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Simulations of nonequilibrium warm dense gold produced by ultrafast heating B. HOLST, V. RECOULES, M. TORRENT, CEA, DAM, DIF, Arpajon, France, Z. CHEN, V. SAMETOGLU, Y.Y. TSUI, University of Alberta, Canada, S.E. KIRKWOOD, University of Ottawa, Canada, M. REID, University of Northern British Columbia, Canada, S. MAZEVET, LUTH, Observatoire de Paris, France, A. NG, University of British Columbia, Canada — The interaction of femtosecond laser pulses with metals produces nonequilibrium states consisting of hot electrons and cold ions. These can last for many picoseconds before relaxing to a thermodynamic equilibrium. Recent experiments using a chirped pulse probe technique provided AC conductivity data of gold at a sufficient time resolution to observe this relaxation process. We developed an ab-initio model that characterizes thermodynamic properties of warm dense matter states in nonequilibrium. Our theoretical scheme combines a standard two temperature model with temperature dependent material parameters and an energy transfer rate that are obtained by means of ab-initio simulations. This enables us to give a prediction for the temperature evolution during the relaxation process. Additionally, we derive the AC conductivity of the nonequilibrium states from our simulations using the Kubo-Greenwood formula. It is used to test our model against measurements. We observe agreement with experiment using an energy relaxation rate, that is smaller than predicted, giving us reason to revisit its determination. We can furthermore provide thermodynamical and structural data of nonequilibrium warm dense gold which are not accessible in experiment.

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