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Density-functional study of U-TRU-Zr and U-TRU-Mo alloys
ALEXANDER LANDA, PER SODERLIND, PATRICE TURCHI, Lawrence Livermore National Laboratory — The U-Zr and U-Mo alloys proved to be very promising fuels for liquid metal fast breeder reactors. The optimal composition of these alloys is determined from the condition that the fuel could remain stable in the bcc phase (γ-U) in the temperature range of stability of α-U phase. In other words, both Zr and Mo play a role of "γ-stabilizers" helping to keep U in the metastable bcc phase upon cooling. In the present study we perform KKR-ASA-CPA and EMTO-CPA calculations of the ground state properties of γ-U-Zr and γ-U-Mo alloys and compare their heats of formation with CALPHAD assessments. Though the U-Zr and U-Mo alloys can be used as nuclear fuels, a fast rector operation on a closed fuel cycle will, due to the nuclear reactions, contain significant amount of TRU elements (Np, Pu, and Am). Above mentioned density-functional theory techniques are extended to study ground-state properties of the bcc-based X-Zr and X-Mo (X = Np, Pu, Am) solid solutions. We discuss how the heat of formation correlates with the charge transfer between the alloy components, and how magnetism influences the deviation from Vegard's law for the equilibrium atomic volume. This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Work at LLNL was funded by the Laboratory Directed Research and Development Program under project tracking code 12-SI-008.

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