STRUCTURAL INFLUENCE ON ELASTIC PROPERTIES OF FIVEFOLD TWINNED NANOWIRES

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Finite element method (FEM) is a powerful research tool for many fields of physics and chemistry. This method can be also utilized in nanotechnology for studying and modelling mechanical properties and behaviour of nanowires (NWs). Attractive objects for this are, for example, noble metal NWs like silver (Ag) and gold (Au), due to their many potential applications, where they are under cyclical mechanical deformation [1,2]. These NWs have fivefold twinned inner structure with pentagonal cross-section [3]. This peculiar structure leads to the presence of inner stresses [4], which can have a considerable influence on the NWs mechanical behaviour.

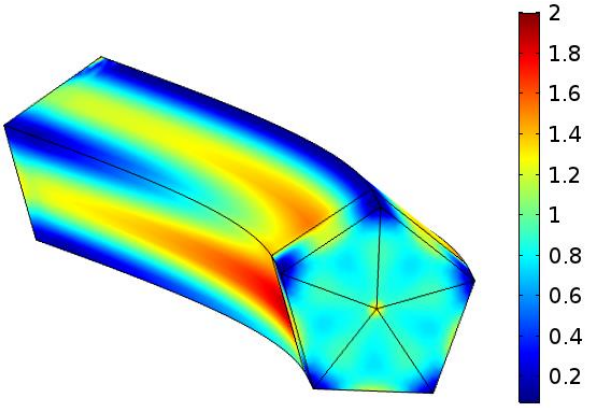

Fig.1 Von Mises stresses (GPa) in Ag NW during cantilevered beam bending test.

In the present work pentagonal Ag and Au NWs were modelled and their mechanical response simulated using FEM. The model taken into account the fivefold twinned structure and the presence of inner stresses. The cantilevered beam bending test was simulated (Fig.1) to further understand the influence of Ag and Au NWs structure on its mechanical behaviour.

References

1. O. Y. Loh, H. D. Espinosa, 2012, *Nat. Nanotechnol.*, 7, 283-295.
2. J.-Y. Lee, S. T. Connor, Y. Cui, P. Peumans, 2008, *Nano Lett.*, 8, 689-92.
3. H. Chen, Y. Gao, H. Zhang, L. Liu, H. Yu, H. Tian, S. Xie, J. Li, 2004, *J. Phys. Chem. B*, 108, 12038-12043.
4. V. G. Gryaznov, J. Heidenreich, A. M. Kaprelov, S. A. Nepijko, A. E. Romanov, J. Urban, 1999, *Cryst. Res. Technol.*, 34, 1091-119.

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