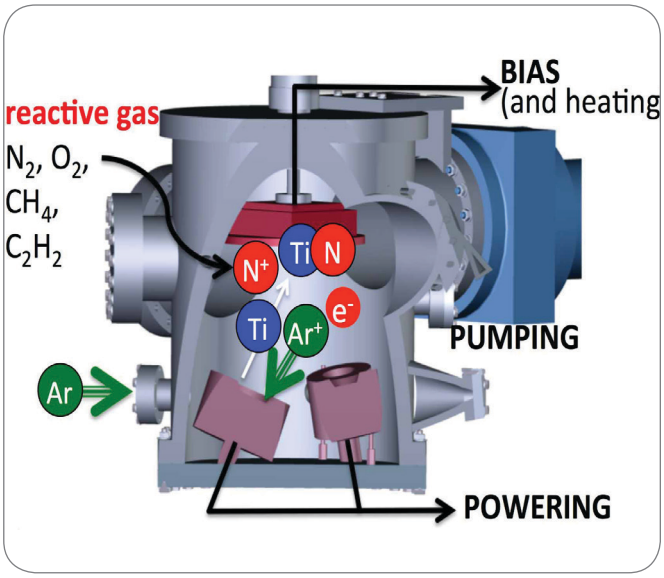
TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

Institute of Materials Science and Technology
Karlsplatz 13/308, 1040 Vienna, Austria
Tel.: +43 (1) 58801 30870
paul.mayrhofer@tuwien.ac.at
www.tuwien.ac.at

Designed surfaces and functional coatings

Ultrathin, tailor-made coatings for highly loaded products and components

High-performance materials and their requirements profile increasingly require application-oriented optimisation. What characterises such ‚tailor-made materials' above all is that the value added process is not defined by the properties or the chemical composition, but rather by the high-performance application, which is planned from the outset. It is particularly clear that the surfaces of tools are subjected to specific demands. This involves a combination of physical, thermal and chemical stress, that radically influences the lifespan and application of not only the tools themselves, but also their components (for example in the automotive and aircraft industries). The optimisation of a particular material by physical, thermal and chemical methods (e.g. shot peening, surface layer hardening, case hardening) is often insufficient. Coating technology, and above all physical vapour deposition (see schematic diagram), provides the opportunity to protect the surfaces of a variety of tools and components with extremely thin (approx. 3-10 µm), but extremely durable, high-performance materials.



Scheme of a PVD prozess

Objective

The knowledge-based development of coatings comprising of several components is central to this research. These types of materials enable the increasing requirements for tailor-made coatings tailor-made for specific applications than ever before.

Coatings protect tools and give them additional and improved properties and functions. Materials consisting of two elements, such as binary nitrides, carbides or borides of certain metals are already well established for this purpose. For a long time, these materials were able to fulfil industry requirements. However, new applications for high-performance materials require new combinations of properties. New possibilities are introduced by materials consisting of more than two components – so-called ternary, quarternery and multinery nitrides, carbides or borides. However, coatings with more components also increase in complexity. The increased use of these coatings therefore requires a knowledge based design concept and a comprehensive understanding of the coating process technology. This task is being addressed by Prof. Paul Mayrhofer and his research team at TU Wien.

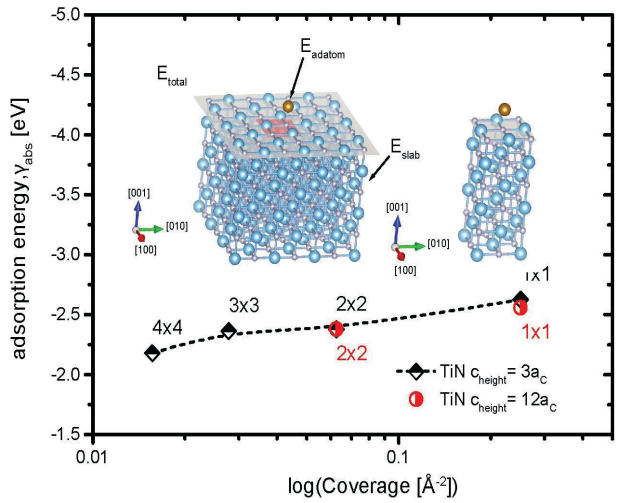
Approach

An important part of this research involves the ‚computer aided design' of coatings materials that allows a precise projection of specific material properties and behaviour. In particular, this involves the use of modern methods of the ‚density functional theory' and continuum mechanics. We mainly use the Vienna Ab Initio Simulation Package (VASP) which was developed in Vienna. Computer supported material development is concerned with both the basic characteristics of the materials, such as the calculation of bond lengths, and their elastic behaviour.
Furthermore, the experimental development of the coatings and the coating processes are being researched. It is not just the different materials that are the focus of attention here, but also special coatings architectures – such as the combination of different layers or phases and chemical or structural gradients.

In both fields – design and development – data, obtained from coating characterizations during thermal, chemical or physical attack, are also taken into account.

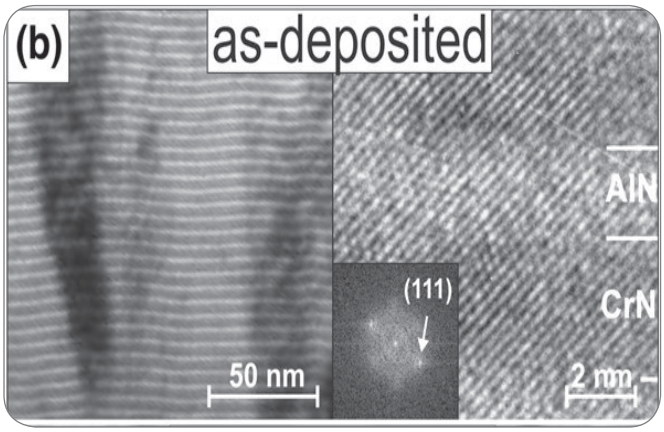
Results

An example of ‚computer aided design' of coatings materials can be found in the adsorption behaviour of different metals to thin films: by calculating the adsorption energies, the selection of coatings systems for particular applications is made easier. In the graph below, the relationship between the size of the super-cells and the adsorption energy is shown. Such calculations are necessary to optimize the computational materials science process. Based on the computer aided design of coatings, the experimental investigations can be focussed to specific targets.



DFT study of the adsorption energy

Material failure often causes production down time or stoppages and often arises as a result of cracks beginning to occur in materials. Though this can seldom be prevented, it is possible, however, to reduce and even stop crack - growth and their propagation by well designed coatings. An example of this was achieved in a TU Wien project, in which a phase-transformation-based volume change of AlN is used to deflect cracks, reduce their propagation and even stop them from further growth. This is only possible through a multi-layer design (see picture below) that also uses the ‚super-lattice effect' to increase the hardness of the layers, as well as their thoughness. In this high resolution transmission electron microscpyimage the AlN and CrN layers can clearly.



Cross section of a CrN/AlN multilayer

Benefits for you

This research opens a new era for targeted design, requirements related development and the investigation of new materials and coatings.
For manufacturers wishing to optimise their products (coatings, target materials, coating processes), TU Wien's combination of computer supported and experimental materials and coatings development offers substantial time and cost savings.

Point of contact:
Prof. Paul Mayrhofer
TU Wien
Institute of Materials Science and Technology
+43 (1) 58801 30811
paul.mayrhofer@tuwien.ac.at
wwwt.tuwien.ac.at
hardcoatings.tuwien.ac.at