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Temperature dependent magnetic properties of the GaAs substrate of spin-LEDs

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Abstract
The temperature dependence of the magnetization of a light emitting diode having a ferromagnetic contact (spin-LED) is measured from 2 to 300 K in magnetic fields from 30 to 70 kOe and it is found that it originates from the GaAs substrate. The magnetization of GaAs comprises a van Vleck-type paramagnetic contribution to the susceptibility which scales inversely with the band gap of the semiconductor. Thus, the temperature dependence of the band gap of GaAs accounts for the non-linear temperature dependent magnetic susceptibility of GaAs and thus, at large magnetic fields, for the spin-LED.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

A formidable challenge in solid state physics is the injection and detection of electron spin in useful semiconducting devices, a field commonly referred to today as spintronics [1]. Among others, one possible approach to detecting spin injection is measuring the polarization of the injected carriers optically via the circular polarization of light emitted from a quantum well within the semiconductor. This structure is often referred to as a spin-LED [2]. Small values of spin injection at room temperature have been detected with such a device having injectors formed from Fe layers and a naturally formed Schottky barrier [3]. Similar results were found for MnAs [4], Fe_3Si [5] and Co_2MnGe [6] injectors. Significantly higher spin injection efficiencies have been found by replacing the Schottky barrier with an oxide tunnel barrier [7] with values as high as 30% at room temperature [8]. Further, the spin polarization depends non-monotonically on the temperature [8, 9]. These effects are a complex superposition of spin relaxation and recombination time effects. One common configuration for spin-LED experiments is to optically detect the degree of electron spin polarization by measuring the degree of circular polarization of the light emitted along the growth direction of the

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quantum well. For this reason measurements on spin-LEDs are often performed in large magnetic fields typically of the order of 20 kOe or above; e.g. [8, 9]. A alternative for circumventing large external magnetic fields is using the oblique Hanle effect [10]. At large external magnetic fields the GaAs substrate gives rise to a large net diamagnetic background in the magnetization measurements which has to be subtracted if one wants to compare the magnetization data with the degree of circular polarization of the emitted light. However, also in the optical data a clear magnetic background at high fields is visible [8, 9] and even for an LED structure with a nonmagnetic Pt electrode the circular polarization of the emitted light at high fields is about 1% [8]. There are three different stages where the external magnetic field may polarize the originally unpolarized electrons: (i) a spin dependent tunnelling probability may be caused by the magnetic field, (ii) the electrons may be polarized while travelling through the drift region or (iii) the electrons may be polarized inside the quantum well before they recombine. Effects (ii) and (iii) are comparable and would require that the semiconductor itself has a net paramagnetic response at least from the electronic states contributing to the transport properties. The observed non-monotonic temperature dependence of the polarization of the spin-LED may be affected by the temperature dependent magnetic properties of GaAs as well. However, since the temperature dependence of the spin polarization of the GaAs-based spin-LED also includes the spin relaxation and recombination time effects [8, 9], there is no one-to-one correlation between the two phenomena.

Here we present detailed temperature dependent magnetization measurements performed on a spin-LED which are compared to the bare GaAs substrate results. It is found that the temperature dependence of the magnetization of the spin-LED at high fields is dominated by the signal from the substrate. In addition to a temperature independent diamagnetic susceptibility, a smaller, but temperature dependent, net paramagnetic contribution exists. This contribution is dominated by a van Vleck-type paramagnetism which is governed by the temperature dependence of the band gap of the semiconductor. We demonstrate that the magnetic susceptibility χ does indeed follow the temperature dependence of the band gap over the entire temperature range from 2 to 300 K. Furthermore this temperature dependence increases significantly if the doping level of the GaAs is increased.

