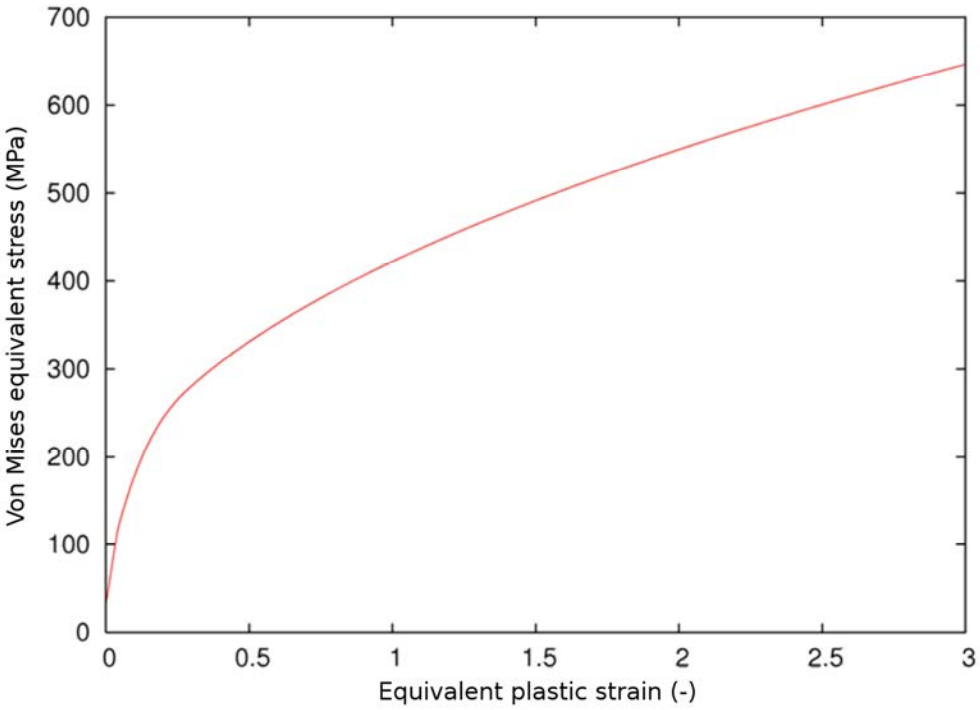

Figure 3-4: Optimized deformation hardening (H in Eq. 2-4).

In Figure 3-3 the local plastic strain at the specimen mid-centre is given as well. An approximate relation between the equivalent plastic strain $\boldsymbol{\varepsilon}_{\mathrm{p}}$ and the contraction of area Z is:

$$\boldsymbol{\varepsilon}_{\mathbf{p}} = \ln\left(\frac{1}{1-Z}\right)$$ *Equation 3-1*

Using the average value on the contraction of area at failure from the test, the equivalent plastic strain at tensile failure can be computed as

$$\boldsymbol{\varepsilon}_{\mathbf{f}} = \ln\left(\frac{1}{1-0.87}\right) = 2.1$$ *Equation 3-2*

3.2 Torsion testing – Experimental set-up and results

See “Skjuvprovning av koppar” (SKBdoc 1193460) for the complete test report. One of the torsion specimens was tested in uniaxial tension, and it was concluded that the material had been deformation hardened during the manufacturing of the specimens. This was accounted for in the optimization through the introduction of initial plastic strains.

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In Figure 3-5 the geometry and dimensions of the specimens used are given.

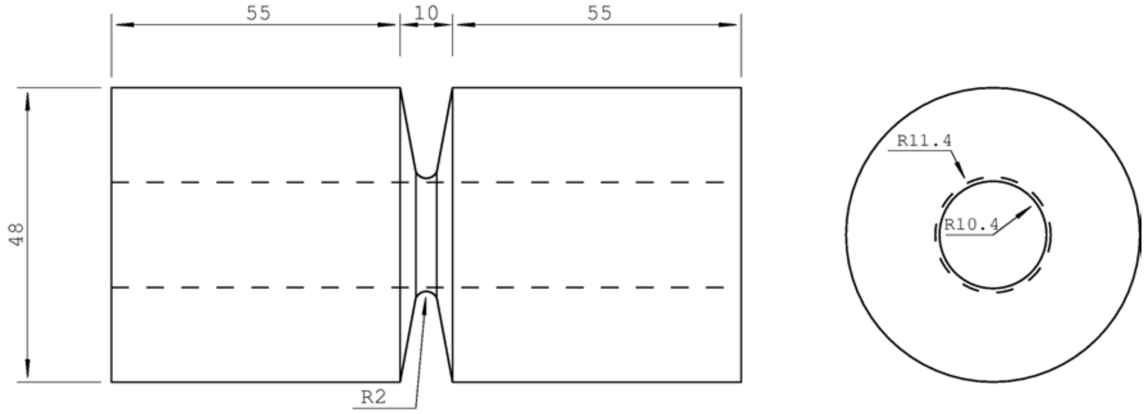


Figure 3-5: Specimen geometry for the torsion testing.

In Figure 3-6 the finite element representation of the specimen geometry is shown.

