INVESTIGATION OF HIGH-ENTROPY ALLOYS FOR USE IN ADVANCED NUCLEAR APPLICATIONS

A thesis submitted in partial fulfilment for the degree of doctor of philosophy at University of Technology Sydney

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Certificate of Authorship / Originality

I certify that the work in this thesis has not previously been submitted for a degree nor has it been submitted as part of the requirements for a degree except as fully acknowledged within the text.

I also certify that the thesis has been written by me. Any help that I have received in my research work and the preparation of the thesis itself has been acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis

Signed:

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Abstract

A preliminary assessment of the suitability of high-entropy alloys (HEAs) for use within a nuclear reactor environment is conducted by combining both experimental and computational techniques. The investigation begins on the V-Zr system where three thin films with stoichiometries (2V:1Zr, 1V:1Zr and 1V:2Zr) were deposited. A metastable amorphous phase was observed and subsequently modelled, for the first time, using static density functional theory (DFT). This methodology is then further developed and the thermodynamics of the binary system were assessed.

Similar computational techniques were then used to investigate CoCrFeNi. Isolated vacancy formation calculations were performed and it was found that vacancies of Co, Fe and Ni are positive, and Cr is negative in energy. This drive for spontaneous segregation of Cr from the FCC matrix is predicted to occur in a vacancy mediated process. It is possible that this mechanism will allow for the formation of a corrosion resistant oxide layer. The addition of Al to form the $Al_xCoCrFeNi$ system, where x is varied from 0 – 2.4 atomic ratio, was then explored. Only when partial ordering was imposed, with Al and Ni restricted to separate sub-lattices, to form an ordering analogous to the B2 NiAl intermetallic, was the BCC packing stable. Decomposition of the ordered BCC single phase into a dual phase (Al-Ni rich and Fe-Cr rich) was also considered.

An algorithm to rapidly screen elemental mixtures to form single phase high-entropy alloys (SPHEAs) was developed. Approximately 186,000,000 compositions of equimolar 4, 5 and 6 element alloys were screened and ~1900 new SPHEAs were predicted using this method.

NbTiV, $Mo_{0.5}NbTiV$, MoNbTiV, $NbTiVZr_{0.5}$, NbTiVZr and $NbTiVZr_2$ were experimentally produced via arc melting. As predicted by the screening method, all alloys were found to form a single phase BCC structure with non-equilibrium dendritic microstructures. Au^{5+} and He^+ ions were used to irradiate TEM samples and a bulk $NbTiVZr_2$ sample. No changes were observed after ~20-25 dpa in the TEM samples and minimal swelling of the BCC matrix was observed in the bulk sample.

The project has revealed that HEA alloys are potentially candidate materials for structural applications in nuclear reactor environments.

Contents

List of Figures

List of Tables