



Candidature for PhD thesis position on
Multi-scale computational-driven design of novel hard nanostructured coatings
and experimental comparisons

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The association of French universities that is called “Sorbonne-Paris-Cité” (SPC) is offering 20 PhD positions to foreign students with excellent scores in their faculty. The present proposition aims to identify the candidate who will apply to the SPC call before end of March 2014.

The goal of the PhD work is to develop new fundamental (basic) and technological (applied) **concepts** for the **design** of novel hard coatings, based on **multi-component transition metal nitrides (TMN)**, with improved performance (hardness, toughness, thermal stability) under service/operation conditions used in the **cutting tool** industry. Industrial needs in this field thrive to increase cutting speed data, which requires the development of new hard coatings with improved thermal stability mechanical properties and wear resistance under more severe work load conditions (temperature, pressure). One path towards such development beyond conventional hard coatings lies in synthesizing compounds with a complex structure, i.e. ternary or quaternary systems. Multicomponent TMN, based on alloying TiAlN coatings with other element X (X=Cr, Ta, Zr, Mo, etc), are promising candidates to fulfil such requirements. Efficient strategies, including new processing routes and new design concepts, based on a chemical/structural tailoring of the coatings, should be addressed to ensure Europe’s leading position in the field of surface engineering. The project aims at contributing to this issue, *both* from a fundamental approach and applied research scheme, by implementing the following **specific innovative objectives**:

- developing combinatorial high-throughput first principles simulations on phase stability and elastic properties of multinary TMN alloys (*chemical design*)
- developing structural concepts for engineering elasticity at the mesoscopic level, i.e. optimizing morphology, microstructure, and interfaces properties (*structural design*)



- implementing advanced, high accuracy, atomic resolution to understand basic mechanisms of growth and structural evolution, and validate the novel concepts in industrial cutting applications.

The best coating candidates will be identified thanks to the relationships between the computed/measured elastic properties and brittle-ductile behaviour, as inferred from known criteria.

The **originality** of the project lies in the implementation of a 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 mesoscopic simulations, effective averaged elastic constants), to tailor the composition, growth morphology and microstructure of Ti-Al-X-N coatings with enhanced properties.

The proposed PhD thesis is embedded in the framework of the transnational M.Era-Net MC2 project “Multi-scale Computational-driven design of novel hard nanostructured Coatings” funded by the ANR (France), Vinnova (Sweden) and FNR (Luxembourg). It is a collaboration of several international research groups from the LSPM in Villeneuve (France), Pprime institute in Poitiers (France), the IFM in Linköping (Sweden) with an industrial partner and the CRP-GL (Luxembourg) in Belvaux. **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 evaluations. Also, 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.**

For further information, please contact

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Applications including a CV (including the Master scores), 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: March 23rd, 2014