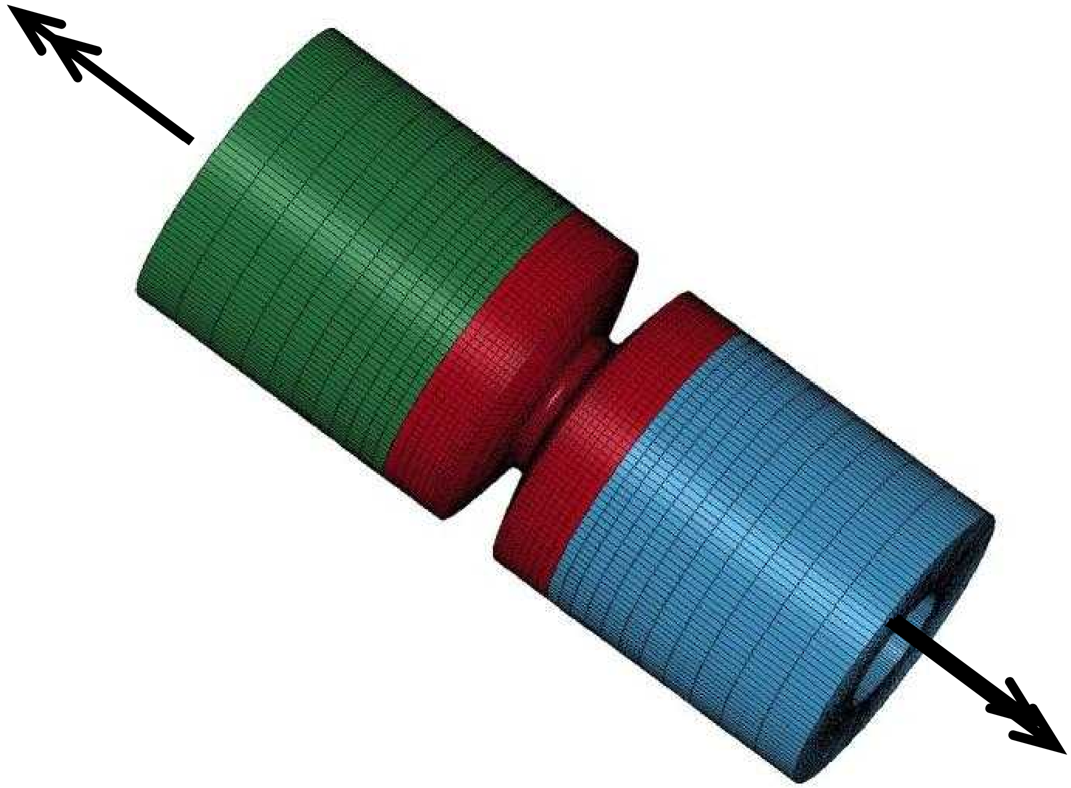


Figure 3-6: Geometry (finite element mesh representation) used for the torsion testing.

An iterative simulation procedure was adopted here as well to optimize the texture parameters for the copper material, where the parameters was changed until a good fit between experiment and model was achieved. In Figure 3-7 results from the tensile test (experimental) are compared to results from the numerical model for the optimized texture parameter $\boldsymbol{\alpha}$, see Table 3-1. In Table 3-1 the parameter values used for the failure model (Equation 2-6) are also given.

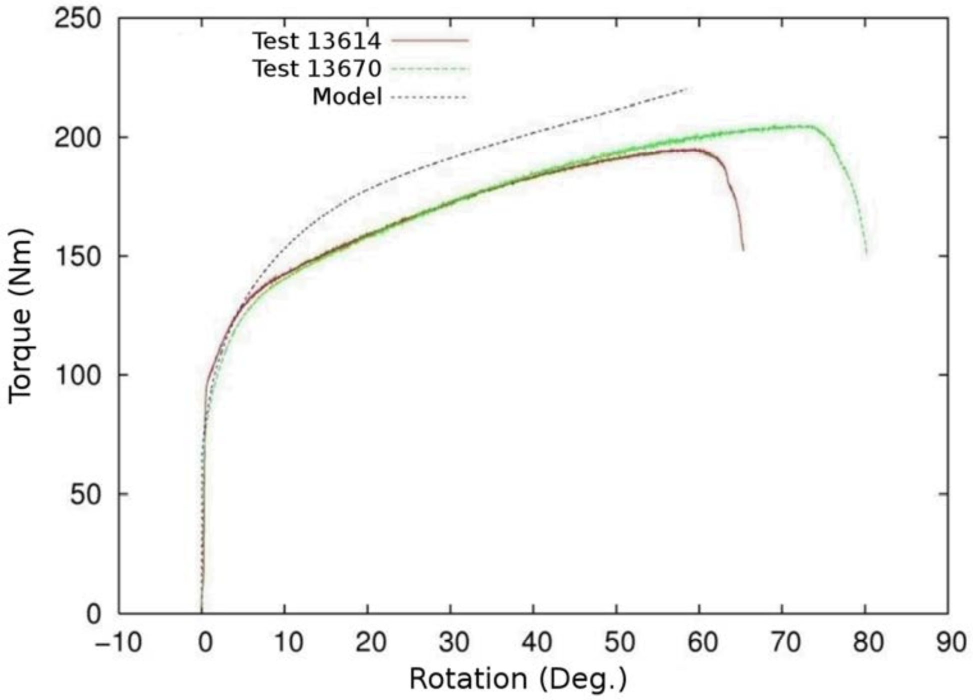


Figure 3-7: Results from test and numerical simulation with optimized parameter values for torsion test. Results (mean values) from the torsion tests used for the optimization were global torsional moment (torque) vs. angle of twist and local angle of twist at specimen centre at material failure.

Table 3-1: Optimized parameter values for Cu-OFP.

α	a	b
0.1	4.0	1.93

The equivalent plastic strain at failure for torsion was evaluated from the simulation by comparing the local angle of twist from the test with the model, giving

$$\varepsilon_f = 4.0 \qquad \textit{Equation 3-3}$$

In Figure 3-8 a graphic representation of the pressure dependent, or stress triaxiality dependent, failure strain function is given together with data from the literature for comparison.

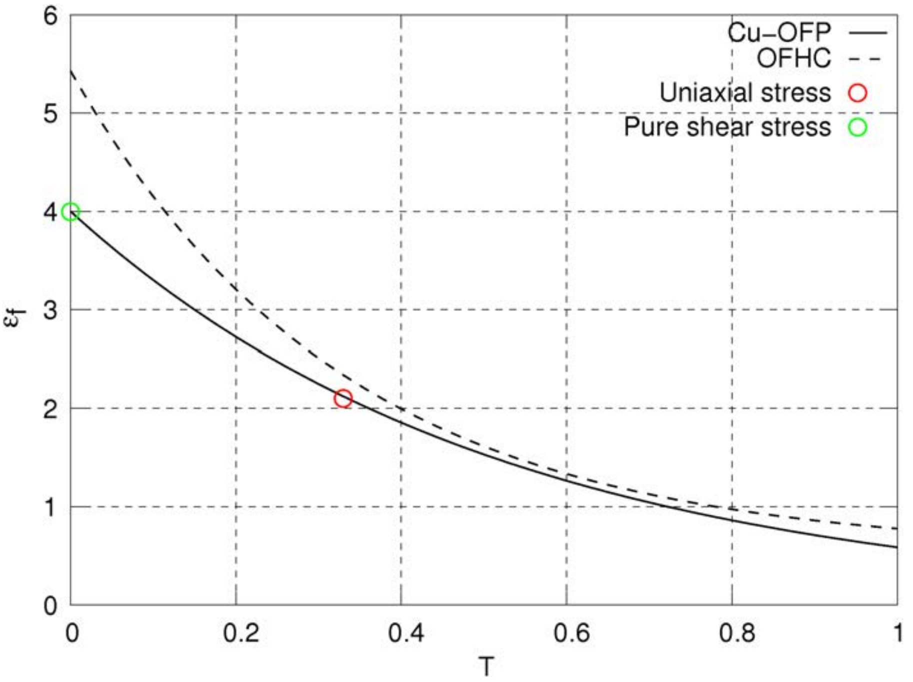


Figure 3-8: Triaxiality dependent failure strain function for Cu-OFP. Data for OFHC at room temperature and strain rate 1/s from Johnson and Cook (1985) shown for comparison.

3.3 Summary of the optimization

Using the computed equivalent plastic failure strain for tension and torsion, see the parameters in Equation 2-5 can be determined, and the result is given in Table 3-1.

