European XFEL Joint Theory Seminar

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XSPIN: a hybrid tool for description of X-ray induced demagnetization

We investigated the role of electronic excitation, relaxation and transport processes in X-ray induced ultrafast demagnetization of magnetic multilayer systems. We report on the results obtained with the newly developed modeling tool, XSPIN, which enables nanoscopic description of electronic processes occurring in X-ray irradiated ferromagnetic materials [1,2]. With this tool, we have studied the specific response of cobalt/platinum (Co/Pt) multilayer system irradiated by an ultrafast XUV pulse at the M-edge of Co (photon energy around 60 eV) [1]. It was previously studied experimentally at the FERMI free-electron-laser facility, using the magnetic small-angle X-ray scattering technique (mSAXS) [1]. The XSPIN simulations show that the magnetic scattering signal from cobalt decreases on the femtosecond timescales considered due to electronic excitation, relaxation and transport processes both in the cobalt and in the platinum layers. The signal decrease scales with the increasing fluence of incoming radiation, following the trend observed in the experimental data. Similar observations [2] were also made for the demagnetization data from magnetic multilayer systems recorded at the L-edge of Co (Co/Pd multilayer system, photon energy about 778 eV), which are also briefly discussed here. Moreover, the results for bulk nickel, which has a higher Curie temperature than Co are presented and contrasted with those for Co. Confirmation of the predominant role of electronic processes for X-ray induced demagnetization in the regime below the structural damage threshold, achieved with our theoretical study, is a step towards quantitative control and manipulation of X-ray induced magnetic processes on femtosecond timescales. Further development of the simulation tool should take into account eventual structural changes of the irradiated materials (if irradiating with high-fluence X-ray pulses) [4] as well as the energy exchange between electronic system and lattice through electron-phonon coupling [5].

[1] K. J. Kapcia, V. Tkachenko, F. Capotondi, A. Lichtenstein, S. Molodtsov, L. Mueller, A. Philippi-Kobs, P. Piekarz, B. Ziaja, npj Computational Materials 8, 212 (2022). [2] K. J. Kapcia, V. Tkachenko, F. Capotondi, A. Lichtenstein, S. Molodtsov, L. Mueller, A. Philippi-Kobs, P. Piekarz, B. Ziaja, Physical Review B 107, 094402 (2023). [3] K. J. Kapcia, V. Tkachenko, F. Capotondi, A. Lichtenstein, S. Molodtsov, P. Piekarz, B. Ziaja, arXiv:2307.04671 [cond-mat.mtrl-sci]. [4] V. Lipp, V. Tkachenko, M. Stransky, B. Aradi, T. Frauenheim, B. Ziaja, Sci. Rep. 12, 1551 (2022). [5] N. Medvedev, V. Tkachenko, V. Lipp, Z. Li, and B. Ziaja, 4open 1, 3 (2018).

Hosts: Beata Ziaja-Motyka and Nils Brouwer

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