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P3.165 Estimation of thermophysicochemical properties in uranium-hydrogen (U-H) system

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Uranium (U), which has three allotropic crystal modifications (alpha-, beta-, and gamma-U), is a strong candidate medium for storing and delivering hydrogen or hydrogen isotopes. Alpha-, beta-, and gamma-U are stable at a temperature of up to 668℃, from 668℃ to 775℃, and above 775℃, respectively. Because the temperature of the uranium hydride (UHx) formation is limited at room temperature or below 250℃, it is assumed that all uranium is in the form of alpha-U. UHx has two allotropic crystal modifications (alpha- and beta-UHx). A common beta-UHx is produced as a single phase above 200℃. In this study, thermophysicochemical properties of the uranium-hydrogen (U-H) system were estimated by introducing an alpha-phase orthorhombic A20 crystal lattice structure in uranium (alpha-U) and a beta-phase cubic beta-tungsten A15 crystal lattice structure in uranium hydride (beta-UHx) and applying the chemical mixing rules. An assumption of hydrogen intervention into the interstitial sites of the orthorhombic symmetry crystal lattice of alpha-U was used to obtain a plausible property estimation. Experimental data in rarity in U-H system were used to calculate and correlate the consistency of the thermal, physical, and chemical properties of the complex atomic structure in a unit cell. As a result, the volume expansion of the beta-UHx was greatly influenced by the hydrogen content, but showed no meaning in the thermal expansion within the engineering concept. In consideration of the heat capacity, the temperature effect from hydrogen - an interstitial heat quantity - in the beta-UHx formation was mainly the attributed factor, but not the hydrogen content.

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