In conclusion, the output from the optimization procedure to be used as input for sub-sequent analyses is:

- Deformation hardening (Figure 3-4)
- Texture parameter (Table 3-1)
- Failure strain parameters (Table 3-1)

4 Discussion on strain rates

4.1 Tensile test

In a standard tensile test the rate of displacement, i.e. velocity, is kept constant according to standards. As long as the deformation of the specimen is homogenous the strain rate is the same in every material point. However, as soon as deformation localizes and necking occurs the strain rate will vary throughout the specimen, with the highest strain rate occurring at the centre of the neck.

To visualize this phenomenon a simulation of a tensile test was carried out. With one end of the bar kept fixed and the other moving at a prescribed constant velocity throughout the simulation, the nominal strain rate was approximately 10^0 1/s. In Figure 4-1 the geometry and equivalent plastic straining is shown before loading and at material failure.

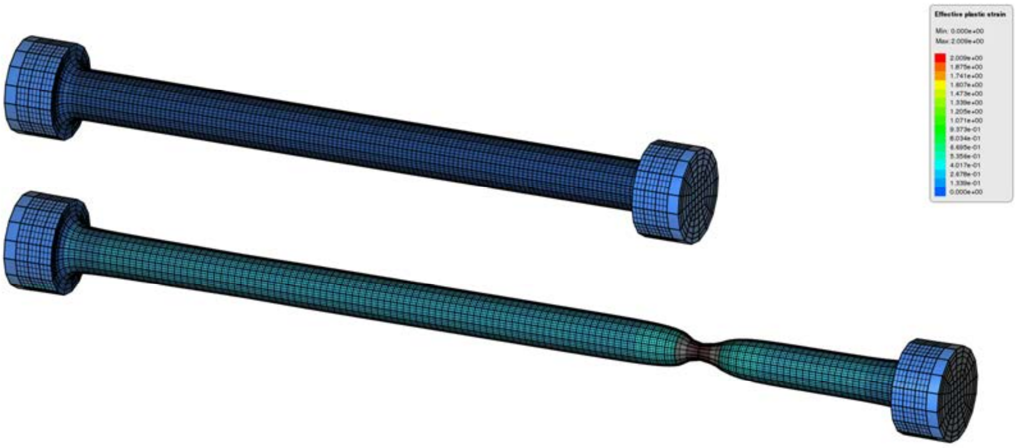


Figure 4-1: Geometry and plastic strains before loading and at material failure.

In Figure 4-2 two curves representing strain rates from the simulation are shown, one corresponding to standard extensometer measurement in tests and one corresponding to the mid-neck material point, i.e. at the centre of the bar. From the results it can be seen that after necking, the material in the bar is subjected to a range of strain rates between approximately 10^0 1/s and 10^2 1/s. When the tensile test is evaluated to determine the material behaviour, i.e. hardening with respect to strain and strain rate, it is with respect to the material centre point in the mid-neck section. Hence, the hardening after necking from a standard tensile test is not valid for a constant strain rate. To have a constant strain rate throughout the tensile test, one would have to design another set-up where the loading is controlled by the degree of necking.

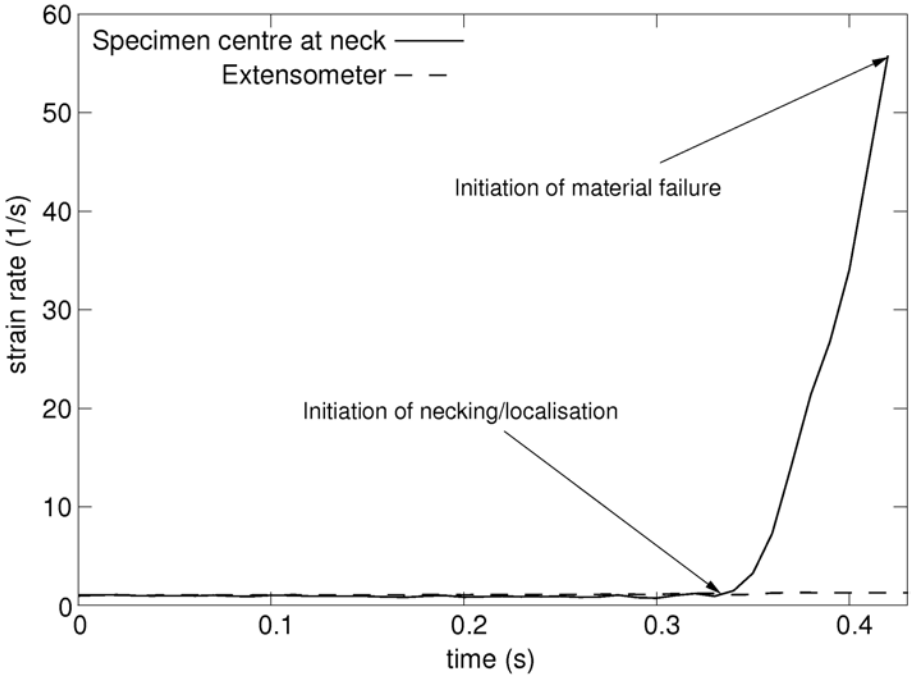


Figure 4-2: Strain rates in simulation corresponding to extensometer measurement and in the specimen centre at the mid-neck section.

4.2 Torsion test

No numerical study of strain rates for the torsion test has been carried out. However, in "Skjuvprovning av koppar" (SKBdoc 1193460) the rate of twist in the test is given as 0.2 degrees per second, ie. 0.00349 rad/s. Approximating the deformation to simple plane shear and that all deformation is localized to a mid section at the notch with dimensions 4 x 1 mm^2, we get that the nominal rate of (uniaxial) extension of the diagonal material fibre is of the order 10^{-2} s^{-1}.

References

Johnson, G. R., Cook, W. H., 1985. Fracture characteristics of three metals subjected to various strains, strain rates, temperatures and pressures. Engineering Fracture Mechanics, 21. doi: 10.1016/0013-7944(85)90052-9

Jonas, J J, Canova, G R, Shrivastava, S C, Christodolou, N, 1982. Sources of the discrepancy between the flow curves determined in torsion and in axisymmetric tension and compression testing. In Lee E H, Mallet, R L. Plasticity of Metals at Finite Strain: Theory, Computation and Experiment, Stanford Stanford University, California, 29 June-1 July, 1982.

Olovsson, L, 2013. Impetus Afea Solver - User guide & keyword manual, version 3.0 beta. Impetus Afea AB.

