Post Doctoral position

Multi-scale computational-driven design of novel hard nanostructured coatings

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Contract terms:
Position available: 1st October 2014 ; duration: 12 months ; salary: on the basis of CNRS standards.

Context:
The proposed work is part of a European **M.ERA-NET** Research project on "**Multi-Scale Computational-driven design of novel hard nanostructured coatings**" (MC2), which gathers 5 partners from Sweden, Luxembourg and France. The project MC2 is sponsored for 3 years (2013-2016) by respective National funding agencies, including the "Agence Nationale de la Recherche (ANR)" for the French teams in Poitiers and Paris. The goal of the project is to develop new fundamental and technological concepts for the design of novel hard coatings, based on multicomponent **transition metal nitrides** (TMN), with improved performance (hardness, toughness, thermal stability) under service/operation conditions used in the cutting tool industry.

Work description:
An innovative multi-scale computational approach to predict phase stability and elastic properties at the *single-crystal* level (first-principles calculations) as well as at the *polycrystal* level (phase-field and kinetic Monte Carlo simulations, effective averaged elastic constants) will be implemented to tailor the composition, growth morphology and microstructure of Ti-Al-X-N coatings with enhanced properties, where X is an alloying element such as Cr, Ta or Zr.
The successful candidate will study the phase stability, the microstructural and the mechanical properties of disordered quaternary TiAlXN nitrides alloys combining advanced ab initio calculations, phase field simulations and effective elastic properties predictions.
The numerical estimates will be compared to experimental determinations using non-conventional techniques such as Brillouin light scattering and picosecond techniques on TiTaAlN and TiZrAlN films elaborated by the partners.

Requirements
- PhD Degree in Physics, Materials Science or Computational Materials Science
- Strong knowledge in computational modeling of materials: ab-initio calculations (VASP, ABINIT, EMTO), Molecular Dynamics (LAMMPS), Phase field simulations, effective elastic properties calculations
- Good skills in computer programming (Fortran, C++)
- Background in Solid State Physics; *optional*: Thin Film Growth processes
- Enthusiasm for research and team-minded
- Able to communicate in English and/or French

For further information, please contact
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Dr. Ferenc Tasnadi (tasnadi@ifm.liu.se, Tel.: +46 13 285709),

Applications including a CV with short work experiences, 2 letters of recommendations, and a letter of motivation (with acquired competences or to be acquired and perspectives) should be sent to djemia@univ-paris13.fr.
Deadline: July 31st, 2014