Magneto-optical spectra of Mn-Ge films

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Abstract. Experimental magneto-optical Kerr effect spectra of Mn-implanted Ge samples are interpreted using an ab-initio theoretical model based on density functional theory. The presence of Mn in the Ge matrix is accounted for considering either Mn precipitation as Mn₅Ge₃ nanoparticles or as perfect dilution. The Mn concentration profile in the sample is also considered in the theoretical model. The computational results are in good qualitative agreement if Mn₅Ge₃ nanocluster formation is assumed. The effect of partial etching of the implanted region is also studied by comparing our experimental and theoretical MOKE spectra data.

1. Introduction
The realization of alloys possessing both semiconductive and magnetic characteristics constitutes one of the most promising research lines in the field of spintronics. Magnetic properties can be achieved in zinc-blende structure semiconductors, conventionally used in microelectronics and optoelectronics, through incorporation of transition metal (TM) impurities in a diluted phase. These materials, referred to as diluted magnetic semiconductors (DMS), with the optimal content of dopant atoms might yield spin-polarized currents. The study of magneto-optical (MO) Kerr effect (MOKE), i.e., the change of polarization experienced by light when reflected by a magnetic sample, gives a deep understanding of the optical and magnetic properties involving electronic transitions in the metallic spin-polarized energy bands, paving the way to novel MO reading/recording devices. We recall that linearly polarized light, incoming on a magnetic surface, becomes elliptically polarized upon reflection: the resulting ellipse has its major axis rotated by an angle θₖ (the Kerr rotation angle) with respect to the initial linear polarization direction.

The aim of this paper is to interpret the experimental MOKE spectra of a Mn-implanted Ge sample in different conditions (namely, (I) as-implanted, and (II) eroded) and to show that morphological/structural information can be obtained via theoretical approaches based on spin density functional theory (SDFT).
2. Technical details

A Ge (100) wafer was implanted at room temperature with 100 keV Mn$^+$ ions with a dose of $4 \times 10^{16}$ ions/cm$^2$. This sample is $\sim 150$ nm thick and the Mn-ion concentration profile, measured by X-ray photoemission spectroscopy (XPS), has a pseudo-gaussian trend with the peak centered at $\sim 60$ nm (see the inset of Fig.1 (a)) with an average Mn volume concentration equal to $\sim 7\%$. The substrate temperature was kept at 300°C during implantation to avoid amorphization. Furthermore, we expect precipitation of Mn-rich nanoclusters, typically Mn$_5$Ge$_3$. In fact, as X-ray diffraction (XRD) patterns and transmission electron microscopy (STM) show, there are nanospheres of the Mn$_5$Ge$_3$ phase dispersed in the matrix and preferentially aligned with their [0001] axis perpendicular to the Ge (100) surface.

Theoretical calculations have been performed with the highly precise all-electron full-potential linearized augmented plane wave (FLAPW) method, within the local spin density approximation (LSDA) to calculate the conductivity tensor $\sigma$ of pure Mn$_5$Ge$_3$ and dilute Mn$_x$Ge$_{1-x}$ (details of the calculations are given elsewhere). Using the Zak formalism to treat multilayered structures, and the effective medium approximation (EMA), we show that the nanoscopic structure of the samples can be taken into account in the calculations obtaining spectra which can be directly compared with experiments (more detail on this procedure has been reported in Ref. [15]). In this way, we can take into account the experimental XPS Mn-concentration profiles and approximate the sample as a sequence of layers, each containing the correct proportion of Mn atoms (assumed as Mn$_5$Ge$_3$ clusters), as extracted from XPS measurement. As a result, the system appears as continuous and homogeneous to the radiation. To obtain the continuum limit, it is necessary to make the thickness of the layers considered in the simulations much smaller than the wavelength used to probe the sample. As a result, the system appears as continuous and homogeneous to the radiation. To obtain the continuum limit, it is necessary to make the thickness of the layers considered in the simulations much smaller than the radiation wavelength; typically the MOKE spectrum converges to this limit with the number of such layers larger than 30.

3. Results

The results obtained are shown in Fig.1 where both cases considered, (I) and (II), are reported. In Fig.1 (a) we show the experimental measurements compared with the theoretical curve obtained for polar geometry at 45° incidence, considering the XPS sample thickness (150 nm). As experimental MOKE rotation angles, we considered the saturation values extrapolated from the hysteresis loop at each wavelength at 12 K. As we can see from Fig.1 (a), the spectrum shows features very similar to experiments, although differing in intensity: this is due presumably to a part of Mn that does not form clusters and is present in an amorphous phase, not contributing to the overall magnetization. Experiments show that only 85% of Mn atoms are in crystalline Mn$_5$Ge$_3$ form while the remaining 15% is in the amorphous phase. Moreover, other contributions such as surface and temperature effects may hinder the magnetic response with respect to the ideal zero temperature calculated system. The calculation well reproduces the overall energy dependence of the spectrum except for a rigid energy shift. Now, let us consider the presence of a Mn$_x$Ge$_{1-x}$ diluted phase and calculate the conductivity tensor at different Mn-concentrations: 6.25%, 8.33% and 12.5%. Then, the sample is simulated as a sequence of layers, whose thickness is adjusted to keep the Mn average concentration constant as given by the XPS profile. The calculated MOKE spectra is compared with experiment in Fig.1 (b). The most striking difference with experiment is the much larger Kerr rotation predicted by theory (on order of magnitude difference) whereas the shape features of the theoretical curve are related to the step-like Mn-concentration profile assumed. Comparing the two simulations, Mn$_5$Ge$_3$ clusters and dilute Mn$_x$Ge$_{1-x}$, we argue that
Figure 1. Experimental (open circles) and theoretical (solid line) polar MOKE spectra. Comparison for the as-implanted sample considering Mn₅Ge₃ clusters (panel (a)) and dilute MnₓGe₁₋ₓ (panel (b)). Panel (c) shows the same comparison for the eroded sample. The inset of panel (a) shows the Mn concentration profile measured by XPS for the as-implanted sample; the vertical dashed line indicates the depth eroded from the sample shown in (c).

the main contribution to the observed Kerr rotation comes from the Mn₅Ge₃ clusters.

Fig. (c) shows the MOKE spectrum as measured after the first 106 nm at the surface were removed upon sputtering the sample with Ar-atoms (as shown in the inset of Fig. (a) - vertical dashed line). Accordingly, the theoretical spectrum was calculated using this same Mn-concentration profile thus dropping the topmost 106 nm surface layer and considering once again Mn₅Ge₃ clusters. The resulting spectrum is very different from the previous one (compare Fig. (a) and (c)). Our calculation within EMA reproduces the sign and the overall trend of the measured spectrum correctly, except for the amplitude. This difference can be ascribed to the damages suffered by the surface upon sputtering and consequent deterioration of the structure of both the Mn₅Ge₃ clusters and the Ge matrix.

In conclusion, we studied the MOKE spectra of Mn-implanted Ge films comparing experimental data and theoretical simulations. The computational results, assuming spherical Mn₅Ge₃ nanoclusters formation, are all in a good qualitative agreement, predicting the correct sign of the Kerr rotation and its order of magnitude. The theoretical predictions have been
successfully tested on Mn-implanted samples subject to different treatments and resulting on different doping profiles. Further studies are presently in progress to improve the simulation model.

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