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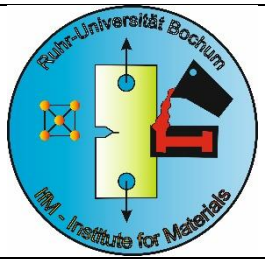
**RUB-SEMINAR**

***MATERIALS SCIENCE AND TECHNOLOGY***




**Date: 15 December 2016 Time: 4:00 p.m. Venue: RUB, IC04 – 408**

# 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.

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