[100] loading of fcc based nano-fibre reinforced composites

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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 data predicted a synergy effect raising the strength above a simple linear interpolation with its maximum at concentrations of 60-80% of reinforcement fibres.

In this paper, the theoretical strength of ideal nano-composites with copper matrix and long iridium fibres is computed for several nano-fibres of different thickness (from a single atom to several atomic distances) by means of ab initio method. The main aim of this work is to verify our former results on bcc metals on the theoretical tensile strength.

A model of the nano-composite is built as a periodic repeating of 3x3x1 fcc-based super-cell containing 36 atoms. 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 Ir as the reinforcing material in Cu matrix since both metals crystallize in fcc 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 working with ultrasoft pseudopotentials and a plane wave basis set. The exchange-correlation energy was evaluated using the generalized-gradient approximation.

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