First-principles Study of Tin Intergranular Segregation in Zirconium

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Abstract

The Zirconium is the major component of zircaloy (2 and 4), this latter has a very weak thermal neutron absorption, satisfactory mechanical properties and good corrosion resistance at high temperature. For these reasons, it has been used in the cladding of nuclear fuel rods for some types of nuclear reactors. In this environment, it is submitted to different severe conditions of temperature and pressure. The zircaloy contains alloying elements for improving of the various properties. Segregation of one or more alloying elements modifies considerably these properties. The objective of this work is to calculate by the first principles the Sn alloying element segregation energy at the symmetrical grain boundary [θ=49.7146°/[2$\bar{1}\bar{1}$0], (03$\bar{3}$7)] in zirconium.

The optimization and convergence calculations show that the most optimal pseudopotentials among five selected pseudopotentials are GGA-PBE-HGH and GGA-PBE-Trouiller Martins. For our study of segregation at grain boundary we chose the second pseudopotential.

Calculation results show that the tin segregation energy at the grain boundary is negative, i.e. unfavorable segregation, but positive for the site of the first plane parallel to the grain boundary, i.e. favorable segregation.

The charge density curves demonstrate the difference between the intergranular zone without, and with tin in various atomic sites.

As perspective of this work: calculation of intergranular segregation energies in Zr for alloying elements Fe, Cr and Ni.

Keywords: First principles calculation; zircaloy; grain boundary; intergranular segregation; alloying element.