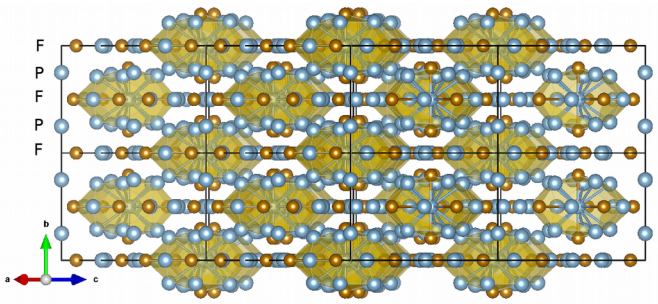
Complex intermetallic / oxide interfaces : theoretical approach at the atomic scale

Scientific project :

Complex intermetallic compounds belong to a class of materials characterized by a large unit cell, containing several tens to several thousands of atoms, usually arranged into regularly packed clusters of high symmetry. It includes intermetallic quasicrystals and their periodic approximants, but also cage compounds like intermetallic clathrates. Their potential lies on their unique electronic and atomic structures, which allows a large flexibility for tuning their properties. Each of the thousands of binary intermetallic compounds known so far has the potential to behave as a new material, opening a vast field to be explored.

The study of the surfaces of these materials is a very active research subject motivated by their original properties potentially useful for various applications - as coatings or catalysts for example. But aside from niche applications for vacuum technologies, surfaces interact with their environment. The objective of the thesis is to determine the influence of the complexity on the oxide layer and the modifications of the atomic and electronic structure of complex intermetallic surfaces, induced by oxidation. It is a first step towards understanding the functional properties of these surfaces under real conditions of use.



Quasicrystalline approximant $Al_{13}Fe_4$ [Scheid et al., Acta Cryst. A (**2019**)]

This project will take place at the Jean Lamour Institute (IJL), on the campus Artem Nancy, gathering more than 5000 people including 3500 students. This project has an international dimension and takes place within the "Integrated European Center for the Development of New Alloys and Metallic Compounds" and the International Lab between IJL and the Joseph Stefan Institute (JSI, Ljubljana, Slovenia). Strong interactions are expected with experimentalists.

Successful candidates should hold (or be about to receive) a master's degree in Materials Science, Chemistry, Physics, or a related area. Good knowledge of quantum mechanics is expected. Candidates who have interest in writing computer code and shell scripts are preferred. Please send a motivation letter and your CV, including names and contact information of two referees.

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