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# Atomistic modelling of tungsten based alloys

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Tungsten alloys are considered for structural applications in fusion reactors, especially for armor materials at the divertor and first wall. This interest is motivated by promising physical properties such as high melting point, low coefficient of thermal expansion, high thermal conductivity and high sputtering resistance. In this context we investigate the thermodynamic and mechanical properties of tungsten based alloys on the basis of atomic scale simulations using both density functional theory calculations and empirical potential methods.

Here, we will first report on the properties of intrinsic and extrinsic (Ti, V, Zr, Nb, Hf, Ta, Re) defects in tungsten, which were considered with the eventual objective to address the potential of dilute W-based alloys in lowering the brittle-to-ductile transition temperature (BDTT). Ti, V, Nb, Hf and Ta substitutional defects are found to have negative formation energies whence these elements tend to form solid solutions with tungsten. By contrast positive formation energies for Zr and Re indicate that there is a thermodynamic driving force for segregation in alloys based on these two elements.

Interstitials generally have large formation energy due to large strain fields associated with the defect core. For Zr, Nb, Hf, Ta and W interstitials, <111> crowdions are the most stable interstitial configurations while for Ti, V and Re, <110> as well as “bridge” configurations show the lowest formation energies. Most interestingly negative values of binding energy for Ti, V and Re in both interstitial configurations indicate that these impurities trap interstitials. Under irradiation conditions interstitial defects will be produced that under normal conditions can readily recombine thanks to the large mobility of <111> type interstitials. In the presence of the aforementioned alloying elements, this process will be impeded, whence a faster defect accumulation rate is to be expected.

To explore this effect further we specifically investigate the W-Ti system. It is shown that the system exhibits a strongly asymmetric phase diagram with a large solubility for Ti in BCC-W. Ti-W mixed interstitials are found to have a strong attractive interaction, suggesting a pronounced tendency for interstitial clustering. These results are discussed in the context of the application of in particular W-Ti alloys for structural elements in neutron rich environments.