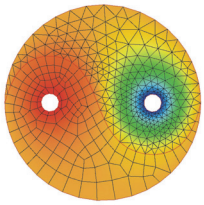
Publishing House
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 9, 2009, No. 1



MODELLING THE INFLUENCE OF THE STRUCTURE ON THE PROPERTIES OF NANOMETALS

ROMUALD DOBOSZ, TOMASZ WEJRZANOWSKI, KRZYSZTOF JAN KURZYDŁOWSKI

Warsaw University of Technology, Faculty of Materials Science and Engineering,
Wołoska 141, Warszawa 02-507, Poland
Corresponding Autor: rdobosz@inmat.pw.edu.pl (R. Dobosz)

Abstract

The mechanical properties of materials depend on their structure. The influence of grain size and grain size distribution on the flow stress of polycrystalline materials (e.g. metals) has been widely reported. The value of the yield point is usually predicted by the Hall-Petch relationship which was established experimentally for micrometer grain sizes. When the grain size is reduced to the nanometric size, the relationship between grain size and flow stress changes for several reasons including activation of the mechanism of grain boundary sliding.

Grain boundaries play a major role in the plastic deformation mechanism of polycrystalline nano-materials, because they possess a significantly large volume fraction of atoms at the grain boundaries. In order to quantitatively model this influence, a two-phase finite element model was developed using the generalized Hill potential theory for modelling the anisotropic plasticity of grain boundaries. The results of the numerical simulations give an insight into the influence of various parameters on the plastic deformation of nano-polycrystalline materials. The simulations were also applied to study the effect of grain size homogeneity on the mechanical properties of nanometals.

Key words: nanometals, plastic deformations, grain boundaries, modelling

1. INTRODUCTION

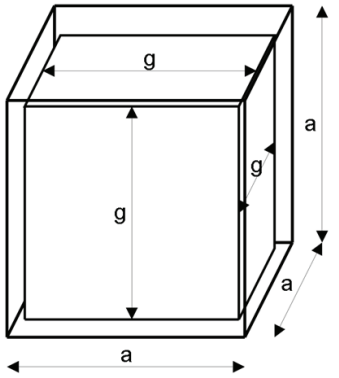
The influence of the grain boundaries on the mechanical properties of metals is usually described by the Hall-Patch relationship (H-P) [2,3] which has been experimentally proved for a wide range of grain sizes. The classic H-P relationship between the yield stress σ_y and the average grain size d is given by the formula:

$$\sigma_y = \sigma_0 + K \cdot d^{-0.5} \qquad (1)$$

where: σ_y is the yield stress, d is average grain size, with σ_0 and K being material constants.

The H-P equation is known to work well for metals with average grain sizes from 1 to 100 μm. Recent advances in nano-technology have made it possible to verify its relevance for grain sizes in the range from 10 nm to 1 μm. It has been found in this context, that for grain sizes in the range 10 – 30 nm, a reduction in the strength of nano-polycrystalline materials is observed [6]. The possible reason for this phenomenon, described as reverse HP (RH-P), is a change in the mechanism of plastic deformation, involving the activation of grain boundary sliding, because of the high volume fraction of atoms located in the grain boundaries (GBs). A simple geometric consideration indicates that if the grain boundaries 1 nm wide, then for an average grain size of 10 nm, the volume fraction of grain boundary atoms is 25 %, see figure 1.

ISSN 1641-8581



$$a = 11nm \quad g = 10nm$$

$$V_f = \frac{a^3 - g^3}{a^3} \cdot 100\% \approx 25\%$$

Fig. 1. *Estimation of the volume fraction of atoms at the grain boundaries.*

The different behaviour of nano-metals can be explained by the difference between the mechanical properties of the grain interiors (GIs) and the grain boundaries. Normally grain boundaries are considered as being 2-dimensional elements of zero thickness. This concept is fully justified if the nominal thickness of the boundaries, approximately 1 nm, is less than 10^{-4} of the standard grain size. However, for nano-polycrystals the thickness of the grain boundaries cannot be ignored. This leads to a two-element situation, one of being the grain boundaries and the other the grain interiors.