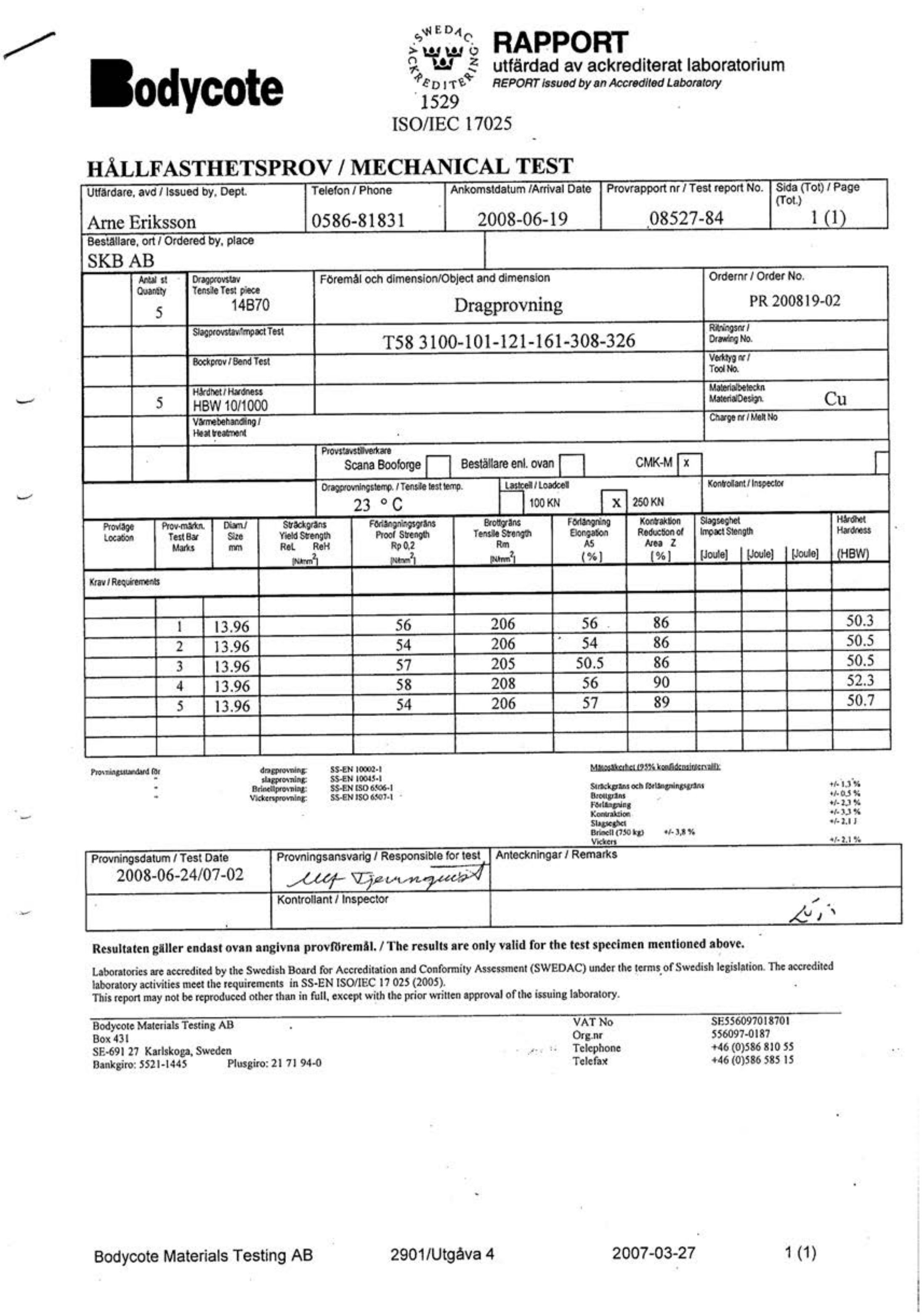
Tome, C, Canova, G R, Kocks, U F, Christodolou, N, Jonas, J J, 1984. The relation between macroscopic and microscopic strain hardening in F.C.C. polycrystals. Acta Metallurgica, 32. doi: 10.1016/0001-6160(84)90222-0

Xue, L, Wierzbicki, T, 2008. Ductile fracture initiation and propagation modeling using damage plasticity theory. Engineering Fracture Mechanics, 75. doi: 10.1016/j.engfracmech.2007.08.012

Unpublished documents

SKBdoc Id, version	Title	Issuer, year
1193460 ver. 1.0	Skjuvprovning av koppar	SKB, 2009
1205273 ver. 2.0	Intryck i kopparmaterial	SKB, 2009

Appendix A



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RAPPORT
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HÅLLFASTHETSPROV / MECHANICAL TEST

Utfärdare, avd / Issued by, Dept.	Telefon / Phone	Ankomstdatum /Arrival Date	Provrapport nr / Test report No.	Sida (Tot) / Page (Tot.)
Arne Eriksson	0586-81831	2008-06-19	08527-84	1 (1)

Beställare, ort / Ordered by, place: SKB AB

Antal st Quantity		Föremål och dimension/Object and dimension	
5	Dragprovstav Tensile Test piece: 14B70	Dragprovning	Ordernr / Order No.: PR 200819-02
	Slagprovstav/Impact Test	T58 3100-101-121-161-308-326	Ritningsnr / Drawing No.
	Bockprov / Bend Test		Verktyg nr / Tool No.
5	Hårdhet / Hardness: HBW 10/1000		Materialbeteckn MaterialDesign.: Cu
	Värmebehandling / Heat treatment		Charge nr / Melt No

Provstavstillverkare: Scana Booforge ☐ Beställare enl. ovan ☐ CMK-M ☒ ☐

Dragprovningstemp. / Tensile test temp.: 23 °C

Lastcell / Loadcell: ☐ 100 KN ☒ 250 KN

Kontrollant / Inspector

Provläge Location	Prov-märkn. Test Bar Marks	Diam./ Size mm	Sträckgräns Yield Strength ReL ReH [N/mm²]	Förlängningsgräns Proof Strength Rp 0,2 [N/mm²]	Brottgräns Tensile Strength Rm [N/mm²]	Förlängning Elongation A5 (%)	Kontraktion Reduction of Area Z [%]	Slagseghet Impact Stength [Joule]	[Joule]	[Joule]	Hårdhet Hardness (HBW)
Krav / Requirements											
	1	13.96		56	206	56	86				50.3
	2	13.96		54	206	54	86				50.5
	3	13.96		57	205	50.5	86				50.5
	4	13.96		58	208	56	90				52.3
	5	13.96		54	206	57	89				50.7

Provningsstandard för dragprovning: SS-EN 10002-1
" slagprovning: SS-EN 10045-1
" Brinellprovning: SS-EN ISO 6506-1
" Vickersprovning: SS-EN ISO 6507-1

Mätosäkerhet (95% konfidensintervall):

Sträckgräns och förlängningsgräns	+/- 1,3 %
Brottgräns	+/- 0,5 %
Förlängning	+/- 2,3 %
Kontraktion	+/- 3,3 %
Slagseghet	+/- 2,1 J
Brinell (750 kg)	+/- 3,8 %
Vickers	+/- 2,1 %

Provningsdatum / Test Date	Provningsansvarig / Responsible for test	Anteckningar / Remarks
2008-06-24/07-02	Ulf Tjernquist	
	Kontrollant / Inspector	

Resultaten gäller endast ovan angivna provföremål. / The results are only valid for the test specimen mentioned above.

