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DocMASE

Education and Culture
Erasmus Mundus

DocMASE Project Proposal 2012-05

Project Title	Theoretical analysis of internal interfaces
Main University and Advisor	**Linköping University (LiU)** (Linköping, SWEDEN) Prof. Igor ABRIKOSOV
Second Univ. and Advisor	**Saarland University (UdS)** (Saarbrücken, GERMANY) Prof. Frank MÜCKLICH
Associated Partner(s)	**SECO Tools** (Fagersta, SWEDEN) Prof. Bo JAHNSSON
Project Description	The project primarily aims at a theoretical, density functional theory (DFT) based simulations of the thermodynamic and dynamical stabilities of both the strained TiAlN and modified Al(Si,Sr) alloys. The calculations are aimed to include vacancies and interstitials to elaborate general understanding of how the interface structure and strain affect the phase evolution in such systems. During your studies you will use state-of-the-art softwares for the solution of quantum mechanical problems on modern powerful supercomputers.. Since the project is highly application-driven, you will master yourself in theoretical materials science but you are also expected to closely collaborate with experimentalists in the frame work of DocMase. It means that your theoretical predictions will be experimentally verify through advanced materials characterization on model materials synthesized and designed just for this purpose. We expect applications from candidates with basic experiences with Linux, numerical methods of theoretical physics/chemistry, electronic structure methods, but specific knowledge in any of these areas is less critical compared to an exceptional intellectual ability.
Previous Publications	H. Lind et al. “Improving thermal stability of hard coatings via a concept of multicomponent alloying” *Appl. Phys. Lett* **99**, 091903 (2011). A. Knutsson et al. “Thermal decomposition products in arc evaporated TiAlN/TiN multilayers” *Appl. Phys. Lett* **93**, 143110 (2008).