When the average grain size is reduced to the nano-metric level, consideration should be given to the influence of grain size distribution on the mechanical properties. Experimental results revealing the special properties of nano-metals with bimodal grain size distribution have been published [5].

rate phases with different mechanical properties. The properties of the grain boundaries were described by the Generalized Hill Potential Theory (GHPT) [1], to account for their anisotropic plasticity. Isotropic properties of the grain interiors have been assumed with the yield stress of individual grains being determined by the HP formula, see equation (1).

2. MODEL DESCRIPTION

Model grain structures with different grain size dispersion were generated by Voronoi tessellation. The numerical models were built with grain interiors and grain boundaries, see figure 2. The thickness of the grain boundaries were modelled at 1nm. The two-phase model was analyzed by the finite element method implemented by Ansys software.

The anisotropic Hill potential theory was used for modelling plastic deformation of the grain boundaries. The Hill's criterion is an extension to the Huber-Mises-Hencky yield criterion for anisotropic materials. This criterion was used under assuming that isotropic hardening is given by:

$$f\{\sigma\} = \sqrt{\{\sigma\}^T [M] \{\sigma\}} - \sigma_0\left(\varepsilon^p\right) \qquad (2)$$

where: σ_0 = reference yield stress and ε^p = equivalent plastic strain. The grain boundary phase is assumed to have three orthogonal planes of symmetry. The material coordinate system is perpendicular to these planes of symmetry and the plastic compliance matrix [M] is written as:

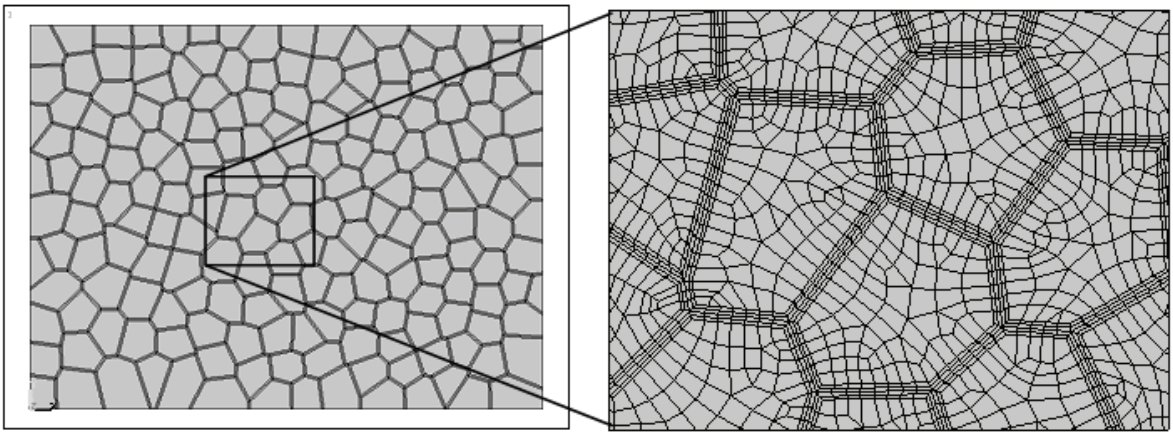


Fig. 2. *The "two-phase" numerical model of the polycrystalline structure.*

In order to model the influence of grain boundaries and grain size dispersion on the flow stress of nano-metals, a "two-phase" finite element model was developed. In this model, it was assumed that the grain boundaries and grain interiors act as sepa-

$$[M]=\begin{bmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2N & 0 & 0 \\ 0 & 0 & 0 & 0 & 2L & 0 \\ 0 & 0 & 0 & 0 & 0 & 2M \end{bmatrix} \tag{3}$$

