First Principles Study of Ideal Composites Reinforced by Coherent Nano-fibres

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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 engineering macro-composites depend on many parameters related to particular design and production technology. However, there are cases for which the situation is not so complicated. For example, the Young modulus of long-fibre composites in the fibre direction can be sufficiently precisely assessed according to a simple linear mixture rule. Preliminary studies on W-Nb, Mo-V and W-V nanocomposite models exhibiting a perfect cohesion on the fibre/matrix interface revealed that the linear mixture rules are valid at the atomistic level e.g. for values of the equilibrium volume and elastic moduli. In case of the theoretical strength, however, the obtained relationships predicted an increase only up to 60-80% of reinforcement fibres. In this paper, the theoretical strength of ideal nano-composites with vanadium or niobium matrices and long molybdenum or tungsten fibres is computed for different thickness of nano-fibres (from a single atom to several atomic distances) by means of ab initio method. The main aim of this work is to verify our preliminary results using a different approach and to compare the obtained results for several models with the main focus on the theoretical tensile strength.

Computational procedure. A model of the nano-composite is built as a periodic repeating of 4x4x1 bcc-based super-cell. Occupying the lattice sites by atoms of either fibre or matrix material enables us to model infinite fibres of various thickness (and atomic concentration) equidistantly spaced in the composite model. This study considers W and Mo as the reinforcing materials in V or Nb matrices since all those metals crystallize in bcc structure with similar lattice parameters but significantly different elastic moduli. Forces and stresses necessary for the relaxation procedure were calculated according to the Hellman-Feynman theorem using the Vienna Ab initio Simulation Package within the projector augmented-wave scheme and a plane wave basis set. The exchange-correlation energy was evaluated using the generalized-gradient approximation.

Results. Computed ground-state properties of the ideal lattice (the equilibrium lattice parameter, the bulk modulus, the Young's modulus and the Poisson's ratio) agree well with experimental data. The maximum tensile stresses and the corresponding critical strains for pure V, Nb, Mo, and W were also successfully compared with available literature data. The maximum tensile stresses in the nanocomposite models exhibit simple increasing dependence on atomic concentration of the reinforcement up to about 60-80%. Above those concentrations they seem to reach the values corresponding to pure reinforcements or even somewhat higher. This indicates a presence of certain synergy effect between the fibre and the matrix that can be caused by the lattice mismatch and the induced transverse tensile or compressive stresses.

Summary. First principles calculations of a tensile strength of nano-fibre reinforced composites under uniaxial loading parallel to the fibres reveal that the theoretical tensile strength monotonously increases up to about 60-80% atomic concentration of the reinforcement and then the computed values seem to become almost saturated.