Simulations for oxygen-free productions

Molecular dynamics simulations of deoxidized and oxidized surface and interface phenomena in oxygen-free productions

***N. Gunkelmann, H.-T. Luu**, Institute of Applied Mechanics, Clausthal University of Technology*

In Short

- Material compounds can be used to achieve tailored properties for automotive, aerospace, manufacturing and industrial applications.
- Oxide layers make it difficult to join workpieces.
- The physical properties of the bonding of the joining partners in the contact zone can be analyzed by molecular dynamics simulations.
- The aim is to find process conditions that lead to particularly high-quality, metallurgically-bonded compounds.

Different metallic material compounds can be used to achieve tailored properties for automotive, aerospace, manufacturing and industrial applications. For example, one goal might be, to produce a structure that has good corrosion resistance on one side and good wear resistance on the other side of the component. In this context, improving the quality of joints is of great importance. During metallic joining, a large number of physical and chemical processes determine the quality and strength of the resulting joint. For an example, in joining by cold roll cladding, the oxidation of the surfaces of the joining partners plays an important role and hinders the formation of high-quality joints. An analytical prediction of the joining process is here no longer possible on an ad-hoc basis, since small variations in the chemical composition significantly change the surface condition and can thus already lead to major changes in the joining process. This is particularly relevant for lightweight materials such as aluminum alloys, where an oxide layer forms within seconds even under high vacuum conditions.

The aim of the scientists of the CRC 1368 Oxygen-free production is to develop and establish a production technology under oxygen-free conditions that opens up new possibilities. Wherever two metals come into direct contact with each other in production technology, it is not the metal atoms that touch each other, but the oxide layers on the respective surfaces that are formed by the oxygen in the environment. These oxide layers make it difficult to join workpieces which is why one expects great advantages from oxide-layer-free materials in roll bonding and other joining techniques.

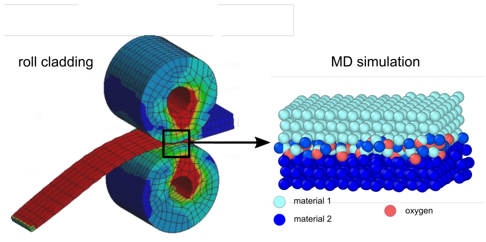

***Figure 1:** Scheme of roll bonding.*

In our subproject, modelling methods will be used to gain a fundamental understanding of the processes and mechanisms in oxygen-free environments. These processes are considered on an atomic level to investigate the physical properties of the bonding of the joining partners in the contact zone using the example of roll bonding. The aim is to find process conditions that lead to particularly high-quality, metallurgically-bonded compounds. The basic dependencies of the bond strength on oxygen concentration, temperature and oxide layer thickness will be investigated for interfaces. The hardness of the materials as an indicator for the quality of the joint will be determined experimentally by nanoindentation and compared with simulation values. Within the framework of a further cooperation with experimentalists from CRC1368, the transport phenomena of oxide-free particles during deoxidation in the plasma fluidized bed will also be simulated. Here it will be shown that the adhesion probability for deoxidized particles is changed, which influences transport limitations in the fluidized bed. The main gain of knowledge of the subproject is the understanding of the atomic mechanisms, which occur in an oxygen-free environment. To fulfill the described objective, the following questions have to be elucidated:

- Which available interaction potentials are suitable for reproducing the oxidation properties?
- How can an MD program tailored to the joining process be implemented to simulate the interfacial phenomena during joining?
- How are the material properties of the composite such as hardness, bond strength and frictional properties affected by the absence of oxygen?
- What is the influence of rough surfaces?
- How does the adhesion probability of particle and particle-wall collisions with deoxidized

nanoparticles compare to the adhesion probability of oxidized particles?

WWW

https://www.simzentrum.de/en/research-projects/sfb1368/

More Information

[1] https://www.sfb1368.uni-hannover.de/en/research/project-area-c/subproject-c05/

Funding

The authors gratefully acknowledge for supports from Simulation Science Center Clausthal/Göttingen. The project was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 394563137 - SFB 1368.