Thermodynamic study of the Neptunium-Zirconium system

Bajaj, S., Garay, A., Arróyave, R., Sevik, C., Cagin, T., Turchi, P.

A. Texas AandM University, College Station, TX - 77840, United States
B. Cinvestav Queretaro, Fraccionamiento Real de Juriquilla, Libramiento Norponiente, # 2000, Santiago de Querctaro, Qro. -76230, Mexico
C. Lawrence Livermore National Laboratory, 7000 East. Avenue, Livermore, CA - 94551, United States

Abstract

In fast breeder nuclear reactors, high burn-up rates lead to fissioning of trans-uranium elements, thus Solving the problems of waste disposal and spent nuclear fuel recycling. Zr is alloyed with such metals so as to increase their melting points and suppress inter-diffusion between the nuclear fuel and cladding. In this work, we study one such metal actinide alloy fuel. Np-Zr, on which little and contrastiong prior information is available. A detailed ab-inito study, implemented with the L(S)DA+U formalism, is performed to better approximate such a localized and strongly correlated system. Also, a thermodynamie model is developed using the CALPHAD method. In this method, the Gibbs energies of all the phases that are likely to take part in equilibrium are described based on empirical models. The thermodynamic model is found to be in close proximity with experimental results.

Author keywords

Ab-inito; CALPHAD; Fast breeder; Metal actinide alloy

Indexed Keywords

Ab-inito; Calphad; Fast breeder; Fast breeders

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Bajaj, S.; Texas AandM University, College Station, TX - 77840, United States
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