Abstract Submitted
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Thermodynamic properties and phase transitions of α, γ and liquid uranium: QMD and classical MD modeling ALEXEY YANILKIN, KIRILL MIGDAL, PAVEL POKATASHKIN, OLEG SERGEEV, All-Russia Research Institute of Automatics — The application of molecular dynamics allows us to take into account the influence of thermal properties on thermodynamic properties and phase transitions. In this work different uranium phases are investigated at finite temperatures by means quantum and classical molecular dynamics. In order to verify simulations the lattice constants, elastic modulus, isotherms, Gruniesen coefficient and heat expansion are calculated for α, γ and liquid phases. The results are in good agreement with experimental data. The stability of high temperature γ phase is discussed. The diffusion coefficient is calculated for liquid phase at different densities and pressure. The boundaries of phase stability are estimated based on QMD results. Furthermore hugoniot calculated is in a good agreement with other calculations and experimental data up to 2TPa. In order to investigate phase transitions EAM interatomic potentials are derived by force-matching method. Different parameterizations are used for different part of phase diagram to improve the reproduction of QMD data. The coexistence and transition rates of two phases are investigated based on Z- and two phase methods.

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