

Study of metastable phase formation for sputtered thin films

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Due to kinetically limited vapor phase condensation processes, metastable phases are commonly obtained during synthesis of thin films, which makes prediction of their structures and properties rather demanding. In this work, metastable phase formation of sputtered thin films were studied using *ab initio* calculations and the CALPHAD (CALculation of PHase Diagrams) approach together with combinatorial experiments. Phase diagrams and metastable phase formation diagrams of the metallic systems were calculated, which agree well with experimental data. Ongoing work on nitride thin films also shows promising results. Application of the research strategy to predict the metastable phase formation for sputtered thin films will be testified further.