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IMPROVING THE DUCTILE-TO-BRITTLE TRANSITION IN TUNGSTEN ALLOYS: AN COMPUTATIONAL SEARCH FOR TOUGHER FIRST WALL MATERIALS IN FUSION REACTORS

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ITER, the first fusion plant that will be able to produce more energy than it consumes, is currently being built in Cadarache (France). In the meantime researchers are planning the next step to commercial fusion reactors, called DEMO. This prototype plant is planned to start operation around 2040, but research for DEMO has already begun. One of the most important aspects that will determine design decisions is the development of new materials with very specific properties. This is particularly important for the so-called 'first wall materials', which come into direct contact with the plasma and have to be able to withstand severe operation conditions.

At present, tungsten alloys are the only potential candidates to serve as first-wall materials for long term operation under conditions relevant for DEMO. They are the only materials that combine good high temperature strength, high thermal shock resistance, good thermal conductivity, low sputter rates, low tritium retention and good irradiation resistance.

However, there is one main disadvantage, which is still very hard to overcome: the ductile-to-brittle transition temperature (DBTT) of tungsten is too high. In the low-temperature range of operating conditions, tungsten would therefore be in the brittle regime. Since this is a highly unwanted property, researchers are looking for a first wall material with a lower DBTT, while keeping all the favourable characteristics of tungsten. One of the possible approaches is to alloy tungsten with other elements. It has been shown that adding tantalum or rhenium indeed changes the ductility of tungsten for the better. There are however a lot of possible alloying elements and concentrations remaining, and the experimental search for new candidates proceeds slowly.

Using ab initio methods, such as density functional theory (DFT), one can speed up experimental work by preselecting the most promising materials via a computational search. DFT is able to compute properties at an atomic scale. As long as the underlying mechanisms for a certain phenomenon are understood well enough, a computer calculation can yield valuable information, that could not be obtained (that easily) from experiment.

In tungsten alloys screw dislocations are of the utmost importance. They are helical distortions of the perfect bcc lattice (see figure). Since these structures are imperfections, they diminish the strength compared to the ideal material. When stress is applied to the material, dislocations are the first to react. This is not always a bad thing, as the movement of dislocations can increase the ductility of a material. Indeed, a brittle material under stress will crack, and eventually breaks when the critical point is

reached. In a ductile material, however, mobile dislocations will relieve a part of the applied stress. In order to improve the ductility of tungsten alloys, one therefore needs to increase the mobility of its dislocations.
In ab initio calculations this mobility can be found in the form of the Peierl stress σ_P. It represents the stress necessary to move a dislocation at zero kelvin. One calculates it by straining the crystal in small steps and relaxing it in between. σ_P is that stress for which the dislocation does not relax to its original shape anymore, but moves to a neighboring position instead.

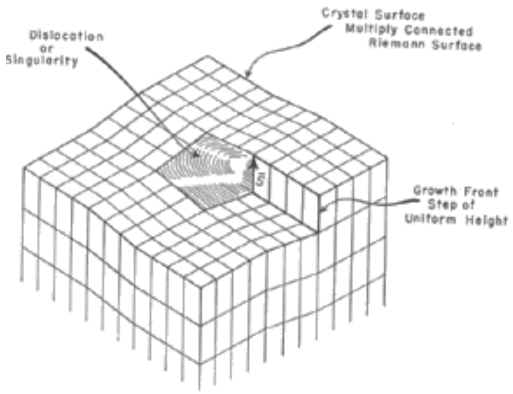

***Figure 1**: Screw dislocation in a cubic crystal*

Goal The purpose of this master thesis is to determine the Peierl stress for a few tungsten alloys. In the first place W and W-Re will be employed as a test system, since a study of these compounds has already been performed in literature [Romaner2010]. Comparison of our results to those of Romaner et al. will validate the procedure. Afterwards other materials systems will be examined, in search of useful alloying elements for the fusion community.

A few less complex indicators of ductility exist as well, such as the Cauchy pressure. A second goal of this thesis is to evaluate to what extent such easy quantities are useful to predict ductility in tungsten alloys. If it turns out that ductility can be predicted with sufficient accuracy using a Cauchy pressure rather than a Peierl stress, the speed by which different alloys can be computationally tested can be enhanced significantly.

Interested students will get a proper training in the use of ab initio computer codes. The necessary expertise and software is available at the Center for Molecular Modelling of Ghent University. For fusion aspects there is a close collaboration with both the Applied Physics Department, which coordinates the fusion research at Ghent University, and SCK·CEN, the Belgian Study Center for Nuclear Energy.

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