F, G, H, L, M and N are material constants that can be determined experimentally. They are defined as:

$$F=\frac{1}{2}\left(\frac{1}{R_{yy}^2}+\frac{1}{R_{zz}^2}-\frac{1}{R_{xx}^2}\right),$$

$$G=\frac{1}{2}\left(\frac{1}{R_{zz}^2}+\frac{1}{R_{xx}^2}-\frac{1}{R_{yy}^2}\right),$$

$$H=\frac{1}{2}\left(\frac{1}{R_{xx}^2}+\frac{1}{R_{yy}^2}-\frac{1}{R_{zz}^2}\right)$$

$$L=\frac{3}{2}\left(\frac{1}{R_{yz}^2}\right),\quad M=\frac{3}{2}\left(\frac{1}{R_{xz}^2}\right),\quad N=\frac{3}{2}\left(\frac{1}{R_{xy}^2}\right) \tag{4}$$

The yield stress ratios; R_{xx}, R_{yy}, R_{zz}, R_{xy}, R_{yz} and R_{xz} can be calculated as:

$$R_{xx}=\frac{\sigma_{xx}^{y}}{\sigma_0},\quad R_{yy}=\frac{\sigma_{yy}^{y}}{\sigma_0},\quad R_{zz}=\frac{\sigma_{zz}^{y}}{\sigma_0},$$

$$R_{xy}=\sqrt{3}\frac{\sigma_{xy}^{y}}{\sigma_0},\quad R_{yz}=\sqrt{3}\frac{\sigma_{yz}^{y}}{\sigma_0},\quad R_{xz}=\sqrt{3}\frac{\sigma_{xz}^{y}}{\sigma_0} \tag{5}$$

where: σ_{xx}^{y}, σ_{yy}^{y}, σ_{zz}^{y}, σ_{xy}^{y}, σ_{yz}^{y}, σ_{xz}^{y} are values of yield stress.

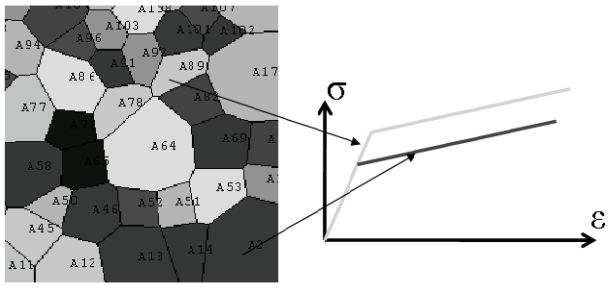


Fig. 3. *The mechanical properties of grain interiors.*

The grain interiors were treated as being isotropic elasto-plastic elements, with their yield point being dependant on the grain size in accordance with Hall-Patch relationship [4], see figure 3. Linear hardening was assumed with $d\sigma/d\varepsilon$ being designated as E_T.

Calculations were performed to obtain the macroscopic tensile stress-strain curves for the nano-polycrystals. The simulations of the plastic deformation of the described two-phase structure were carried out for copper, with the following constants K = 0.14 MN m$^{-3/2}$ and σ_0 = 33 MPa for the grain interiors. Work hardening was assumed as E_T = 12 GPa for the GIs and E_T = 0.6 GPa for the grain boundaries.

The mechanical properties of the grain boundaries, as described by the *Rij* dimensionless coefficients, were varied in the range from 1 to 20. For the largest values of *Rij*, approaching 20, the grain boundaries were stronger than the interior of the larger grains. For smaller values, near to 1, the resistance of the grain boundaries to plastic deformation was equal to that of monocrystals.

The two σ_0 parameters used in the simulation have different physical meanings. That in the HP equation (1) describes the resistance to plastic deformation of mono-crystals. The, other, applied in the Hill theory, describes the resistance of the material to the plastic flow. Within the scope of the analyses reported here they have been assumed as being numerically equal.

The material parameters used in the computations are presented in table 1.

