Ab initio study of elasticity of nano-fibre reinforced composites.

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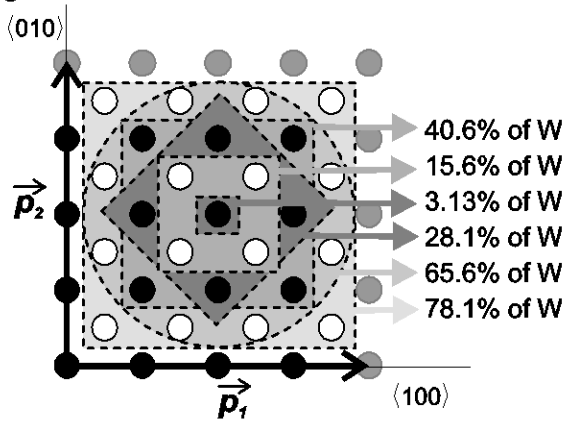
Ab initio calculations of the bulk modulus of composite lamina having continuous nano-fibre reinforcements are performed using pseudo-potential plane-wave code. Obtained results are used to verify validity of macro-scale empirical relations for composites (rules of mixtures) on the nano-scale. All quantities are computed from the dependence of crystal energy on a crystal volume. Results for tungsten nano-fibres in niobium matrix will be presented as a particular example of the ab-initio analysis.

A model of the nano-composite is built by periodic repeating of 4x4x1 bcc-based super-cell displayed in the following figure.



The crystal basis of our super-cell contains 32 atom in both A (solid circles) and B (open circles) ⟨001⟩ planes. The gray solid circles belong to other (adjacent) super-cells. The dashed contours define considered interfaces between tungsten (W) wire and niobium (Nb) matrix in investigated lamina models of different atomic concentration of W.

The equilibrium volume of each lamina model and the lamina bulk modulus were computed. Atomic positions within the cell were relaxed in order to minimize the interfacial stresses. The dependence of the computed composite bulk modulus B on the atomic concentration of W (nearly corresponding to the volume fraction V_f of tungsten fibres) should follow the simple rule of mixture for an ideal composite

$$B = B_f V_f + B_m (1 - V_f) \tag{1}$$

where B_f and B_m are bulk moduli of the fibre (W) and matrix (Nb), respectively (here, $B_f > B_m$). Our results confirm on atomistic level that deviations from relation (1) observed for real composites are caused by their imperfections, particularly by reduced interface cohesion. On the other hand, the atomic volume linearly decreases with W concentration.

Keywords: ab-initio calculations, bulk modulus, nano-composites, mixture rule