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Numerical Investigation of Size Effects in Tension and Torsion of Micro-scale Copper Wires using a Strain Gradient Modified Johnson-Cook Constitutive Model

While material behaviour on the micro to nanoscale may be investigated using various experimental methods, it is of interest to develop complementary 3-dimensional (3D) numerical approaches to simulate material deformation at such small scales. In particular, these simulations provide a means to shed further light on key mechanisms at play, especially in the region of plastic strain. The size effect in tension and torsion of micro-scale copper wires is numerically investigated in this study using a strain gradient modified Johnson-Cook method. This 3D algorithm is implemented by self-compiled subroutines using the ABAQUS/Explicit solver. The simulated flow stress and yield stress in torsion of micro-scale copper wires were observed to increase with the decrease of the wire diameter, which correlates well with experimental findings reported in the literature. A similar size effect, although not as significant as that in torsion, was also observed in the simulated tension experiments, again in line with existing experimental reports. This work contributes to the efforts of the research community in the simulation material behaviour at the micro- to nanoscale, especially when considering the combined influence of both size effect and strain rate.

Keywords:
Tension/torsion simulation, johnson-cook theory, strain gradient plasticity, size effect, finite element method.

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INTRODUCTION

The knowledge of material properties on the micro- to nanoscale is of great importance for the predictable and reliable manufacture of small-scale structures. Different from the meso-macro scale, where material properties can be considered constant and relatively easy to calibrate when implementing numerical simulations, establishing accurate material constitutive models at smaller scale remain challenging due to increased instrumentation requirements and the prevalence of more complex mechanisms such as the size effect. This effect, which results in the increase in the flow stress of material as the volume of the deformed region reduces, has been reported in many experiments [1] such as tension, compression, torsion, indentation and scratching of various metal/polymer wires and foils.

Numerical tools such as molecular dynamics modelling (MD), crystal plasticity finite element method (CPFEM), multiscale approaches including finite element combined with atomistic method (FEAt), bridging scale method (BSM), coupled atomistic and discrete dislocation plasticity (CADD) approaches and quasi-continuum (QC) method have been developed by the research community to investigate and model this size effect. However, prohibitive computational cost, unrealistic space/time scale involved, and implementation complexity can hinder the applications of these methods. On the other hand, the low-order strain gradient plasticity theory (SGP), which is built on the framework of von Mises plasticity, considers the size effect by introducing a material characteristic length and strain gradient. The relative ease of implementation and robust physical derivation render SGP an efficient and reliable method to investigate material behaviour at the micro to sub-micro scale. In addition, the Johnson-Cook (JC) theory [2] which considers the effect of strain hardening, strain rate and the temperature has been widely utilised in the simulation of meso to macro scale deformation of metallic materials.

To solve the aforementioned issues in numerical simulations at micro and sub-micro scales, this study reports the implementation of a 3D Finite Element (FE) approach whereby the material constitutive model is described by combining the JC and the SGP theories. The combination of these theories forms a novel framework within which the effect of strain hardening, strain rate, temperature and size effect could be investigated thoroughly. As a result, the bridge between different scales is expected to be facilitated and the material library at small scales is expected to be enriched for future simulations.

MATERIALS AND METHODS

The FE simulations carried out in this work concern the torsion and uniaxial tension of copper wires. The numerical studies are performed using the ABAQUS/Explicit module and the SGP-modified JC algorithm is realised using the embedded subroutines. The copper wires are constrained on all degrees of freedom (DOF) on the base part and only the *x* direction of the grip part is ascribed to move under a quasi-static strain rate of 0.1 in tension (see Fig. 1). The stress in tension is calculated as an average value of the von Mises stress of the gauge section. For the torsion simulations, the grip and base parts are subjected to a rotation of 1.57 (radians) in the *UR1* direction and the remaining DOFs are constrained. The shear strain is calculated using $a\theta/L$, where L is the gauge length, a is the radius of the wire and θ is the torsion angle. The diameters of the simulated copper wire were varied and included the following values: 18 µm, 30 µm, 42 µm and 105 µm. These values were selected to be able to compare the simulation results against the experimental data published in [1]. The material properties used in this work can be found in [2].

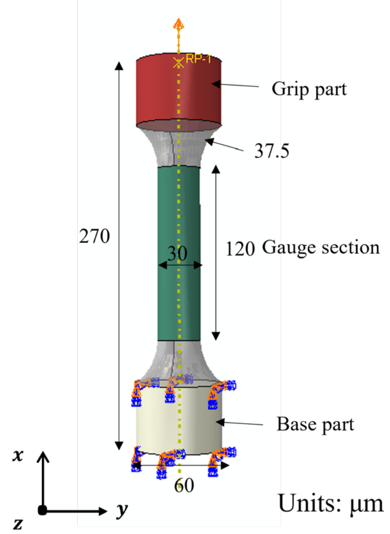

Fig. 1. Schematic illustration of one of the simulated dog-bone-shaped specimens.