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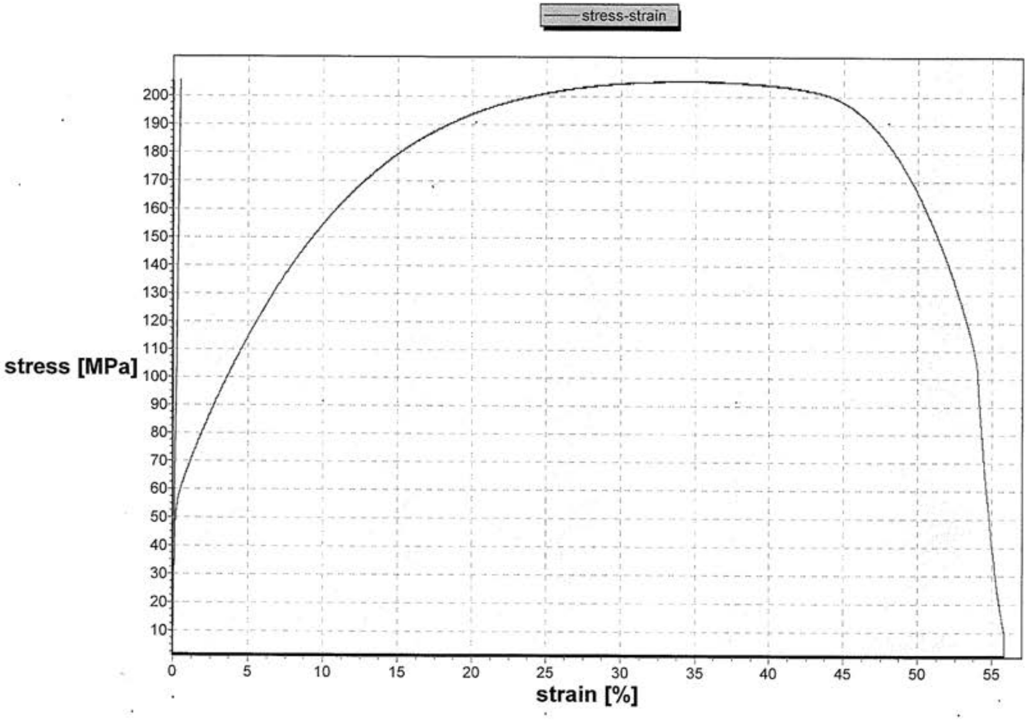
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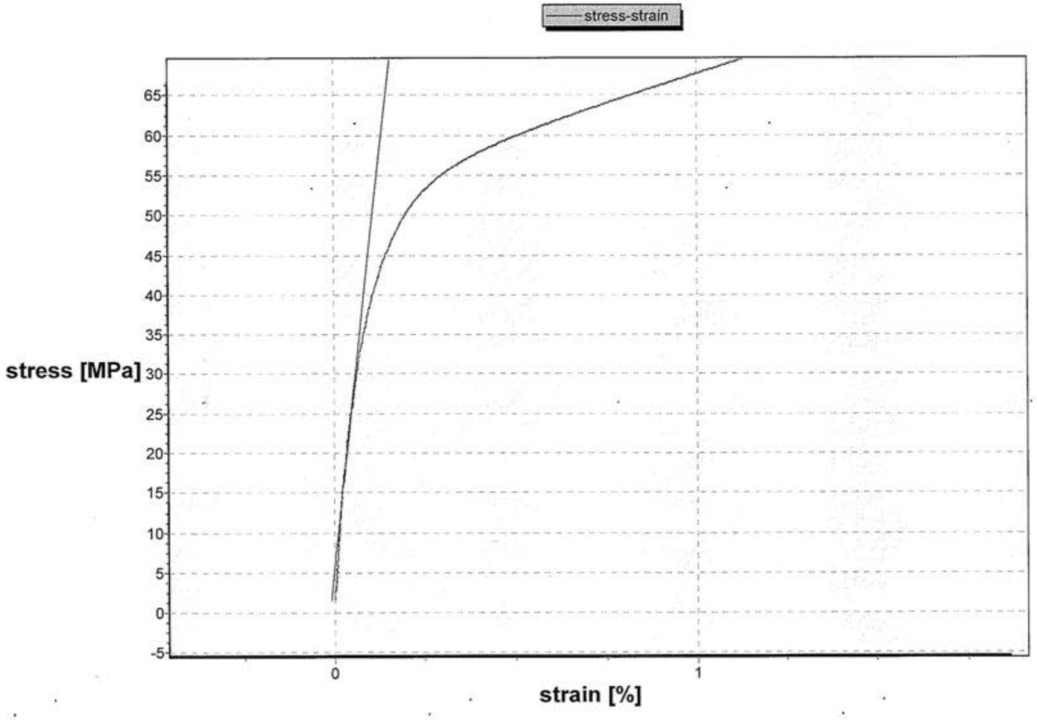
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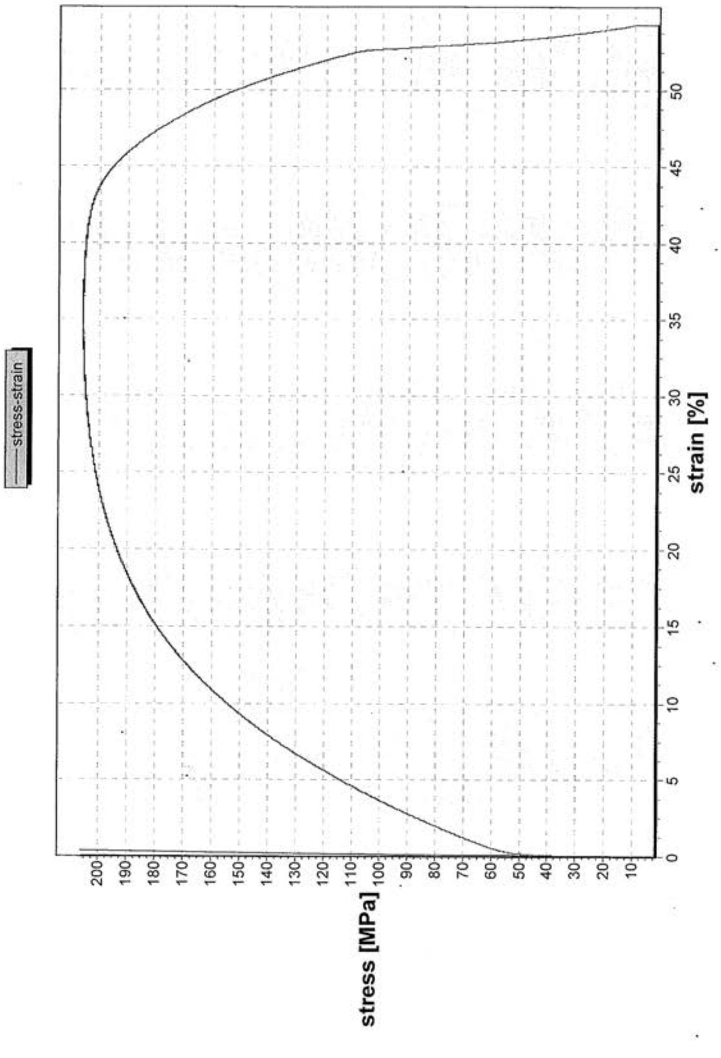
