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Erasmus Mundus

DocMASE Project Proposal 2012-02

Project Title	***Modeling of the microstructure evolution in functional surfaces***
Main University and Advisor	**Linköping University (LiU)** (Linköping, SWEDEN) Prof. Magnus ODÉN
Second Univ. and Advisor	**Saarland University (UdS)** (Saarbrücken, GERMANY) Prof. Frank MÜCKLICH
Associated Partner(s)	**SECO Tools** Prof. Bo JAHNSSON
Project Description	The project is devoted to modeling the microstructure evolution of nanostructured wear-resistant functional surfaces based on transition metal nitride alloys. This type of film can be synthesized having a homogeneous composition by e.g. PVD processes. The coating might undergo precipitation hardening through spinodal decomposition during heat treatments or high temperature applications. The ability to model the spinodal decomposition and its effect on mechanical properties can be utilized as a tool to design and tailor films to desired properties. The project will apply a multiscale modeling approach. We intend to use first-principles density-functional theory (DFT) for a relatively small system (~100 atoms) to solve the quantum mechanical problem combined with thermodynamic (CALPHAD) methods to model the microstructure evolution on the μm scale utilizing continuum models and the phase field method. The multiscale modeling approach has experienced certain success. However, presently the different methods used for different scales are not interfacing fully and are often treated separately. For example, DFT calculations emphasize the electronic subsystem, while atomic motions are often neglected. Classic CALPHAD models for large time and length scales often lack adequate experimental information, which is compensated by oversimplified interpolations. Instead we will perform the simulations in such a way that the DFT calculations are relevant and appropriate for the subsequent step where microstructure evolution and material properties are established. Thus, a consistent scheme for multiscale modeling will be developed. The phase field models are based on formulating the total free energy of the system which will provide the driving force for the diffusion controlled spinodal decomposition. Examples of required input data that can be generated from DFT calculations are: • Thermodynamic properties of homogenous solid solution phases • Anisotropic elastic properties as a function of composition and pressure • Lattice parameter as a function of composition and pressure • Surface tension for diffuse interfaces, e.g. gradient energy. Some experimental information regarding the microstructure evolution is required to tune the phase field models and DFT calculations: • Differential scanning calorimetry for in situ study kinetics and evolved heat • Characterization by atom probe tomography of the microstructure after heat treatments
Previous Publications	F. Tasnádi *et al:* Significant elastic anisotropy in Ti(1-x)AlxN alloys, *Appl. Phys. Lett.* **97** (2010). B. Alling *et al:* Pressure enhancement of the isostructural cubic decomposition in Ti1-xAlxN, *Appl. Phys. Lett.* **95** (2009) 181906.