Stability and Novel Ordered Phases Prediction in Unclear Fuel Materials

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First-principles calculation has been progressing significantly in recent years, its application to nuclear materials is extending to various aspects. In this talk, the highlights of study on stability of Uranium binary alloys will be introduced.

Uranium binary alloys have been widely adopted in fast nuclear reactors, but information on their stability, especially under extreme conditions of high pressure is very limited. In this study, we systematically investigated the stability of U-X (X = 3G-6G transition metal elements Sc, Ti, V, Cr, Y, Zr, Nb, Mo, Hf, Ta, W) binary systems at the ground state and under high pressure using first-principles calculations, and predicted the existence of various novel ordered phases. For each U-X system, a comprehensive structure searching for the pressure range of 0-200 GPa at several typical with compositions have been conducted. For the four stable or metastable structures which were explored, the precise electronic structure, interatomic bonding features were evaluated, as well as the dynamic stability checked by phonon spectrum, and the phase transformation property were investigated based on the formation enthalpy.

For U-Zr system, the stable phase U_2Zr and metastable phases U_3Zr and U_4Zr under pressure were discovered for the first time. It is revealed that all these phases are metallic; the ionic interactions between U and Zr and covalent interactions between adjacent U atoms were observed. Furthermore, a unique hybrid feature of first-order and second-order phase transition was discovered in U_2Nb, and its mechanics were understood by the Landau model. Furthermore, it is predicted that the U-X systems have similar stability behavior under high pressure. In particular, hybrid phase transitions have also been observed in U_2X (X=Zr, Ti, Hf). These provided rich information and new knowledge on the phase diagrams of uranium binary alloy systems.

References

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