55th Annual Technical Meeting of the Society of Engineering Science (SES2018)
October 10 - 12, 2018, Leganés, Madrid, Spain

Two-phase mean-field estimate for the effective stiffness tensor of nanocrystalline materials of cubic symmetry

Katarzyna Kowalczyk-Gajewska[1,*], **Marcin Maździarz**[1]

[1] Institute of Fundamental Technological Research of Polish Academy of Sciences, Pawińskiego 5B,

02106 Warsaw (kkowalcz@ippt.pan.pl,mmazdz@ippt.pan.pl)

Two variants of an anisotropic two-phase model of a nano-grained polycrystal has been built in the spirit of [1, 2] and called Mori-Tanaka (MT) and Self-Consistent (SC) core-shell models and verified by means of the atomistic simulations. In the simulations, at variance with the available literature [1, 2], all 21 components of the anisotropic elasticity tensor $\bar{\mathbf{C}}$ are acquired by performing six independent numerical tests for several samples of the polycrystalline material. The closest isotropic approximation of this tensor is found using the Log-Euclidean norm [3]. The dependence of the obtained overall bulk and shear moduli on the average grain diameter is analysed. In the mean-field approach the thickness of the shell is specified by the *cutoff radius* of a corresponding atomistic potential, while the grain shell has the stiffness tensor corresponding to the lower zero-order bound of $\bar{\mathbf{C}}$. Under such assumptions, in the case of grain cores with cubic elastic symmetry, the effective stiffness tensor of a bulk polycrystal is specified by an explicit formula. In the recent study [4] it has been shown that the obtained estimates are in satisfactory qualitative and quantitative agreement with the results of atomistic simulations performed for nano-crystalline copper. In particular, in accordance with the atomistic simulations, the predicted bulk modulus does not depend on, while the shear modulus decreases with the grain size.

In the present study it will be checked whether the observed difference in the dependence of the bulk and shear moduli on the grain size is valid for other metals with cubic lattice symmetry, especially when they differ in their Zener anisotropy factor specified as a ratio of two shear moduli defining anisotropy of a single crystal.

The simulations were performed at the Interdisciplinary Centre for Mathematical and Computational Modelling of Warsaw University (ICM UW) and the computing cluster GRAFEN at Biocentrum Ochota. The research was partially supported by the project No. 2016/23/B/ST8/03418 of the National Science Centre, Poland.

REFERENCES

[1] B. Jiang and G.J. Weng. *J. Mech. Phys. Solids*, 52 (2004) 1125.

[2] L. Capolungo, M. Cherkaoui and J. Qu *Int. J. Plasticity*, 23 (2007) 561.

[3] M. Moakher and N. Norris *J. Elasticity*, 85 (2006) 215.

[4] K. Kowalczyk-Gajewska and M. Maździarz *Int. J. Eng. Sci.*, under review, (2018).