2. Experimental details

The experiments were carried out using a spin-LED formed from a CoFe ferromagnetic electrode separated by a MgO tunnel barrier from a single $GaAs/Al_{0.08}Ga_{0.92}As$ quantum well grown on a p-doped GaAs(001) wafer (Be doping of the order of 1 to 2×10^{17} cm^{-3}). The measurements were performed in magnetic fields up to 70 kOe and at temperatures from 2 to 300 K using a superconducting quantum interference device (SQUID) magnetometer. The magnetic field was applied both in and out of the sample plane. For comparison, n-doped GaAs(001), nominally undoped GaAs(001), n-doped Si(001) and sapphire (Al_2O_3(0001)) wafer pieces were investigated under the same conditions.

For all SQUID measurements of the GaAs wafer pieces great care was taken to reduce the background signal of the sample holder (typically a clear drinking straw) to a minimum. For all in-plane and out-of-plane measurements the wafer pieces were cut to such a size that they could be held inside the straw by clamping it without any further means of holding the sample in place (typically another piece of straw or a small cotton ball). Furthermore, we confirmed that the small depressions in the straw due to the sample edges do not give rise to any significant magnetic background by measuring an already used but emptied sample holder. To determine the volume of the sample its weight was measured and the literature value of the density of GaAs was taken ($\rho_{GaAs} = 5.32$ g cm^{-3} at 300 K) to derive the volume of the sample. This

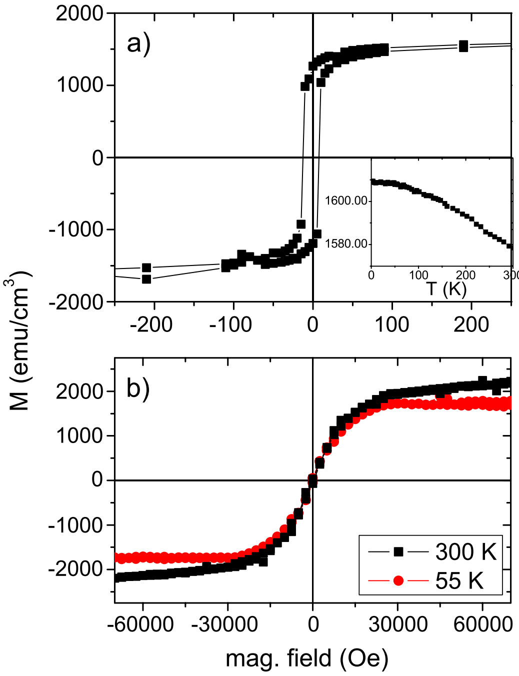

Figure 1. (a) Magnetic hysteresis of the spin-LED recorded in the film plane. The inset shows the temperature dependence of the magnetization at 1500 Oe. (b) Hysteresis measured out of the film plane at two different temperatures. The diamagnetic background was derived from the 55 K data and subtracted from both data sets.

procedure gives rise to the largest error (typically 3% depending on the size of the sample) for all χ values measured for GaAs. Although the absolute value of χ cannot be accurately determined for this reason its relative change with temperature can be determined with much higher precision.

3. Results and discussion

Figure 1(a) shows a magnetic hysteresis loop recorded in the film plane of the spin-LED on p-doped GaAs(001) at 300 K. Since the field is applied along the easy magnetization direction of the CoFe electrode (in this case ∼35 Å thick), the magnetization saturates at low fields around 150 Oe. The inset shows the temperature dependence of the magnetization measured in an applied magnetic field of 1.5 kOe ensuring magnetic saturation of the CoFe film. The magnetization smoothly decreases with temperature since the magnetic behaviour is dominated by the CoFe electrode at low fields. However, if the same sample is measured out of the plane, i.e. along its magnetic hard axis, a field of ∼25 kOe is necessary to fully rotate the magnetization of the CoFe out of the plane which is consistent with the shape anisotropy of the CoFe film having a magnetization of about 1550 emu cm^{-3}. If the sample is measured in such high magnetic fields the contribution of the substrate has to be subtracted to determine the magnetization of the CoFe film. Figure 1(b) shows two hysteresis loops measured at 55 and 300 K respectively. The diamagnetic contribution from the substrate was determined from the slope of the measured magnetization from 30 to 70 kOe at 55 K. In this field regime the magnetization of the CoFe film is independent of the magnetic field. The same diamagnetic background was subtracted from both data sets. Surprisingly, the hysteresis at 300 K is not