Table 1. *Material parameters for the analyzed models. R_{xx}/R_{yy} and R_{xy} represent the flow stress of the grain boundaries in the directions parallel/perpendicular to the grain boundary plane and the shear flow stress, respectively.*

	E, GPa	N	σ_y, MPa	E_T, GPa	R_{xx}	R_{yy}	R_{xy}
Grains interior	120	0.336	Equation (1)	12	-	-	-
Grain boundaries	120	0.336	33	0.6	1~20	1~20	1~20

3. RESULTS AND DISCUSSION

3.1. Variation of the flow stress of grain boundaries

Calculations were performed to obtain an insight into the variation of the flow stress of the grain boundaries in two orthogonal directions, parallel and perpendicular to the surface of the grain boundary, and the shear stress, see table 1. The results of simulations are presented in figure 4. These results

clearly demonstrate the strong influence of the grain boundaries properties on the properties possessed by the polycrystalline aggregate. Depending on the combination of the flow stress of the grain boundaries the macroscopic yield point varies from 200 to 1200 MPa.

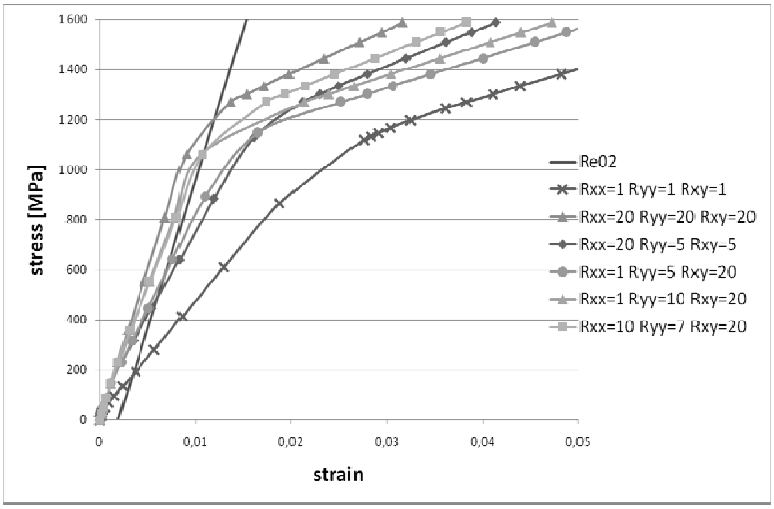


Fig. 4. *The macroscopic stress-strain curves obtained for the two-phase model with varied properties of the grain boundaries (see also table 1).*

aggregates, see figure 5. It would appear that the resistance to grain boundary sliding, which is represented by R_{xy}, depends on the difference between the properties of the grain interiors and the grain boundaries.

3.2. Grain size distribution effect

The influence of the grain size distribution on the flow stress was analyzed for a set of polycrystalline aggregates with the parameters listed in table 2. Six structures with an average grain size 10, 16, 21, 32, 43, 65 nm with three different grain size dispersions were analyzed. The grain size dispersion was described by the coefficient of variation *C*V defined as:

$$CV = \frac{SD}{\bar{E}} \tag{6}$$

where SD is the standard deviation and $\bar{E}$ is the average grain size of the structure. The three values of CV analysed were 0.07, 0.2 and 0.41.

Table 2. *Material properties for modelling grain dispersion effect.*

	E, GPa	v	σ_y, MPa	E_T, GPa	R_{xx}	R_{yy}	R_{xy}
Grains interior	120	0.336	H-P	12	-	-	-
Grain boundaries	120	0.336	33	0.06	10	15	10

