Empa, Swiss Federal Laboratories for Materials Science and Technology

Laboratory for Joining Technologies & Corrosion

Empa
Materials Science and Technology

Master Project

Investigating the structure and properties of metal/ceramic interfaces by means of atomistic simulations: Designing an interatomic potential for the Cu/AlN system

Metal/ceramic interfaces are of great importance both scientifically and technologically, with applications in structural composites, electroceramic devices, environmental coatings and low-temperature brazing materials. Ag-Cu binary alloys are routinely used as brazing fillers to join different solid materials. The Laboratory of Joining Technologies & Corrosion at Empa have designed a new type of brazing materials composed of alternating nanolayers of Cu-Ag and AlN. Our experimental observations reveal semi-coherent interfaces between Ag and AlN and incoherent interfaces between Cu and AlN. A fast outflow of Cu is observed during the heating of such nanolayered systems, and is attributed to the fast diffusion of Cu along the metal/ceramic interfaces. However, the systematic experimental investigation of the Cu diffusion and outflow is impossible due to the small time and length scales for such processes.

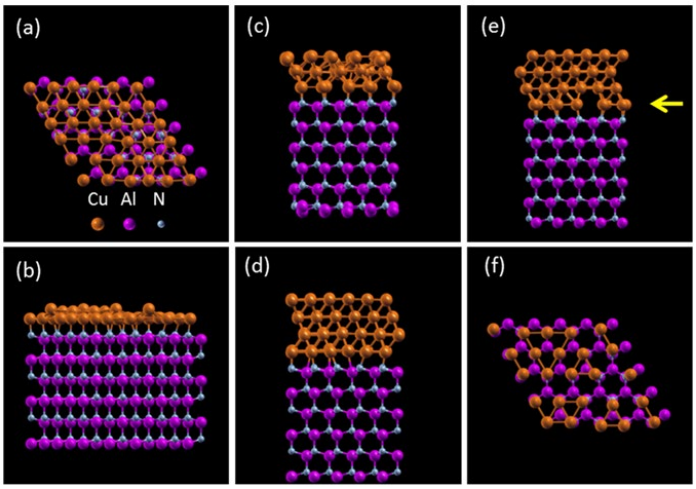

Figure 1. *DFT model calculation of the atomic structure of different (relaxed) Cu slabs on a N-terminated AlN(0001) slab [1].*

Atomistic simulations are proven to be a useful tool for investigating the dynamics of such nanoscale phenomena. Due to the complex interactions between metals and ceramics, the heterogeneous interfaces between them are usually investigated by means of first principles methods such as density functional theory (DFT). However, DFT models are limited to a few hundreds of atoms and, thus, limited to coherent or semi-coherent interfaces. To gain an initial insight into the properties of the Cu/AlN interfaces, we started with such types of interfaces, as shown in Figure 1.

Scope of the thesis

The goal of this project is to use such DFT data to construct an interatomic potential for the Cu/AlN system by fitting the Cu-Al and Cu-N interactions using pair potentials. Due to a small number of parameters, such a simplified model with pair potentials will allow for molecular dynamics simulations with millions of atoms and provides a direct access to the structure and properties of incoherent interfaces between Cu and AlN. The practical work will predominantly be executed at Empa in Dübendorf.

Contact

If you are interested or want to learn more, please contact Dr. Lars Jeurgens (lars.jeurgens@empa.ch)

[1] Pigozzi, G., Antušek, A., Janczak-Rusch, J., Parlinska-Wojtan, M., Passerone, D., Antonio Pignedoli, C., ... Jeurgens, L. P. H. (2012). Phase constitution and interface structure of nano-sized Ag-Cu/AlN multilayers: Experiment and ab initio modeling. Applied Physics Letters, 101(18), 181602.