Electronic Scattering Dynamics and Ultrafast Magnetization Dynamics

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Abstract: A dynamical model for Elliott-Yafet type scattering of carriers and its importance for the demagnetization dynamics after ultrafast optical excitation is reviewed. It is pointed out that the demagnetization in 3d ferromagnets as well as recent experimental results on "novel" materials are still in need of a microscopic explanation.

Introduction

Ultrafast demagnetization dynamics in itinerant ferromagnets has been well established, and explained phenomenologically on the basis of a three-temperature model. More recently, demagnetization has been observed in half-metallic ferromagnets, and there is an enormous current interest in the optically induced magnetization dynamics of systems with different sublattices and magnetic alloys.

There are a number of different theoretical ideas as well as specific models that are contenders for such a microscopic explanation. Different approaches typically treat one aspect of the problem particularly well: coherent dynamics during during the exitation pulse, elementary magnetic excitations, spin-flip scattering transitions, and transport [1-5].

In the following, we will concentrate on the dynamical description of spin-flip scattering transitions, i.e., the dynamical Elliott-Yafet mechanism [3,4]. A treatment beased on dynamical distribution functions is valid even at ultrashort timescales and away from quasi-equilibrium. In the Elliott-Yafet mechanism, the spin expectation value of the carriers is changed by scattering transitions due to a spin-diagonal interaction mechanism, such as the carrier-carrier Coulomb or the carrier-phonon interaction. The spin-orbit coupling is responsible for the spin-mixed character of the single-particle states, which act as the initial and final states for scattering transitions. Here, we focus on carrier dynamics in Heusler alloys.

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Dynamical carrier scattering in Heusler compounds

A dynamical model for the numerical calculation of the band and momentum resolved distribution carrier distribution functions $f_s(\vec{k}, t)$ has been described in Ref. [2] and applied to half-metallic Heusler compounds of the $Co_2Mn_{1-x}Fe_xSi$ material system [6]. The model describes carrier-carrier Coulomb scattering at the level of Boltzmann scattering integrals, includes a simplified spherically symmetric band structure and a constant spin-mixing parameter. It is therefore well suited to compare the influence of different band structures on the spin-dependent carrier scattering after ultrafast excitation. In Ref. [6], it was found that a fast demagnetization is possible by spin-flip transitions after optical excitation, but these transitions follow different scattering pathways for Co_2FeSi (CFS) and Co_2MnSi (CMS) because of the different line-ups of the minority band-gap with the Fermi energy. In particular, it was found that hole scattering dynamics plays an important role, which makes the line-up of the minority band less important a difference between the two compounds than one would anticipate.

For Heusler alloys, sample quality may be an issue, and the interpretation of magneto-optical measurements of the magnetization dynamics is made more complicated by the possible existence of defects [7]. Müller et al. [7] discussed the fast magnetization dynamics in the case of CMS with regard to possible Co antisite defect states (DO3-disorder, Co on Mn positions) close to the Fermi level. These defect states were predicted for CMS by ab-initio calculations [8].

Here we analyze the influence of defects on the magnetization dynamics in CMS in the framework of our dynamical calculation of carrier distribution functions. To this end, we introduce in the calculation the presence of defects by adding a defect band with a flat dispersion 150 meV below the Fermi energy, similar to Ref. [9].

Figure 1 (left panel) shows the magnetization dynamics for CMS without defects, as well as two different defect concentrations. The case of 100% Co antisites is only presented to elucidate trends of the model because at this defect concentration the overall band structure should be changed considerably. For both cases with defects we obtain a more pronounced quenching and a faster demagnetization by up to a factor of two. The reason for this change in dynamics can be traced back to the minority band line-up in the right panel of Fig. 2. The dynamical calculations show an increase of occupation of the minority band 5 by about 1/3 in the band structure with defects compared to the defect-free case after optical excitation. The excited carriers subsequently flip their spin and contribute to the demagnetization. This increase of occupation in band 5 can be explained only if the defect band serves as an intermediate state for two-photon pumping into the minority band 5 from lower lying minority bands. A few such multi-photon pathways are added as green arrows in Fig. 1.

The present model calculation shows that already a small concentration of impurities may increase the quenching and speed up the demagnetization dynamics

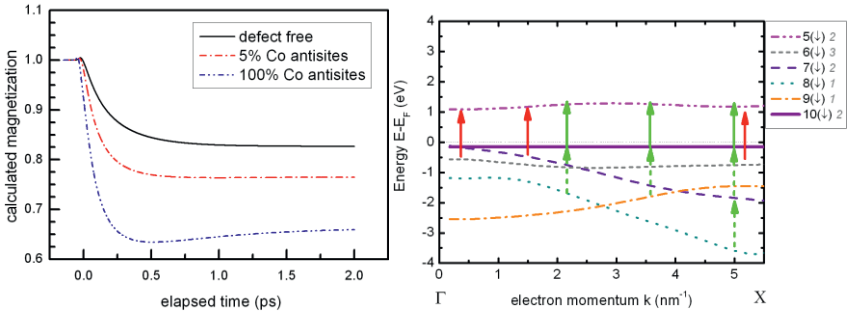

Fig. 1. Computed demagnetization dynamics for the Heusler compound (left) and dispersion of selected bands including transitions driven by the optical excitation. The vertical band (solid line) close to zero energy is the defect band, single (red) arrows indicate minority-spin transitions without defects, multiple stacked (green) arrows indicate new transitions due to the defect band.

due to a higher number of minority carrier states below the Fermi energy, if the impurities form a continuous band close to an unoccupied band above the Fermi level.

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