The Role of Point Defects in Self-Passivating Alloys for Fusion Reactor First Walls

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To address the growing demand for low carbon energy, the UK government has recently committed to building the world's first nuclear fusion power plant by 2040, the Spherical Tokamak for Energy Production (STEP). One of the challenges faced by the STEP project concerns the oxidation of the reactor's tungsten-based first wall, which may occur during a loss of coolant accident or during remote handling maintenance. To mitigate the oxidation of tungsten, there has been a growing interest in the use of 'smart alloys' for use in future tokamak fusion reactor designs. In particular, the ternary alloy W-11.4Cr-0.6Y has been identified as a potential candidate for fusion reactor first walls owing to its favourable oxidation resistance and self-passivating behaviour. However, the role of the alloying elements, Cr and Y, is not fully understood on a mechanistic level. To investigate this behaviour, we have employed molecular statics using the LAMMPS code and density functional theory using the VASP code to study the behaviour of the binary W-Cr alloy, the favourability of a range of point defects in bulk W, and the formation energies of the oxide phases which have been observed experimentally. By combining these, we present our current understanding of the role of Cr and Y in these smart alloys and why this composition in particular offers the greatest oxidation resistance.

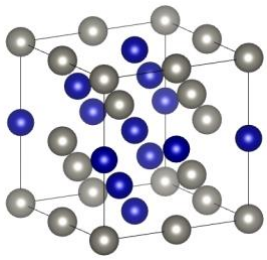

Figure 1: A representative SQS unit cell of $W_{0.5}Cr_{0.5}$.

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