QUANTUM MOLECULAR DYNAMICS STUDY OF THERMOPHYSICAL PROPERTIES OF NUCLEAR ENERGY METALS: FROM MELTING TO THE CRITICAL POINT

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We present the latest advances in modeling the thermodynamic, transport, and optical properties of metals over a temperature range from melting to the critical point using the quantum molecular dynamics method. The focus is on key metals used in nuclear energy, such as zirconium [1, 2], nickel [3], and hafnium [4]. The study investigates their thermal expansion, enthalpy, electrical resistivity, and normal spectral emissivity.

We demonstrate the calculated dependencies of density, enthalpy, isobaric and isochoric heat capacities, the Grüneisen parameter, and the speed of sound on temperature along the critical isobar for these metals. Additionally, estimates of their critical parameters, obtained from quantum molecular dynamics simulations of supercritical isotherms, are provided. The results of resistivity calculations for zirconium, hafnium, and nickel over a wide temperature range are also discussed.

The obtained results are compared with available experimental data from the literature, as well as with the latest experiments conducted using the ultrafast pulse heating of conductors by electric current method as part of a joint computational-experimental project.

Special attention is given to ab initio calculations of the normal spectral emissivity for these metals in the liquid phase along the critical isobar. These data can significantly improve the accuracy of pyrometric temperature measurements for heated liquid metals. The results are of great interest for understanding the behavior of materials under extreme conditions.

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References

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