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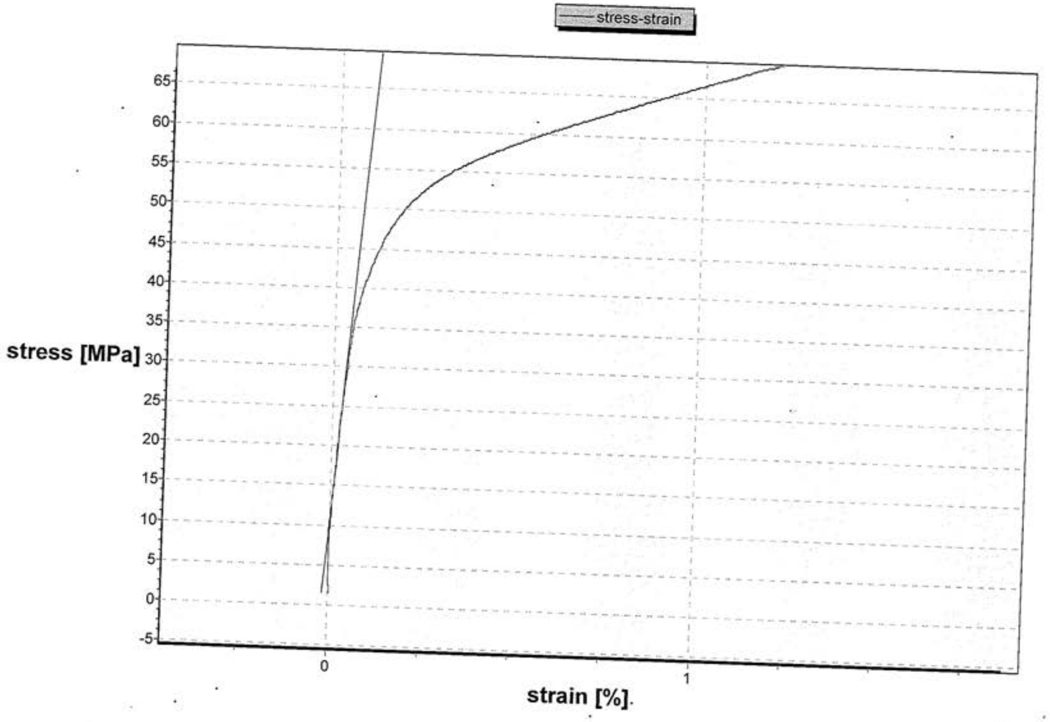
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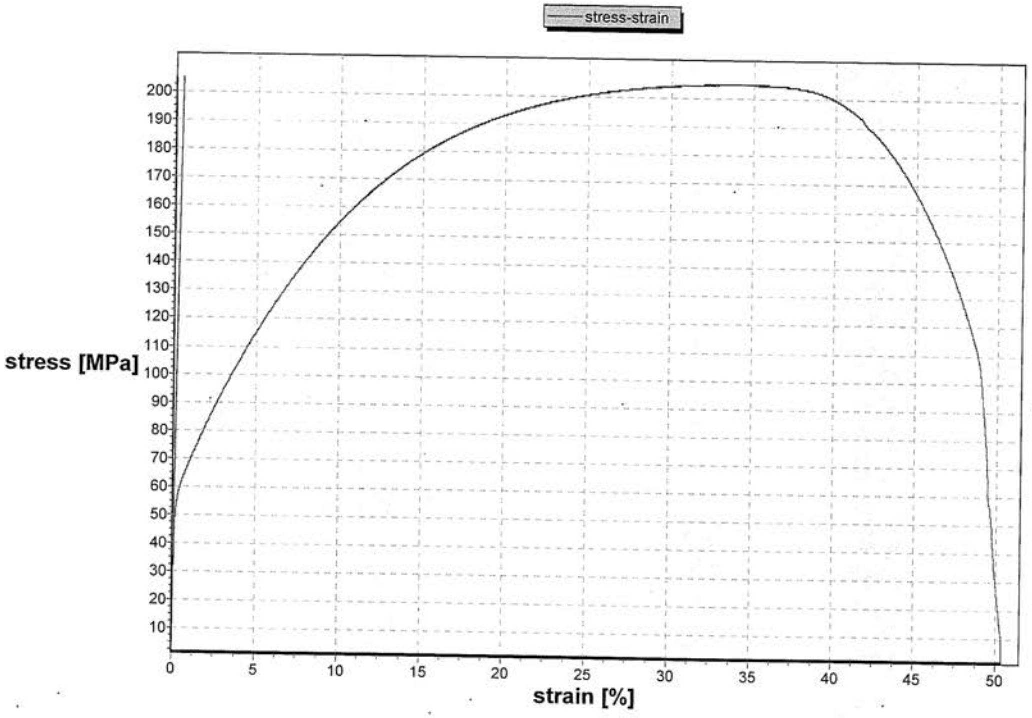
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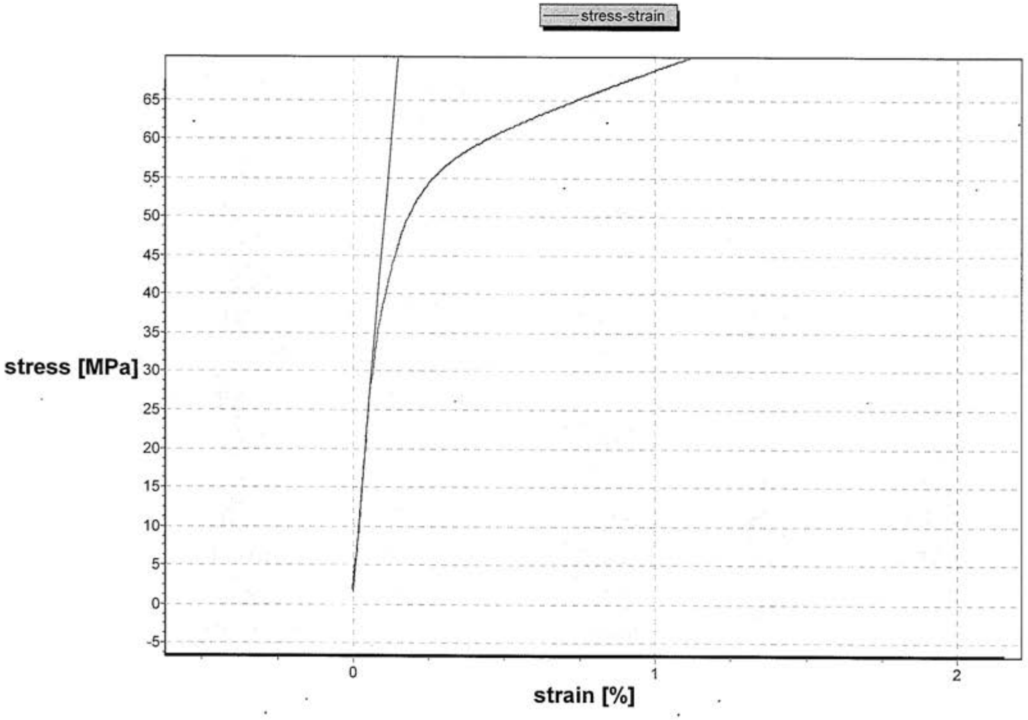
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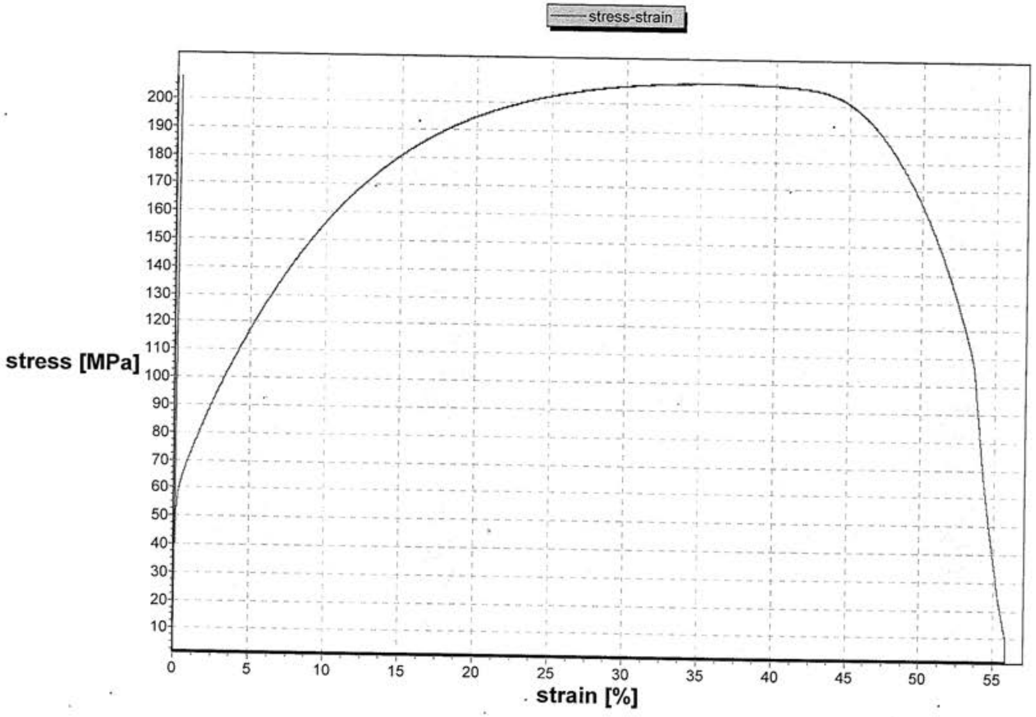