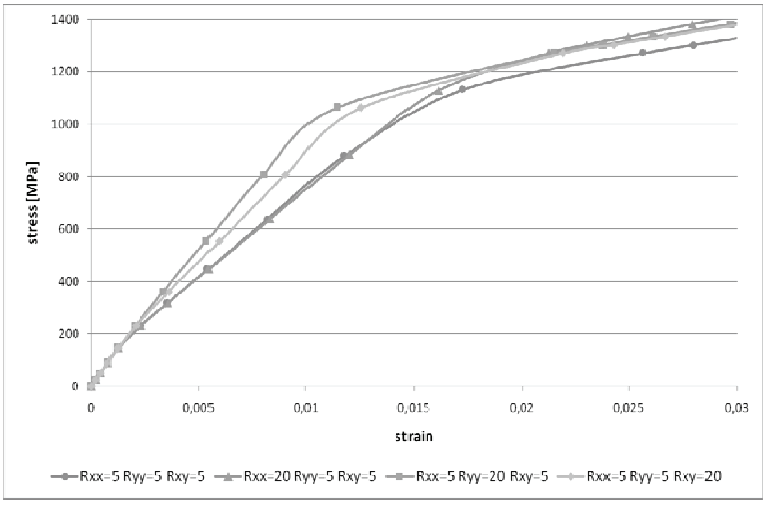


Fig. 5. *Influence of the R_{ij} parameters on the stress-strain curve of analyzed structure.*

The results of the calculations show that parameters R_{yy}, defining the resistance of the grain boundaries to the plastic deformation in the direction perpendicular to the grain boundary plane, has the highest influence on the flow stress of the polycrystalline

Figure 6 presents the results of the calculation for all the situations modelled. It is clearly shown that the flow stress does depend on the grain size distribution. The variation of the yield stress for the same grain size can be greater than 140 MPa.

4. CONCLUSIONS

Since the structure of grain boundaries differs from that of the grain interior, their plastic properties also differ. The impact of these differences on the macroscopic properties of the polycrystalline materials is particularly pronounced for ultrafine grained structures.

The simulation reported here give quantitative estimates of the grain boundary effect on the flow stress of nano-crystalline metals. The simulation, based on a two phase model, explains the so-called reverse Hall-Patch dependence, as being due to the increasing volume fraction of atoms

located in the grain boundaries. Grain boundary sliding and the variations in the mechanical properties of the grain interiors and grain boundaries play a key role in controlling the plastic deformation of polycrystalline nano-materials.

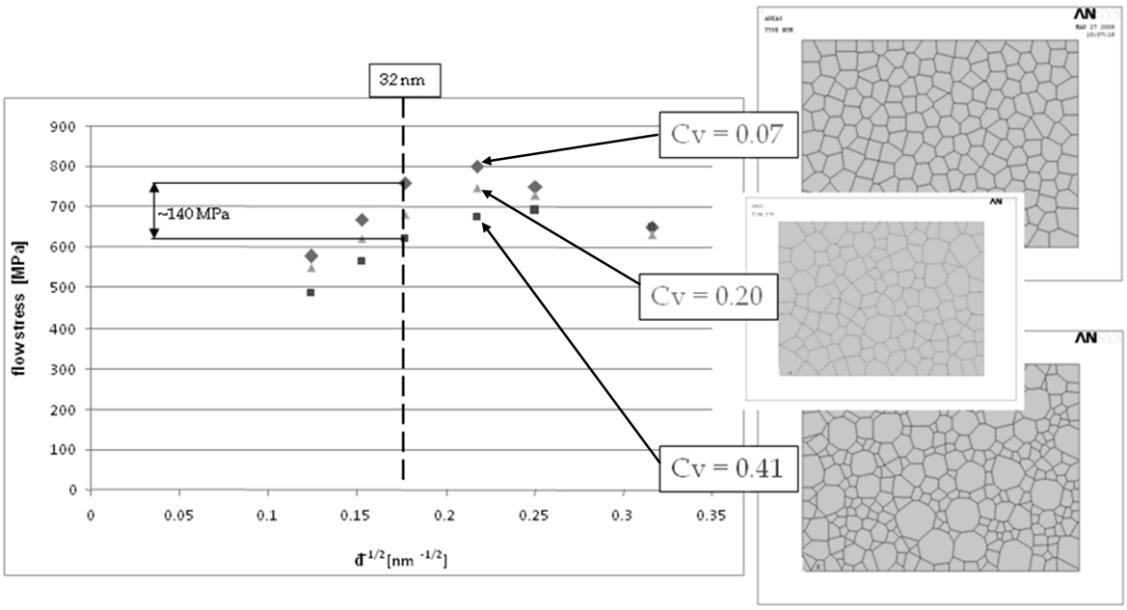


Fig. 6. *Influence of grain size distribution on flow stress of modelled nano-materials.*

