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Thermodynamic properties of UMo alloys from first principles

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UMo alloys appear to be the most promising nuclear fuels for the conversion of highly enriched fuels that are currently used in research reactor cores, such as U_3Si_2, UAl alloys, or U_3O_8. These alloys have been selected because of their high uranium density, as well as their cubic crystal structure that guarantee isotropic swelling under irradiation. It is therefore crucial that we get some basic understanding of their thermal properties via the determination of phonon spectra and density of states. However, while a lot of work has been dedicated to the electronic structure of UMo with respect to the Mo content, there is little data related to the phonon dispersion curves.

In this work, we run ab initio molecular dynamics and we use TDEP method [1–3] and its SIFC extension [4] in order to calculate the phonon spectra of UMo alloys over the whole range of Mo concentrations. We compare the results with those of pure bcc uranium and molybdenum, as well with experimental results [5] in order to get a consistent and comprehensive picture of UMo thermodynamic properties. We show how the interplay between the addition of Mo and the temperature stabilizes the uranium bcc structure and we calculate a number of thermal properties derived from the phonon density of states, such as Gibbs free energies, phonon and electron thermal conductivities, Gruneisen parameters, expansion coefficients, {\it etc.}

Refs
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Primary authors: CASTELLANO, Aloïs (CEA – The French Alternative Energies and Atomic Energy Commission, Arpajon, France); BOUCHET, Johann (CEA – The French Alternative Energies and Atomic Energy Commission, Arpajon, France); BOTTIN, François (CEA – The French Alternative Energies and Atomic Energy Commission, Arpajon, France); DORADO, Boris (CEA – The French Alternative Energies and Atomic Energy Commission, Arpajon, France)

Presenter: CASTELLANO, Aloïs (CEA – The French Alternative Energies and Atomic Energy Commission, Arpajon, France)