Investigation of thermophysical properties of metals near the liquid–gas coexistence curve: Ab initio calculations and experiment

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We present our current advances in describing the thermodynamic, transport, and optical properties of metals from the vicinity of melting up to the critical point by the quantum molecular dynamics method. We focus on the analysis of thermal expansion, enthalpy, resistivity, and normal spectral emissivity. Calculated dependences of density, enthalpy, the isobaric and isochoric heat capacities, the Grüneisen parameter, and the speed of sound on temperature along the critical isobar for Zr, Mo, and Pb are going to be demonstrated. New experimental data on electrical pulse heating of zirconium wires are also presented. We note an excellent agreement between the measured enthalpy of fusion and calculated value. The results of the first-principle calculations of the resistivity for Zr and Pb in a wide temperature range will be discussed. Ab initio calculations of the normal spectral emissivity for Zr and Pb in the liquid phase along the critical isobar will be presented. This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).