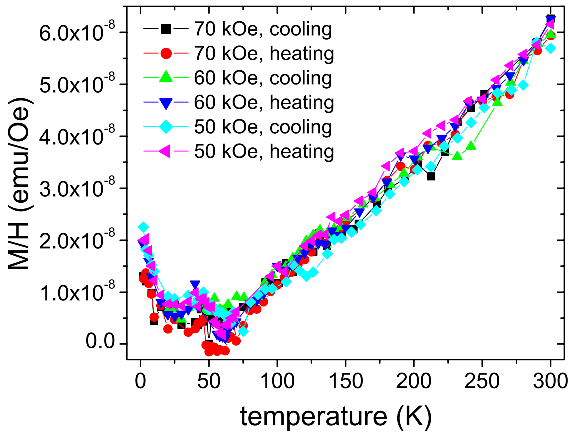

Figure 2. Temperature dependent measurements of the spin-LED structure. The magnetization of the complete stack was measured at magnetic fields of 50, 60 and 70 kOe while ramping the temperature up and down. By dividing the magnetization by the applied magnetic field a value proportional to the susceptibility was derived. The maximum diamagnetic signal at 55 K was subtracted, to focus on the temperature dependent part.

flat at high fields when the diamagnetic background of the 55 K data is subtracted, but shows an additional, net paramagnetic contribution. Only subtracting different background signals for the measurements at different temperatures reveals a flat hysteresis which is expected for CoFe films. This is a first indication that χ for the GaAs substrate changes with temperature, which may explain the magnetic background at high fields in the electroluminescence (EL) data in [3–8].

The temperature dependence of the net diamagnetic background can be derived from the magnetization measurements shown in figure 2. The spin-LED structure was measured at magnetic fields of 50, 60 and 70 kOe from 2 to 300 K while cooling and heating. The magnetization of the ferromagnetic electrode is assumed to be independent of the applied magnetic field. Its contribution was subtracted from the measured magnetization prior to dividing the data by the applied magnetic field. Since the resulting curves for the three magnetic fields are identical within the accuracy of the SQUID measurement this rules out field dependent effects and justifies the assumption of a field independent magnetization of the CoFe electrode. Note that the largest diamagnetic signal, which is measured around 55 K, is also subtracted from the data and thus they are proportional to the temperature dependent contribution to χ of GaAs. Furthermore, figure 2 displays the data in emu Oe^{-1}, thereby providing a quantity which is only proportional to χ. A net paramagnetic signal is obvious in figure 2 which increases with temperature between 55 and 300 K and at lower temperatures as well. The low temperature paramagnetic contribution is due to the sample processing and will be discussed in greater detail elsewhere [11] and we focus on the paramagnetic contribution between 55 and 300 K.

To confirm that the temperature dependent background of the spin-LED originates from the GaAs substrate we performed similar temperature dependent measurements from 50 to 70 kOe on various pieces of p- and n-doped GaAs(001) wafers. For the latter substrates the Si dopant level was typically of the order of 1 to 2 $\times$ 10^{17} cm^{-3}; for the p-type wafers used as substrates for the spin-LEDs the dopant was typically Be of comparable concentration. For comparison, measurements on nominally undoped GaAs(001), Si(001) and sapphire wafers were also made under the same conditions. Whereas sapphire shows a temperature independent

