Leoben, July 7, 2017

PhD position:
Ab initio study of impact of interfaces on mechanical properties of hard coatings

A **3-year PhD position**, with a foreseen start **from November 1, 2017**, is open in the Computational Materials Science (CMS) group[1] at the Department of Physical Metallurgy and Materials Testing, **Montanuniversität Leoben, Austria**.

The CMS group focuses on applying atomistic modelling techniques to the current materials science problems. The interests span from structural (structure prediction, phase stability, defects, etc.) to functional properties (e.g., surface adsorption, electronic and optical properties) and cover various material classes, from bulk intermetallic alloys to nitride and oxide thin films to carbon and gold nanostructures. A particular strength of the group lies in a close collaboration with experimentalists, both at the Montanuniversität Leoben, TU Wien as well as from abroad.

The position is available within a **basic research project** titled "Impact of interfaces on mechanical properties of hard coating materials" funded by the Austrian Science Fund (FWF)[2]. The project aims on **combining high-resolution micromechanics experiments with atomistic modelling** to reveal the very elemental mechanisms responsible for superlattice-induced enhancement of mechanical properties (e.g., toughness) and deriving design rules that can be used to produce novel nitride-based materials with yet improved and/or application-tailored properties. The successful applicant will employ **quantum mechanical calculations** to study tensile and shear strength as a function of the multilayer architecture (bi-layer period, lattice parameter mismatch, crystal structure, etc.) and environmental properties (temperature, atmosphere supposedly leading to segregation of impurities into the interface).

The experimental part of the project will be carried out at **TU Wien, Vienna, Austria**, in the group of Dr. Matthias Bartosik and Prof. Paul H. Mayrhofer[3]. The working place will be Leoben or Vienna, depending on the candidate's preference, and in any case will involve a very intensive collaboration with the group in Vienna.

The **interested candidate** should have a Master degree (or equivalent) from Materials Science, Physics, Chemistry or a related subject, be strongly self-motivated, have good communication skills (English, German is optional), and be willing to work in a team. A prior experience with atomistic modelling is desirable, hands-on knowledge of any DFT code is strongly beneficial but not essential. The gross monthly salary is €2,017.00 (14× per year).

Accompanying letter, academic CV, transcript of a study record, and two recommendation letters shall be sent to Dr. David Holec (`david.holec@unileoben.ac.at`) **before the application closing date on August 11, 2017**. Evaluation of the applications and interviews with the short-listed candidates will follow immediately after that deadline.

[1] `http://materials.unileoben.ac.at/en/1457/`
[2] `http://www.fwf.ac.at/en/`
[3] `http://wwwt.tuwien.ac.at/research/chair_of_materials_science/EN/`

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