Master Thesis:
Applications of *ab initio* molecular dynamics in cemented carbides sintering

Background
Sandvik Coromant is a global market-leading manufacturer of tools and tooling systems for cutting operations as well as of blanks and components with 8000 employees in 130 countries. Products are manufactured in cemented carbide, high-speed steel and other hard materials such as diamond, cubic boron nitride and special ceramics. Sandvik Coromant's research and development focuses on the development of new materials and products and the improvement of production processes and production equipment.

Cemented carbides are produced by powder metallurgy and consists of a binder phase (often cobalt), tungsten carbides and in many cases additions of cubic carbides. The common production route of cemented carbides comprises mixing and milling of starting powders in alcohol with a polymer binder, spray-drying to granules, powder compaction, pre-sintering and sintering at temperatures in the range 1400-1500°C. The sintering is followed by several operations such as grinding and coating.

To increase the understanding of the physical processes many of the productions steps are modeled using different simulation methods. The condition during *e.g.* sintering makes it difficult to follow the microstructural evolution, making modeling an important tool to understand and improve the material synthesis.

Assignment
During sintering of cemented carbides, the evolution of the microstructure can be controlled by changing the chemical potentials in the raw material powders, or in the atmosphere. The transport of elements trough the liquid binder phase however differs between elements. In this project we will calculate, using *ab initio* molecular dynamics simulations, the mobility of different elements in the liquid binder. It is furthermore the aim to investigate how interactions between elements affect the diffusion rates.

The work will contain the following steps
- Literature study
- Simulation of liquid self-diffusion using *ab initio* molecular dynamics
- Evaluation of mobility from the simulations
- Report

Duration
20 weeks, corresponding to 30 credits

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