ELASTICITY AND STRENGTH OF NANO-FIBRE REINFORCED COMPOSITES FROM FIRST PRINCIPLES

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Introduction

Composites represent one of widely used successful ways to improve mechanical properties of materials, in particular their elastic moduli, strength and fracture toughness. Resulting properties in real composites can be, at least in some cases, predicted from properties of the constituents using simple linear rules of mixtures. Such linear relations are often used for Young's moduli as well as for the strength of composites.

In this paper, the equilibrium volume, elastic moduli and theoretical strength of ideal nano-composites with vanadium matrix and long molybdenum fibres are computed for different thickness of nano-fibres (from a single atom to several atomic distances). The main aim of this work is to verify the validity of linear mixture rules at atomic level and reliability of our preliminary results [1].

Computational details

A model of the nano-composite is built as a periodic repeating of 4x4x1 bcc-based super-cell (Fig. 1).

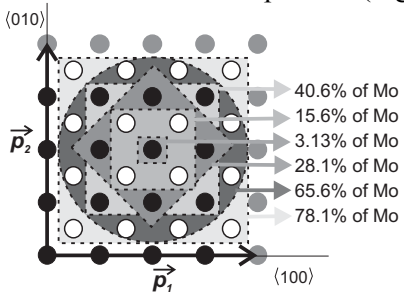

Figure 1: The super-cell model.

The crystal basis of the super-cell contains 32 atoms in two adjacent A (solid circles) and B (open circles) (001) planes. The grey solid circles belong to other super-cells. The dashed contours schematically define considered interfaces between molybdenum (Mo) wire and vanadium (V) matrix in investigated composite models of different atomic concentrations of Mo. In order to get few more different concentrations, the V wires in Mo matrix were also considered. Molybdenum concentrations of 59.4%, 71.9% and 84.4% were obtained this way.

Calculation procedure consists of several steps. The ground-state of the crystal was found by optimizing the super-cell shape as well as the atomic positions within the cell. Then the crystal system was elongated in [001] direction to simulate uniaxial loading applied in the direction parallel to the lamina fibres. The lateral stresses were relaxed at any elongation by varying lengths of the corresponding cell edges (lengths of the $\boldsymbol{p_1}$ and $\boldsymbol{p_2}$ translation vectors in Fig. 1) and the tensile stress σ was assigned to the current engineering strain ε. If no other instability precedes, the maximum tensile stress σ_{max} can be considered to be the theoretical tensile strength of the nano-composite.

For calculations of energy we utilized the Vienna Ab initio Simulation Package (VASP) [2]. This code uses projector augmented-wave potential and plane wave basis set. The cut-off energy for the basis set was 290 eV. The exchange-correlation energy was evaluated using the generalized gradient approximation of Perdew and Wang [3]. The 3x3x12 *k*-points mesh was used in all our calculations. The solution was considered to be self-consistent when the energy difference of two consequent iterations was smaller than 0.1 meV. Forces and stresses (unlike the calculations in Ref. 1) for structure relaxations were calculated according to Hellman-Feynman theorem.

Results and discussion

In order to check properly the reliability of presented calculations, we used the super-cell with all atomic positions occupied by the same kind of atoms for calculations of ground-state properties. The computed values of the equilibrium lattice parameter a_0, the bulk modulus B, the Young modulus E_{001} and Poisson ratio ν for pure molybdenum and pure vanadium are listed in Table 1 along with the experimental data [4,5].

The agreement between computed and experimental values of a_0 is within 2% which is acceptable. The agreement in case of elastic moduli and Poisson ratio for molybdenum is also very good (mostly within 5%). On the contrary, computed elastic moduli for vanadium significantly overestimate those observed experimentally.

