1ST CLAUSTHAL CONFERENCE ON CIRCULAR ECONOMY

Revolutionizing Sustainability: Advanced Oxidation-Free Manufacturing in the Circular Economy

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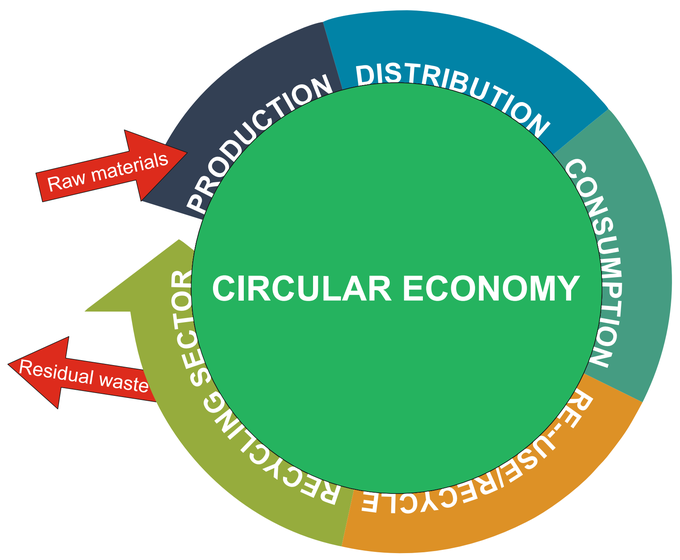
CLAUSTHAL CONFERENCE ON CIRCULAR ECONOMY

23. – 24. November 2023

Hoang-Thien Luu, Nina Merkert* (nina.merkert@tu-clausthal.de)
Institute of Applied Mechanics, TU-Clausthal Adolph-Roemer-Straße 2A D-38678 Clausthal-Zellerfeld

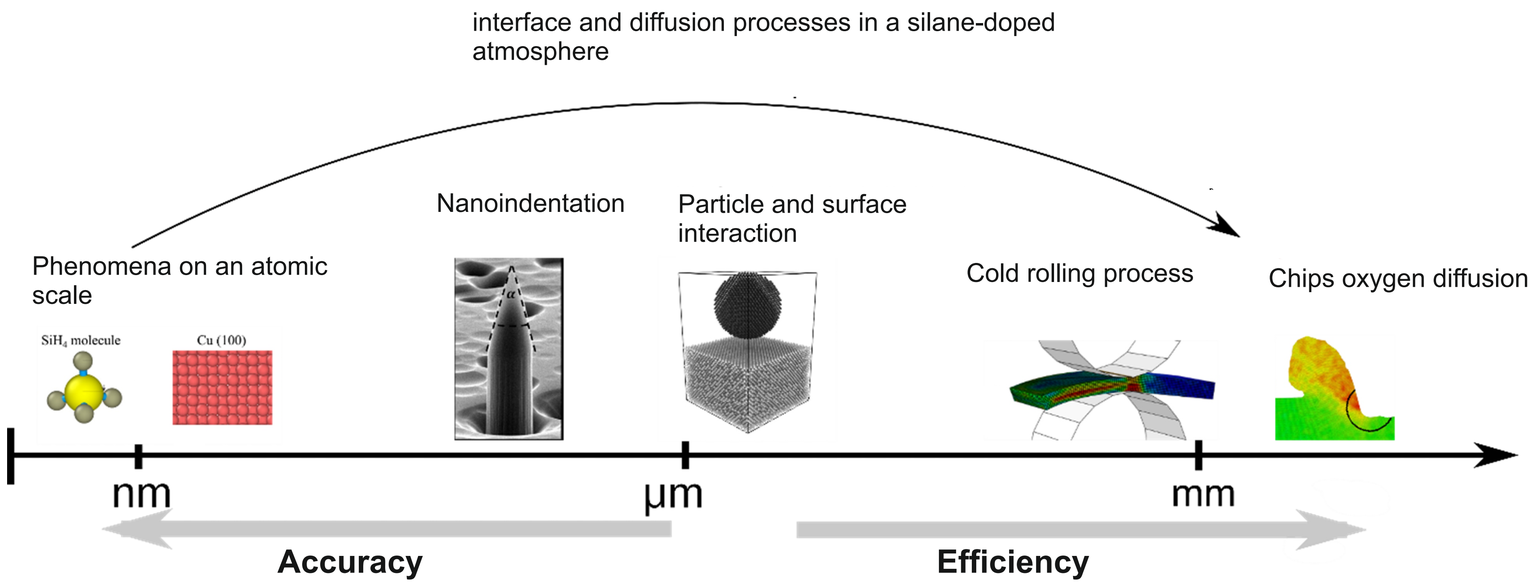
Abstract

Metal products have the potential to undergo mechanical treatment and recycle back into the production process, which allows for the manufacturing of new materials and participating a significant role in the circular economy. The initial step in the circular economy is production, whereas the last and least effective phase is metal recycling. In addition to helping to raise recycled content, efficient **oxidation free production** also raise the rate of end-of-life recycling. This is particularly important when a varied combination of components is highly desired in modern products. By using molecular dynamics simulations, we have the opportunity to gain insight into the essential role of oxide reduction in the atmosphere and on the material surface before and during the production. Beyond being of better quality, products that absence of impurities including oxides also help cut down on waste and raw materials, as well as the cost of recycling.