The classical JC model describes the flow stress as:

$$\sigma_{JC} = [A + B(\bar{\varepsilon}^{pl})^n][1 + C\ln(\frac{\dot{\bar{\varepsilon}}^{pl}}{\dot{\varepsilon}_0})](1 - \hat{\theta}^m) \quad (1)$$

Based on the SGP theory, the flow stress using Taylor's model is given as:

$$\sigma = M\alpha Gb\sqrt{\rho_s + \rho_g} \quad (2)$$

ρ_s can be determined by material tests where the strain gradient is negligible and thus classic JC is applicable:

$$M\alpha Gb\sqrt{\rho_s} = \sigma_{JC} \quad (3)$$

Substituting (3) into (2), the flow stress becomes:

$$\sigma = \sigma_{JC}\sqrt{1 + \frac{\rho_g}{\rho_s}} \quad (4)$$

ρ_g is calculated as:

$$\rho_g = \bar{r}\frac{\eta}{b} \quad (5)$$

Substituting (3) and (5) into (4), the flow stress is now [3]:

$$\sigma_{flow} = \sigma_{JC}\sqrt{1 + (\frac{18\alpha^2 G^2 b}{\sigma_{JC}^2}\eta)^{\mu}} \quad (6)$$

where $\frac{18\alpha^2 G^2 b}{\sigma_{JC}^2}$ is defined as material characteristic length l. μ is introduced to represent the density of GNDs needed to accommodate the strain gradient in the deformation zone. Equation (6) describes the material constitutive model which combines the JC and the SGP theories. The incremental plastic strain gradient $\Delta\eta_{ijk}^p$ can be calculated using the formulation below [4].

$$\Delta\eta_{ijk}^p = \Delta\varepsilon_{ik,j}^p + \Delta\varepsilon_{jk,i}^p - \Delta\varepsilon_{ij,k}^p \quad (7)$$

In this work, (7) is reformulated as:

$$\Delta\eta_{ijk}^{p} = \sum_{k=1}^{8} N_k(\xi,\eta,\zeta)(\Delta\bar{\varepsilon}_{ij}^{pl}) \quad (8)$$

Similar to the effective strain which can be expressed as $\varepsilon = \sqrt{\frac{2}{3}\varepsilon_{ij}\varepsilon_{ij}}$, under rate-proportional loading, $\Delta\eta^p$ can be calculated as:

$$\Delta\eta^p = \sqrt{\frac{1}{4}\Delta\eta_{ijk}^{p}\Delta\eta_{ijk}^{p}} \quad (9)$$

The JC shear failure criterion is also included in the developed model. More specifically, the failure strain $\bar{\varepsilon}_f^{pl}$ is calculated as follows:

$$\bar{\varepsilon}_f^{pl} = (d_1 + d_2 e^{d_3\frac{p}{q}})(1 + d_4 ln\,(\frac{\dot{\bar{\varepsilon}}^{pl}}{\dot{\varepsilon}_0}))(1 + d_5\hat{\theta}\,) \quad (10)$$

Next, a summation of incremental failure strain is performed over all increments to calculate the failure criterion as follows:

$$\omega = \Sigma(\frac{\Delta\bar{\varepsilon}_f^{pl}}{\bar{\varepsilon}_f^{pl}}) \quad (11)$$

Once ω exceeds a critical threshold, i.e., a value over 1, the affected elements are deleted in the next solver step. The equivalent plastic strain $\bar{\varepsilon}^{pl}$, von Mises stress q and hydro stress p that are needed for the algorithm are obtained by the VGETRM utility subroutine at the end of each increment.

RESULTS

All the simulated stress-strain curves of copper wires in tension are displayed in Fig 2. Following the notation reported in [5] the normalized torque Q/a^3 is also plotted against the surface shear strain κa in torsion as shown in Fig 3, where κ is the twist per unit length of the wire.

From Fig. 2, it is observed that the stress-strain curves of wires with different diameters in tension are all superimposed when using only the classical JC method built in Abaqus. This is expected because the classical JC approach does not take strain gradient into account and thus, cannot simulate the size effect. The maximum simulated flow stress in tension using the classical JC model was found to be around 231.8 MPa. In torsion, the simulated flow stress using the built-in JC method fluctuated slightly between 277.3 MPa-290.9 MPa. For this reason, in Fig. 3, only the average value of 283.3 MPa is plotted for the classical JC simulation.

