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Study and simulations of quick diffusion in Zr-based alloys

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ABSTRACT

Zirconium and its alloys are widely used in the nuclear industry. Under normal conditions, Zr-alloys are polycrystalline and contain a high density of grain and interphase boundaries. These boundaries function as paths for accelerated matter movement. The movement of fast diffusing elements (Co, Fe, Cr, Ni) in Zr alloys along boundaries produces technologically important changes in the materials in nuclear reactors at normal temperatures (~550K) e.g.: segregation, phase precipitation, hydrogen absorption, etc.

In this work, diffusion parameters for fast diffusion in Zr at low temperature were assessed for Co and Cr. An improved database for DICTRA (DIffusion-Controlled-TRAnsformation) software for fast diffusion was obtained. The diffusion parameters in grain boundaries of α -Zr for Cr and Co were used from a particular kinetic diffusion model [1]. Simulated profiles were compared with previous experimental work [2]. The results of the comparison and the adequacy of the improved database are discussed.

Diffusion profiles on grain boundaries in α -Zr for Cr and Co are presented in the temperature range of 380-460K.

Keywords: Diffusion, nuclear materials, zirconium, DICTRA.

1. INTRODUCTION

Zirconium based materials are widely used in nuclear power reactors in view of their special properties: good corrosion resistance, adequate mechanical properties and a low capture cross section for thermal neutrons. These materials are usually found in service with a high density of grain and interphase boundaries. Albeit the operating temperatures are not extremely high, these alloys undergo important changes during operation, associated with irradiation, corrosion and the movement of alloy solutes by diffusion. This is especially important with the interest in increased burn-up fuels and other measurements to keep the alloys inside the reactors for longer periods of time. Understanding the changes that can happen to these alloys in the reactor environment is, thus, of paramount importance. Several of these changes are associated with the change of position of atoms in the lattice and one of the important mechanisms for this is diffusion.

In other technological sense, the CANDU (CANada Deuterium Uranium) reactor uses hundreds of pressure tubes (Zr based alloys) to contain the fuel and coolant. These tubes are in contact with alloy steels (with Cr, Co and other possible elements) at 300°C under normal conditions. Finally a

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