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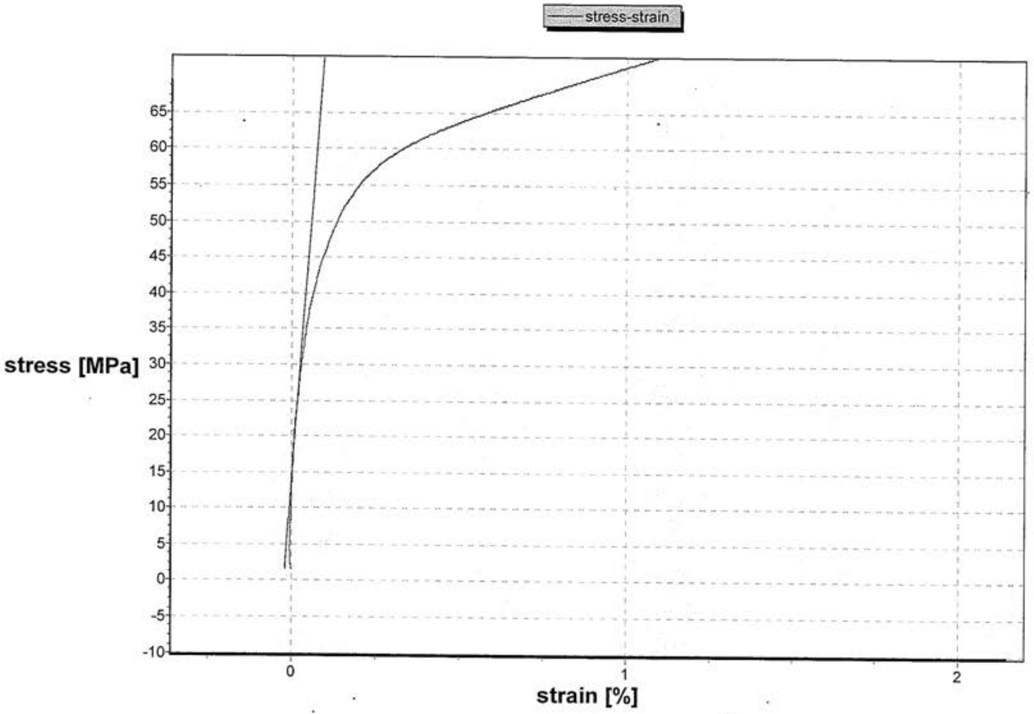
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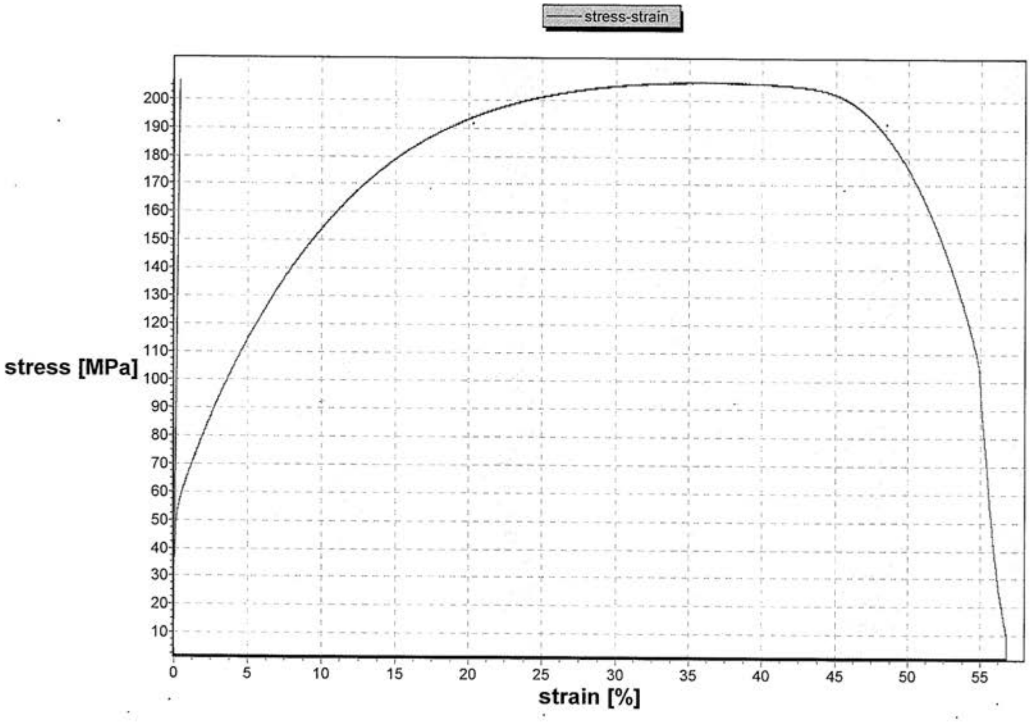
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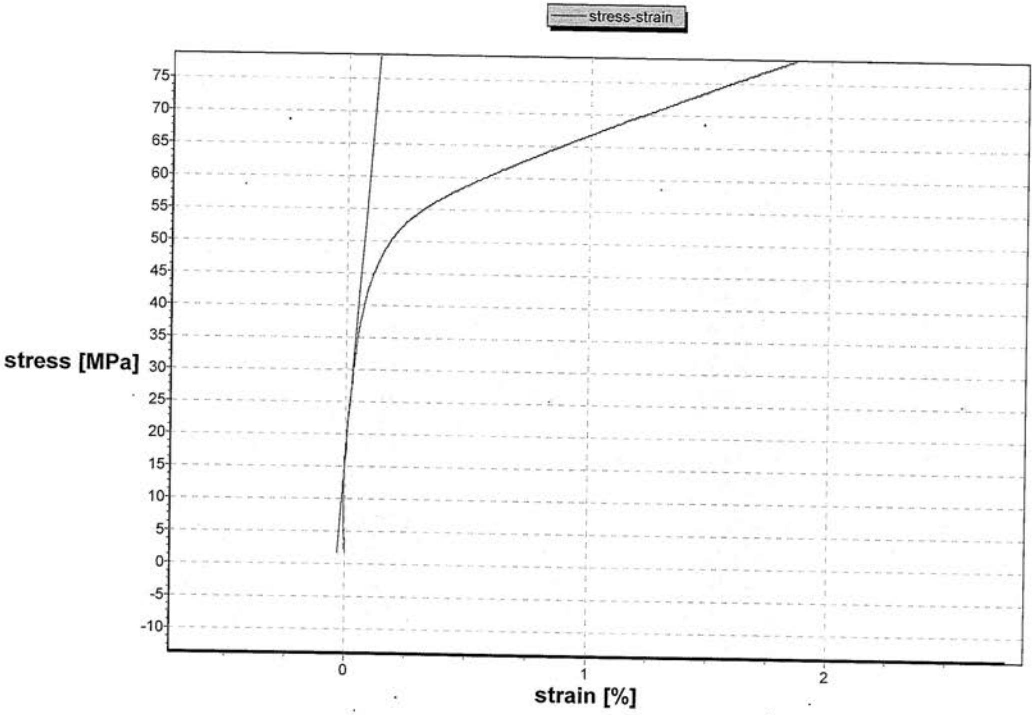
strain [%]