When using the SGP-modified JC method, both the flow stress and Q/a^3 increased in different proportions with the decreasing of wire diameters. In tension, the simulated stress-strain data are the highest for the 18 µm wire, i.e., that with the smallest diameter. This was expected and is aligned with the experimental results in [1], which are also reported in both Fig. 2 and Fig.3. The same observation can be made for the simulations in torsion. The stress-strain data in torsion for the 30 µm and 42 µm wires are relatively close, which is similar in trend to the experimental findings. Although a good agreement between the trends and the order of magnitude of the numerical and experimental data is observed, actual values differ. This may be due to the fact that the experimental results in [1] were achieved on copper wires that had been annealed. The annealing process likely resulted in an enlarged grain size and smaller dislocation density [6] compared to standard copper wires which have been considered as the baseline when implementing the proposed SGP-modified JC constitutive model.

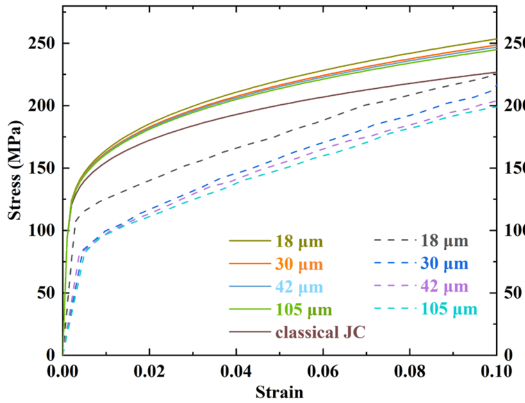

Fig. 2. Stress-strain curves for copper wires in tension with diameters of 18 µm, 30 µm 42 µm and 105 µm. The dashed curves show the experimental results reported in [1].

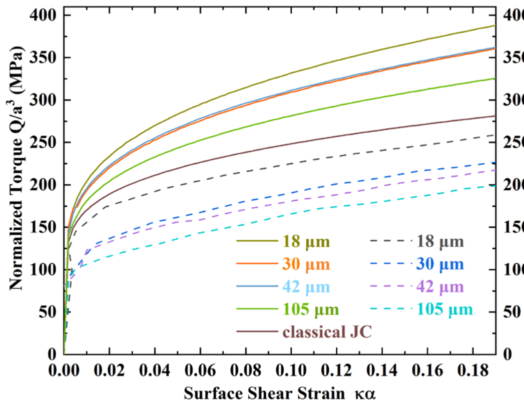

Fig. 3. Plots of normalized torque-twist curves for copper wires with diameters of 18 µm, 30 µm 42 µm and 105 µm. The dashed curves show the experimental results reported in [1].

The extracted yield stress data in tension at the strain of 0.1 and in torsion at the surface shear strain of 0.19 are displayed in Fig. 4 for all wire diameters considered. The yield stress using the classical JC theory remains nearly identical (around 231.8 MPa for tension and 271 MPa for torsion) regardless of the diameter. When using the proposed SGP-modified JC model, it is clearly noted from Fig. 4 that the simulated yield stress increases with a reduction in the wire diameter. This size effect is also observed to be more pronounced in torsion than that in tension, as was also reported in [1] based on experimental findings.

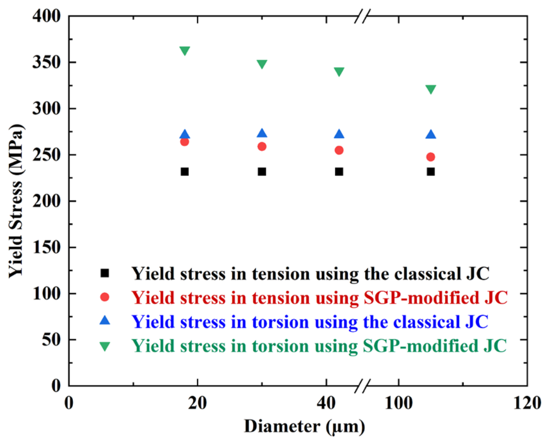

Fig. 4. Simulated yield strength data (for a strain of 0.1 in tension and a surface shear strain of 0.19 in torsion) for copper wires with diameters of 18 µm, 30 µm 42 µm and 105 µm.

DISCUSSION

Using the developed SGP-modified JC constitutive model in the FE simulations, the numerical results were found to be consistent with the experimental findings from [1] which reported the existence of a size effect for micro-scale copper wires. As expected, such size effect cannot be simulated using the classical JC theory only. Fleck et al. [5] pointed out that, the size effect was more prominent in torsion. This was also observed in the simulations presented here.

