DFG-Project Schm-746/68-2

„Molecular Dynamics Modelling and Validation of the Production and Correlation Between the Microstructure and the Characteristics of SiC/SiN-Nanolaminates"

Begin of the Project: 01.10.2007
End of the Project: 31.03.2011

Goals and approach:

The continuously increasing requirements onto structural components have made it necessary to overthink the well established methods and materials of interest in materials science, iron and high performance steels were partially replaced by ceramic materials in the past. The probably most prominent ceramic is diamond, which is considered to be the hardest known material. Under man made non-oxyde ceramics, the highest importance surely have silicone carbide and silicone nitride. Both materials are often used in the industry for componets consisting entirely out of ceramics. Ceramic materials are very brittle due to strong angular dependency of the covalent bond and hence not shapeable. Coating of a previously formed component by a ceramic material will improve the mechanical and thermal stability while at the same time circumventing the problem of ductility.

In this project, thin single- double- and multiple-layers made from SiC and SiN on Si as well as on steel are developed and systematically analysed. These layers are combined together for applications with a requirement for increased abrasive and wear properties. The layers are deposited using the method of reactive magnetron sputtering and are analysed experimentally by the X-ray and electron diffractometry method. On the atomistic level, their characteristics are simulated using molecular dynamics method. One of the focal points of the project is the collaboration between the research group at IMWF Uni-Stuttgart and the Institute for Material Science I at KIT during every step of the production process of the SiC and SiN nanolaminates, hereby using experiment as well as simulation methods. With the help of close synchronisation of the modelling process and the experiments, better multi-layered laminates shall be produced, in order to overcome the trial-and-error method of production.

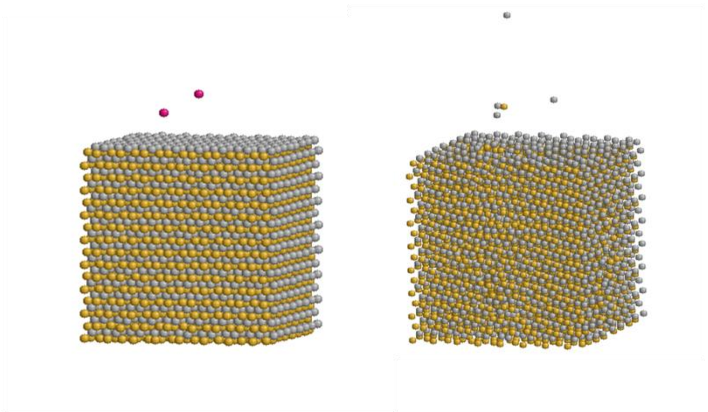

Figure 1: Sputtering of SiC, after impact of two argon ions onto SiC target (left), five atoms are back sputtered (right).

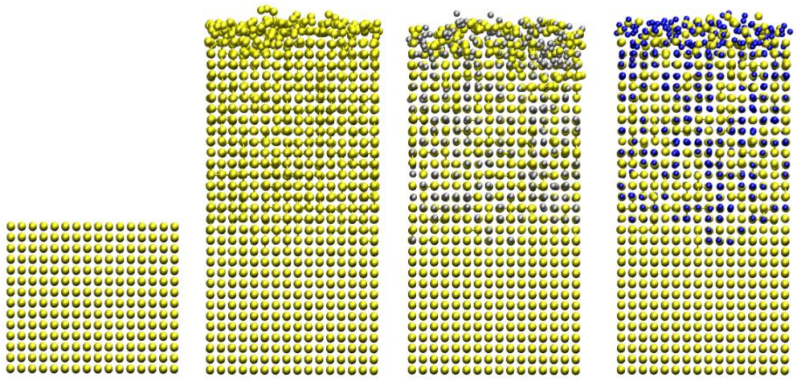

Figure 2: Starting from the left: Silicon substrate, pure silicon coating, silicon carbide coating and silicon nitride coating on a silicon substrate.

Partner:

Joint project of the Institute for Material Testing, Material Science and Strength of Materials (IMWF), University of Stuttgart and the Institute for Material Research I, Karlsruhe Institute of Technology (KIT)

Acknowledgment:

This project is supported by the German Research Foundation DFG in the project SCHM 746/68-2 and ZI 1174/3-2. We would like to thank for the financial support.

List of publications:

1. A.-P. Prskalo, S. Schmauder, C. Ziebert, J. Ye, S. Ulrich, *Molecular dynamics simulations of SiC and* Si_3N_4, Surf. Coat. Technol. (2009), in press.

2. C. Ziebert, J. Ye, S. Ulrich, A. Prskalo, S. Schmauder, *Sputter deposition of nanocrystalline β-SiC films and molecular dynamics simulations of the sputter process*, J. Nanosci. Nanotechnol. (2009), 10 (2010) 1120-1128

3. A.-P. Prskalo, S. Schmauder, C. Ziebert, J. Ye, S. Ulrich, *Molecular dynamics simulations of the sputtering process of silicon and the homoepitaxial growth of a Si coating on silicon*, Computational Materials Science (2010), doi:10.1016/j.commatsci.2010.08.006

Contact:

Dipl.-Phys. Alen-Pilip Prskalo

Institute for Material Testing, Material Science and Strength of Materials IMWF

University of Stuttgart

Pfaffenwaldring 32

70569 Stuttgart

Phone: +49 711 685 62579

Fax: +49 711 685 62635

Email: alen-pilip.prskalo@imwf.uni-stuttgart.de