

DocMASE Project Proposal 2015-05

Project Title	<i>Three-dimensional microstructures of superhard nitrides</i>
Main University and Advisor	Linköping University, Professor Magnus Odén
Second University and Advisor	Saarland University, Professor Frank Mücklich
Project Description (with image , if applicable)	<p>This is a phase-field modeling project, which aims at predicting and take advantage of the 3-dimensional microstructures that evolves when an alloy with an immiscible composition phase transforms. Our prime interest is different types of transition metal nitrides, which are used as superhard coatings. The nanostructure that evolves in these materials is complex and strongly affects the macroscopic properties of the material.</p> <p>Our goal is to bridge the phenomenological phase-field approach closer to the microscopic <i>ab initio</i> simulation of transition metal nitrides.</p> <p>You will be working with developing existing supercomputer phase field code and perform calculations. You will also be working with <i>ab initio</i> approaches and experimental techniques to obtain relevant input data for the phase field simulations. Different experimental techniques such as tomography based approaches (e.g. atom probe tomography) will be used to verify your calculations.</p> <p>You will be part of a strong research team working on many different aspects of microstructure evolution, which will give you the opportunity to gain knowledge also on aspects outside your project.</p> <p>Besides doing research you must fulfill the course requirements imposed by Linköping University, Saarland University, and DocMase.</p>
Previous Publications	<p>A. Knutsson, J. Ullbrand, L. Rogström, N. Norrby, J.S. Johnson, L. Hultman, J. Almer, M.P.J. Jöesaar, B. Jansson, M. Odén: "Microstructure evolution during the isostructural decomposition of TiAlN-A combined in-situ small angle x-ray scattering and phase field study" <i>J. Appl. Phys.</i> 113 (2013) 213518.</p> <p>J. Barrirero, M. Engstler, N. Ghafoor, N. de Jonge, M. Odén, F. Mücklich: "Comparison of segregations formed in unmodified and Sr-modified Al-Si alloys studied by atom probe tomography and transmission electron microscopy" <i>J. Alloy. Compd.</i> 611 (2014) 410.</p> <p>K. Grönhagen, J. Ågren, M. Odén: "Phase-field modelling of spinodal decomposition in TiAlN including the effect of metal vacancies" <i>Scr. Mater.</i> 95 (2015) 42.</p>
References	
Requirements of the candidates / Requirements during the doctoral programme (courses, seminars, etc.)	<p>A solid background in Material Science and/or Solid State Physics is required. In order to graduate from the program the student must fulfil all requirements for a PhD at both Linköping University and Universität des Saarlandes. PhD duration should be 4 years, the actual duration depends on achievements. 90 ECTS course credits must be completed before graduation among which a maximum of 30 ECTS can be accounted for by courses taken during the Master studies on advanced level if the supervisor approves their relevance. The remaining ECTS course credits must be completed through additional course work.</p> <p>You should go to international conferences and present your work and publish your findings in international peer-reviewed archive journals.</p>