The reason behind this difference in material behaviour between tension and torsion is that, in uniaxial tension, the hardening is mainly due to the statistically stored dislocations which can be relatively moderate for a given wire diameter. In torsion, and for the same wire diameter, the strain gradient = and more pronounced non-homogeneity of deformation introduce an increased amount of geometrically necessary dislocations (GND). For a given surface shear strain, a thinner wire i.e., a smaller a, would introduce a larger strain gradient and greater density of GND. A faster and greater hardening in thinner wires would thus be observed. The material characteristic length, which is a homogenous representation of internal structures and dislocations, and the equivalent plastic strain/ shear strain are attributed to this size effect.

One should also notice that the developed model does not capture the size effect in the initial elastic region. This is the reason why the simulated yield point (around 94MPa in tension) and normalized torque (around 140 MPa in torsion) values are constant in Fig. 2 and Fig. 3.

CONCLUSIONS

The presented results demonstrate that the developed SGP-modified JC model and its implementation via 3D FE simulations can be used to study the size effect in micro-scale tension and torsion of copper wires. Given that the model also intrinsically considers the influence of the strain rate, strain hardening and temperature, it paves the way for the further simulation of micro and nano-scale manufacturing processes which are not taking place in a quasi-static mode, such as in ultraprecision machining for example.

In future simulations, the contribution of the strain rate and processing temperature against that of the strain gradients will also be investigated based on the developed model. As stated by Pañeda [7], for a typical dislocation density of $10^{15}/m^2$, equation (6) holds at a scale above 100 nm. This means that the developed model should be used in future studies where the size of the processed material region is above this threshold.

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Conflicts of interest
The authors declare no conflict of interest.

APPENDIX

A, B, C, m, n coefficients of the JC model
$\Delta\bar{\varepsilon}^{pl}$ incremental equivalent plastic strain
$\dot{\varepsilon}_0$ reference strain rate
$\dot{\bar{\varepsilon}}^{pl}$ equivalent plastic strain rate
$\hat{\theta}$ temperature term
d_1, d_2, d_3, d_4, d_5 parameters of JC failure criterion
ρ_s density of statistically stored dislocation
ρ_g density of geometry necessary dislocation
G shear modulus (GPa), b burgers vector (nm)
a empirical coefficient which takes value between 0.3 and 0.5
$\bar{r}$ Nye-factor which is assumed to be 1.90 for face-centred cubic (fcc) polycrystals
M Taylor factor, 3.06 for fcc metals
$N_k(\xi, \eta, \zeta)$ shape function vector
$\Delta\varepsilon^{p}_{ik,j}$ plastic strain components

REFERENCES

[1] D. Liu, Y. He, X. Tang, H. Ding, P. Hu, and P. Cao, ‘Size effects in the torsion of microscale copper wires: Experiment and analysis’, *Scripta Materialia*, vol. 66, no. 6, pp. 406–409, Mar. 2012. doi.org/10.1016/j.scriptamat.2011.12.003

[2] G. R. Johnson and W. H. Cook, ‘Fracture characteristics of three metals subjected to various strains, strain rates, temperatures and pressures’, *Engineering Fracture Mechanics*, vol. 21, no. 1, pp. 31–48, Jan. 1985. doi.org/10.1016/0013-7944(85)90052-9

[3] X. Lai, H. Li, C. Li, Z. Lin, and J. Ni, ‘Modelling and analysis of micro scale milling considering size effect, micro cutter edge radius and minimum chip thickness’, *International Journal of Machine Tools and Manufacture*, vol. 48, no. 1, pp. 1–14, Jan. 2008. doi.org/10.1016/j.ijmachtools.2007.08.011

[4] H. Gao, Y. Huang, W. D. Nix, and J. W. Hutchinson, ‘Mechanism-based strain gradient plasticity— I. Theory’, *Journal of the Mechanics and Physics of Solids*, vol. 47, no. 6, pp. 1239–1263, Apr. 1999. doi.org/10.1016/S0022-5096(98)00103-3

[5] N. A. Fleck, G. M. Muller, M. F. Ashby, and J. W. Hutchinson, ‘Strain gradient plasticity: Theory and experiment’, *Acta Metallurgica et Materialia*, vol. 42, no. 2, pp. 475–487, Feb. 1994. doi.org/10.1016/0956-7151(94)90502-9

[6] P. A. El-Deiry and R. P. Vinci, ‘Strain Rate Dependent Behavior of Pure Aluminum and Copper Micro-Wires’, *MRS Online Proceedings Library*, vol. 695, no. 1, p. 421, Mar. 2011. doi.org/10.1557/PROC-695-L4.2.1

[7] E. Martínez-Pañeda and C. Betegón, 'Modeling damage and fracture within strain-gradient plasticity', *Int J Solids Struct*, vol. 59, pp. 208-215, May 2015. doi.org/10.1016/j.ijsolstr.2015.02.010

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