5


stress-strain
stress [MPa]
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
0
1
2
strain [%]

Appendix B

Optimized deformation hardening (*H*) as tabulated values (true strain, true stress MPa).

0.000,	30.000
0.041,	115.375
0.044,	119.013
0.047,	122.595
0.050,	126.121
0.053,	129.590
0.056,	133.005
0.059,	136.366
0.062,	139.673
0.065,	142.926
0.068,	146.127
0.071,	149.275
0.074,	152.372
0.077,	155.419
0.080,	158.414
0.083,	161.360
0.086,	164.257
0.089,	167.105
0.092,	169.905
0.094,	172.658
0.097,	175.364
0.100,	178.023
0.103,	180.637
0.106,	183.205
0.109,	185.729
0.112,	188.209
0.115,	190.645
0.118,	193.038
0.121,	195.390
0.124,	197.699
0.127,	199.967
0.130,	202.195
0.133,	204.383
0.136,	206.531
0.139,	208.641
0.142,	210.712
0.145,	212.745
0.148,	214.742
0.151,	216.702
0.154,	218.626
0.157,	220.514
0.160,	222.368
0.163,	224.188
0.166,	225.974
0.169,	227.726
0.172,	229.447
0.175,	231.135
0.178,	232.792
0.181,	234.419
0.184,	236.015
0.187,	237.581
0.190,	239.119
0.193,	240.628
0.196,	242.109
0.199,	243.563
0.202,	244.990
0.205,	246.391
0.208,	247.767
0.211,	249.117
0.214,	250.443
0.217,	251.746
0.220,	253.025
0.223,	254.281
0.226,	255.515
0.229,	256.728
0.232,	257.919
0.235,	259.091
0.238,	260.242
0.241,	261.374
0.244,	262.488
0.247,	263.583
0.250,	264.661
0.253,	265.723
0.256,	266.767
0.259,	267.796
0.262,	268.810
0.265,	269.809
0.268,	270.795
0.271,	271.766
0.274,	272.725
0.277,	273.672
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0.286,	276.443
0.289,	277.346
0.292,	278.240
0.295,	279.125
0.298,	280.001
0.301,	280.870
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0.310,	283.440
0.313,	284.285
0.315,	285.126
0.318,	285.962
0.321,	286.795
0.324,	287.624
0.327,	288.449
0.330,	289.270
0.333,	290.087
0.336,	290.900
0.339,	291.710
0.342,	292.516
0.345,	293.319
0.348,	294.118
0.351,	294.913
0.354,	295.705
0.357,	296.494
0.360,	297.279
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0.366,	298.839
0.369,	299.614
0.372,	300.386
0.375,	301.155
0.378,	301.921
0.381,	302.684
0.384,	303.443
0.387,	304.200
0.390,	304.953
0.393,	305.704
0.396,	306.451
0.399,	307.196
0.402,	307.938
0.405,	308.677
0.408,	309.413
0.411,	310.147
0.414,	310.878
0.417,	311.606
0.420,	312.331
0.423,	313.054
0.426,	313.774
0.429,	314.492
0.432,	315.207
0.435,	315.919
0.438,	316.629
0.441,	317.336
0.444,	318.041
0.447,	318.744
0.450,	319.444
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0.465,	322.909
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