Table 1: Computed and experimental values of selected ground-state properties of pure Mo and V.

		a_0 (nm)	B (GPa)	E_{001} (GPa)	ν
V	calc.	0.298	189	199	0.32
	expt.	0.303	157	151	0.34
Mo	calc.	0.315	268	412	0.24
	expt.	0.315	270	394	0.26

The dependence of the computed composite average atomic volume V_0 on the atomic concentration of Mo (nearly corresponding to the volume fraction V_f of molybdenum fibres) was found to be a linear function. As can be expected, the atomic volume linearly increases with Mo concentration.

Values of the Young modulus E_{001} also follow more or less linear trend that interpolates between the moduli of both components. Our atomistic results suggest that deviations from the simplest linear mixture rules observed for real composites are caused by their imperfections, particularly by reduced interface cohesion.

Computed maximum values of the uniaxial tensile stress σ_{max} for pure V and Mo are listed in Tab. 2 together with available literature data [6,7]. Since no mechanical instability was found before reaching the inflection point in Mo [6], we extrapolate the term theoretical strength also to other composite data.

Table 2: Computed maximum tensile stresses and related critical strains.

Element		σ_{max} (GPa)	ε_{max}
V	present	19.2	0.17
	Ref. [7]	19.8	0.22
Mo	present	28.3	0.13
	Ref. [6]	28.8	0.12

Fig. 2 displays the σ_{max} values for all investigated composites. They exhibit a simple increasing dependence on atomic concentration of Mo up to about 60%. Above this concentration they seem to reach a saturated value of about 29 GPa, slightly higher than that of a pure Mo. This stress synergy effect is in a perfect agreement with previous calculations [1] based on an energy minimization.

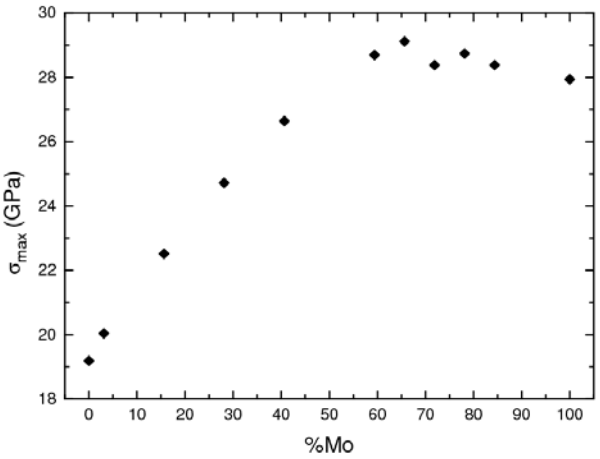

Figure 2: Maximum tensile stress as a function of molybdenum concentration.

Conclusions

Elasticity of nano-fibre reinforced composites (Mo+V) under uniaxial loading parallel to the fibres was studied by means of first principle calculations. Computed results show that the theoretical tensile strength increases with increasing molybdenum atomic concentration up to about 60% and then the computed values seem to become saturated.

Acknowledgement

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References

1. Černý, M. and Pokluda, J., *Proc. 12th Eur. Conf. Compos. Mater.*, Biarritz, France (2006); *Proc. 12th Int. Conf. Fract.*, Ottawa, Canada (2009).
2. Kresse, G. and Hafner, J., *Phys. Rev. B* **48**, 13115 (1993); Kresse, G. and Furthműller, J., *Phys. Rev. B*, **54**, 11169 (1996); Kresse, G. and Furthműller, J., *Comput. Mat. Sci.*, **6**, (1996), 15.
3. Perdew, J. P. and Wang, Y., *Phys. Rev. B* **41**, (1992), 13244.
4. Kittel, C., Introduction to Solid State Physics, John Wiley & Sons (1976).
5. Simmons, G. and Wang, H., *Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook*, MIT Press (1971)
6. Luo, Mo., Roundy, D., Cohen, M. L. and Morris, J. W. Jr., *Phys. Rev. B*, **66**, 094110 (2002).
7. Černý, M. and Pokluda, J., *Phys. Rev. B*, **76**, 024115 (2007).