

Coupling Ab Initio Calculations to PVD Synthesis of Thin Films – A Multi-Methodic Approach

Authors:

Christian Gutschka, Jochen M. Schneider

Experimental and simulation-based screening methods are increasingly used in Materials Science to reduce the time and cost associated with conventional laboratory experimentation. In thin film research, particularly for Physical Vapor Deposition (PVD), combinatorial sputter deposition has become an established technique for rapid materials exploration. However, predictive ab initio methods such as Density Functional Theory (DFT) remain limited in accurately describing key properties of PVD films, including alloy solubility and mechanical behavior. This is particularly relevant for novel ceramic coating materials, such as carbides, nitrides, and borides, where the extreme cooling rates during PVD promote metastable and previously unexplored solid solutions. Reliable predictions in these non-equilibrium phase spaces would significantly improve experimental optimization.

A major challenge is that phase equilibria in PVD-grown thin films differ substantially from equilibrium phase diagrams commonly obtained from CALPHAD calculations. Nevertheless, more than a decade ago, a hybrid model combining combinatorial sputter deposition experiments with DFT and CALPHAD data was introduced [1-3]. The model incorporated substrate temperature, target power, and residual film stress, and demonstrated promising predictive accuracy for both metallic and ceramic thin film systems.

This PhD project aims to extend the methodology by eliminating the dependence on existing CALPHAD databases and incorporating interfacial energy contributions arising from microstructural effects such as preferred crystal orientation and grain geometry. The present study focuses on metallic W-Cu thin films and begins with a systematic assessment of model sensitivities to experimental and DFT-derived input data.

[1] Chang K., et al. Sci. Technol. Adv. Mater. 2016;17:210.

[2] Liu S., et al. Acta Mater. 2019;165:615.

[3] Liu S., et al. Acta Mater. 2020;196:313.