Elastic strain engineering based on quantum-mechanical calculations

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It is well known that stresses and strains in materials may result in stabilization of rather exotic phases that would otherwise not exist in strain-free bulk materials. For example, biaxial planar stresses acting within interface planes in multilayers can alter thermodynamic properties, structural parameters, elastic properties and/or magnetic and electronic state of thin layered materials very significantly. So-called elastic strain engineering is an approach that exploits these mechanisms to (i) fine-tune materials characteristics according to specific needs or (ii) stabilize new phases with unprecedented properties.

Quantum-mechanical calculations represent an excellent tool to describe changes induced by not only small and moderate strains belonging to linear-elasticity regimes but also rather extreme strain levels. The talk will provide a few selected examples of the elastic strain engineering applied to different classes of materials including elemental metals, transition-metal nitrides and half-metallic transition-metal oxides. In particular, nano-scale superlattices containing metastable phases will be discussed as systems that are critically important for future development of advanced lamellar composites with application-dictated stiffness and hardness.

Combining theoretical and experimental methods we focus on elastic properties of AlN/CrN superlattices in which CrN stabilizes AlN in a metastable B1 (rock salt) cubic phase in the form of nm-thin layers (New Journal of Physics 17 (2015) 093004).

The Materials Science and Technology Seminar is jointly organized by ICAMS (Interdisciplinary Centre for Advanced Materials Simulation) and the IfM (Institute for Materials). Members of the RUB Materials Research Department MRD and of the DGM Regionalforum Rhein-Ruhr are cordially invited to participate in the seminar. For further information, please contact: Mrs. Christa Hermichen christa.hermichen@rub.de, phone: +49 234 32 29310.