THEORY-GUIDED STRAIN ENGINEERING OF NANO-SCALE PHASES WITH UNPRECEDENTED PROPERTIES: AN INSIGHT FROM AB INITIO CALCULATIONS

FRIAK Martin

Institute of Physics of Materials AS CR, v.v.i., Brno, Czech Republic, EU

Abstract

Stress/strain conditions in nano-structured composites have recently emerged as a new ground-breaking materials-design concept providing exotic phases that would otherwise not exist in strain-free bulk systems. This state-of-the-art method results in advanced materials with unprecedented properties that significantly extend frontiers of current materials science. In order to efficiently explore this uncharted territory, it is very advantageous to combine experimental and theoretical tools. In particular, quantum-mechanical (so-called ab initio) modeling techniques can serve as a reliable guide when fine-tuning chemical compositions or identifying optimum strain conditions. Ab initio calculations represent an invaluable source of information and provide a deeper insight and fundamental understanding. As an example of such a theory-guided strain engineering, biaxial planar stresses acting in plane parallel to heterogeneous multi-layers can alter quite uniquely thermodynamic properties, structural parameters, elastic properties as well as magnetic and electronic states of thin films. The talk will review recent approaches to the theory-guided strain engineering of nano-scale phases and illustrate the strength of this concept on a few selected examples.

Author did not supply full text of the paper/poster.