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Electron and ion dynamics study of iron in warm dense matter regime by time-resolved XAS measurements and from first-principles T. OGITSU, A. FERNANDEZ-PAELLA, A. CORREA, Lawrence Livermore National Laboratory, K. ENGELHORN, B. BARBREL, D. G. PRENDERGAST, D. PEMMARAJU, Lawrence Berkeley National Laboratory, M. BECKWITH, D. KRAUS, S. HAMEL, Lawrence Livermore National Laboratory, B. I. CHO, L. JIN, J. WONG, GIST, P. HEINMAN, SLAC, G. W. COLLINS, Lawrence Livermore National Laboratory, R. FALCONE, Lawrence Berkeley National Laboratory, Y. PING, Lawrence Livermore National Laboratory — We present a study of the electron-phonon coupling of warm dense iron upon femtosecond laser excitation by time-resolved x-ray absorption near edge spectroscopy (XANES). The dynamics of iron in electron-ion non-equilibrium conditions was studied using ab-initio density-functional-theory (DFT) simulations combined with the Two Temperature Model (TTM) where spatial inhomogeneity of electron (and ion) temperature(s) due to short ballistic electron transport length in iron was explicitly taken into consideration. Detailed comparison between our simulation results and experiments indicates that the ion temperature dependence on specific heat and on electron-phonon coupling also plays a relevant role in modeling the relaxation dynamics of electrons and ions. These results are the first experimental evidence of the suppression of the electron-phonon coupling factor of a transition metal at electron temperatures ranging 5000-10000 K. This work was performed under DOE contract DE-AC52-07NA27344 with support from OFES Early Career program and LLNL LDRD program

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