Metals and Circular Economy

Validation of simulation models



MD simulations were performed at various scales in cooperation with other experimental specialists.

Validation of the force field for MD simulations

- Suitable interatomic potentials for modeling various processes of oxygen-free production were investigated.
- Surface interfacial phenomena and mechanical processes at the atomic level were implemented and the results carefully examined.

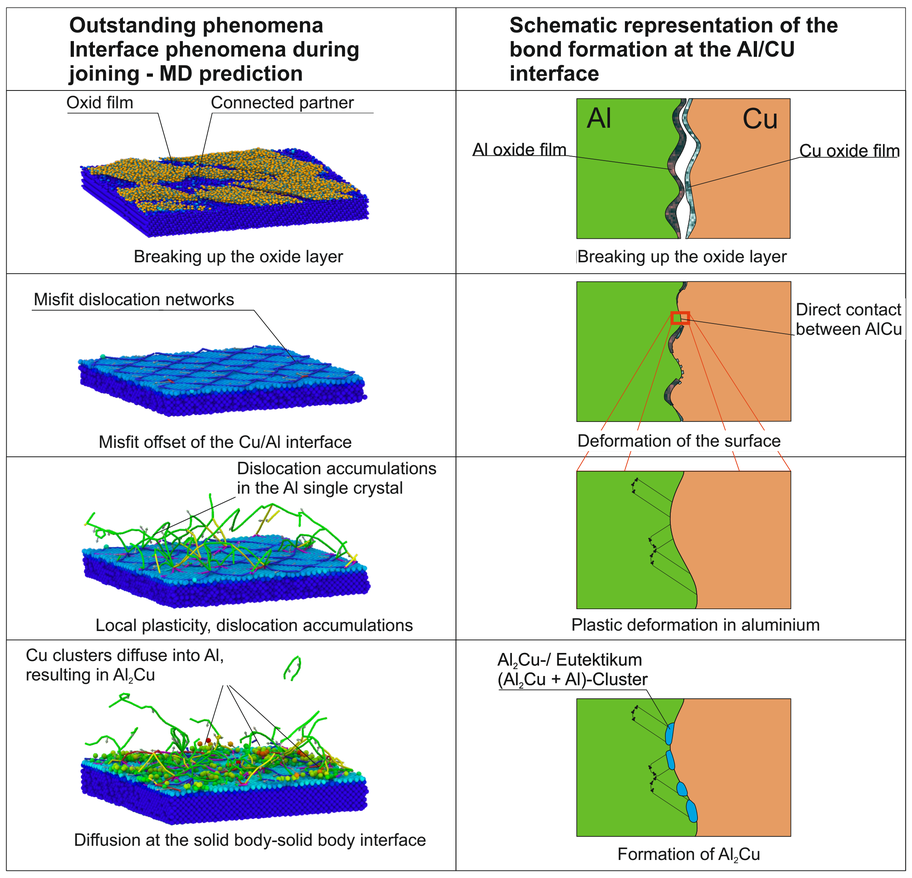
Interface phenomena during joining

The behavior of the oxide layer

- Nanoindentation simulations on Al covered by a native oxide layer lead to plastic deformation in the Al substrate.
- If the deformation is large enough, the oxide layer breaks and cracks appear

Insights into Al and Cu diffusion under oxidation-free conditions

- MD simulations show that diffusion at the oxide-free Cu-Al interface occurs within 1 ns.
- The results are in great agreement with the Gunnier-Preston theory (GP zone).
- Heterogeneous diffusion processes are observed, leading to the formation of Al_2Cu or a eutectic (Al_2Cu + Al) asIndicate primary phase.



Insights into the bond formation of Cu and Al (solid-solid) during the joining process. Left) MD prediction, right) Schematic of the joining process.

TU Clausthal

SWZ Clausthal – Göttingen
Simulation Science Center

Technische Universität Clausthal
Adolph-Roemer-Straße 2A
D-38678 Clausthal-Zellerfeld
Telefon: +49 5323 72-0
Fax: +49 5323 72-3500