Band Occupation and Optical Response of Gold far from Equilibrium

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The excitation of metals with short-pulse lasers is an often applied method to create warm dense matter states. Here, the large energy input drives the electronic system far out of equilibrium. The subsequent relaxation processes reveal many properties of the system but also strongly influence the outcome of any measurement within the relaxation time. In particular, the optical response depends strongly on the occupation of electronic states within the bands, the number of electrons per band as well as the response of the ionic lattice/ion fluid.

Here, we investigate the behaviour of gold after excitation with very short pulses of visible and VUV light that promote additional electrons into the sp-band. Within the first few 100 femtoseconds, we can assume a stable lattice and thus keep the known band structure in our calculations. First we demonstrate that the number of electrons per band is sufficient to describe probing in the optical limit (k->0). Then we present a system of rate equations that describes this band occupation. For excitations with optical lasers, only d-electrons can be promoted into the sp-band and a two-band model is sufficient. With VUV light like from the FLASH laser at DESY, f-electrons can also be excited and we need a three-band model to describe the band occupation. We show similarities and differences of the two excitation methods. Based on these predictions for the band occupation, we are able to calculate the optical properties, like the reflectivity, of the probe and make predictions of their expected behaviour for time-resolved measurements.