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COMPUTATIONAL MATERIALS DESIGN : VANADIUM ALLOYS FOR DEMO

Keywords: Computational materials design, structural materials, vanadium alloys, mechanical properties of materials, computer simulations, DFT

In collaboration with SCK.CEN – the Belgian Nuclear Research Centre in Mol.

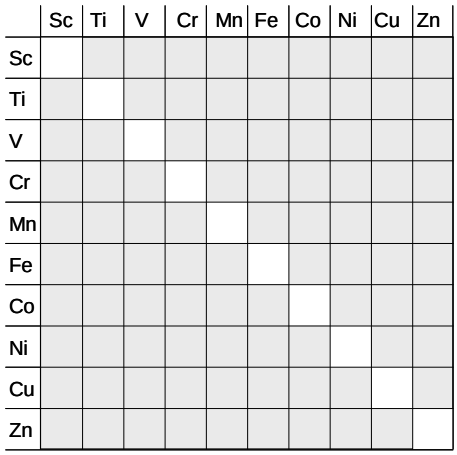

***Figure 1**: Graphical version of the goal of this thesis. For every combination of two alloying elements, the value of a predicted property appears in the matrix. There is one such a matrix for*

The performance as well as the economic feasibility of commercial fusion reactors critically depends on the choice of the right materials for all of its many components. DEMO is the name of the first prototype of a commercial fusion plant. It will be operational around 2040, and will be designed based on the expertise that will have been acquired with ITER. ITER is the first test plant that will be able to produce more energy than it consumes, and is currently being built in Cadarache (France).

At present, materials research for DEMO components is an active research field. One of the material classes that are being examined, are structural materials with specific properties. Steel is ubiquitously used as a structural material in industrial constructions. For application in the specific environment of a fusion plant, however, low activation structural materials are required. In common structural materials, the neutron flux of the reactor would lead by transmutation to a large amount of long-lived isotopes. This would either change the properties of the material beyond an acceptable level, and/or would lead to a prohibitively large amount of highly radioactive waste at the end of the life cycle of the reactor.

The main candidate for low activation structural applications in DEMO are vanadium-based alloys (see Refs. [1] & [2] for reviews). The alloy that has been studied most, is V-4Cr-4Ti (bcc vanadium with 4% chromium and 4% titanium). In order to come to this conclusion, many vanadium alloys have been tested experimentally. It is too time-consuming to examine *all* possible alloys by experiments only. It becomes increasingly more feasible, however, to tackle such a task by means of ab initio computer simulations.

Goal In this master thesis, we will examine the model system V-6X-6Y (bcc vanadium with 6% of element X and 6% of element Y), where X and Y are any of the ten 3d transition metals. For every alloy, we will compute a series of basic mechanical properties that are directly or indirectly related to the actual materials performance. Every property can be summarized in a 10×10 symmetric matrix (see Fig. 1,

which is empty, so far). In this way, it will be possible to see at a glance which combination of alloying elements optimizes the given property. This might lead to new suggestions for vanadium alloys that deserve further experimental and theoretical examination.

Interested students will get a proper training in the use of ab initio computer codes. Software for performing screening studies is being developed at Ghent University, and will be available for this master thesis work as well.

[1] Votinov et al., Journal of Nuclear Materials 233-237 (1996) 370
[2] Tavassoli, Journal of Nuclear Materials 302 (2002) 73

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