The results show that resistance to plastic deformation of grain boundaries in the direction perpendicular to the grain edge has stronger influence on plastic deformations of modelled structures than stiffness in the parallel direction and resistance to the shear strain. The result confirm that grain boundary sliding is not a critical mechanism of plastic deformations for structures with grain sizes lower then ~30 nm.

Another important finding was the influence of grain size distribution in nanostructures. It has been shown that the mechanical properties of nano-materials are dependent on both the average grain size and the grain size distribution.

ACKNOWLEDGEMENTS

This work has been supported by Grant No 110/COS/2006/02 awarded by the Polish Ministry of Science and Higher Education.

REFERENCES

1. ANSYS Inc., Release 11.0 Documentation for ANSYS.
2. Hall, E.O., The Deformation and Ageing of Mild Steel, Proc. Roy. Soc., B64, 747, 1951.
3. Petch, N.J., The cleavage strength of polycrystals, J. Iron Steel Inst., 174, 1953, 25-28.
4. Rao, S.I., Dimiduk, D.M., Parthasarathy, T.A., Uchic, M.D., Tang, M., Woodward, C., Athermal mechanisms of size-dependent crystal flow gleaned from three-dimensional discrete dislocation simulations, Acta Mteri-alia, 56, 2008, 3245-3259.
5. Rollett, A.D., Saylor, D., Fridy, J., El-Dasher, B.S., Brahme, A., Lee, S.-B., Cornwell, C., Noack, R., Modeling Polycrystalline Microstructures in 3D, Proc.AIP Conf., vol. 712, 2004, 71-77.
6. Wei, Y.J., Anand, L., Grain-boundary sliding and separation in polycrystalline metals: application to nanocrystal-line fcc metals, J. of the Mechanics and Physics of Solids 52, 2004, 2587-2616.

ANALIZA WPŁYWU STRUKTURY NANOMETALI NA ICH WŁAŚCIWOŚCI MECHANICZNE

Streszczenie

Właściwości mechaniczne materiałów są ściśle związane z ich budową wewnętrzną. Wpływ wielkość ziaren i niejednorodności struktury na odkształcenie plastyczne materiałów polikrystalicznych (zwłaszcza metali) jest często rozważany w literaturze. Zmiana wartości granicy plastyczności, określana zazwyczaj zależnością Halla-Petcha (H-P), jest zgodna z danymi eksperymentalnymi dla mikrometrycznych wielkości ziaren. W przypadku kiedy wielkość ziarna osiąga poziom nanometryczny zależność H-P przestaje obowiązywać, co wiąże się miedzy innymi z aktywacją mechanizmu odkształcenia, jakim jest poślizg po granicach ziaren.

Znaczący udział objętościowy atomów umieszczonych w obszarach pomiędzy poszczególnymi ziarnami powoduje, że granice ziaren pełnią decydującą rolę w odkształceniu nanomateriałów. W celu ilościowego opisu wpływu właściwości granic ziaren na odkształcenie polikryształów, zbudowany został przy pomocy metody elementów skończonych 'dwu-fazowy' model, uwzględniający anizotropowe właściwości granic ziaren. Wyniki symulacji ilustrują wpływ szeregu parametrów na odkształcenie materiałów nanokrystalicznych.

Submitted: November 4, 2008
Submitted in a revised form: December 9, 2008
Accepted: December 9, 2008