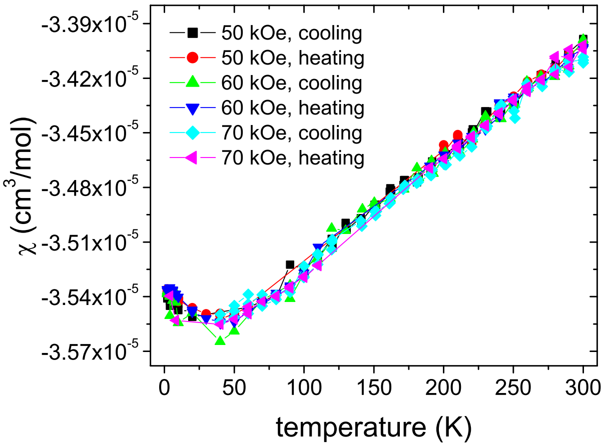

Figure 3. Measured χ for n-type GaAs(001) which was used as the substrate for the spin-LED. The magnetization was recorded at three different magnetic fields from 50 to 70 kOe while ramping the temperature up and down. χ was derived by dividing the magnetization by the applied magnetic field.

diamagnetic signal from 2 to 300 K within the accuracy of the SQUID magnetometer (not shown), Si and GaAs show a temperature dependent magnetization. The observed variation of the magnetization with temperature between 55 and 300 K is qualitatively the same for Si and GaAs but less pronounced (a factor of 2–3 smaller) for Si. Since in the case of Si this is close to the sensitivity limit of the SQUID magnetometer, we will discuss only the GaAs in the following.

Figure 3 shows the data collected on n-doped GaAs(001) measured at magnetic fields between 50 and 70 kOe between 2 and 300 K. The measured magnetization has been divided by the respective applied magnetic field revealing χ. Note that in figure 2 we show the molar χ for easy comparison with the widely used literature value of $(-3.33 \pm 0.10) \times 10^{-5}$ cm^3 mol^{-1} from [12] which corresponds to $(-1.22 \pm 0.04) \times 10^{-6}$ emu cm^{-3} Oe^{-1}. For the n-doped GaAs(001) our measurement reveals $(-3.39 \pm 0.02) \times 10^{-5}$ cm^3 mol^{-1} at 300 K which is in good agreement with the literature. However, at 55 K we measure a susceptibility of $(-3.55 \pm 0.02) \times 10^{-5}$ cm^3 mol^{-1}. The temperature dependence of χ which can be calculated by linear interpolation between these two values is $(6 \pm 2) \times 10^{-9}$ cm^3 mol^{-1} K^{-1} which is significantly larger than the value of 1.2×10^{-9} cm^3 mol^{-1} K^{-1} reported in [12]. Various other n-doped GaAs(001) wafer pieces were measured applying the magnetic field in the sample plane along the edge of the sample ({110} directions) and across the in-plane diagonal as well as perpendicular to the plane ({100} directions). We found no significant dependence on the crystallographic direction as expected. However, χ measured at 300 K varied between -3.3 and -3.5×10^{-5} cm^3 mol^{-1}, which is, within the uncertainty of our measurement, consistent with the literature value. We attribute these discrepancies to uncertainties in the determination of the mass and thus the volume of the sample, and to the different filling factors of the SQUID for various orientations of the sample. The variation of χ with temperature ranged between 4 and 6×10^{-9} cm^3 mol^{-1} K^{-1} and is therefore significantly and systematically higher than the value reported in the literature [12].

The temperature dependent magnetic background is qualitatively the same for the n-doped GaAs(001) wafer and the spin-LED having the p-doped GaAs(001) substrate shown in figure 2(b). Assuming that the quantum well makes a negligible contribution to the magnetic signal due to its small volume, this also holds on a quantitative basis. Also the ferromagnetic CoFe electrode is fully saturated in the high magnetic fields applied for the above measurements and therefore only gives rise to a field independent offset, which can be subtracted. With these assumptions we can determine a temperature dependence of χ of about $5(2) \times 10^{-9}$ cm^3 mol^{-1} K^{-1} for the p-doped GaAs(001) of the spin-LED which compares well with the value for the n-doped GaAs(001) wafer discussed above and is significantly higher that for the undoped GaAs. Thus, the temperature dependent magnetic background of the spin-LED as shown in figure 2 can be fully ascribed to the temperature dependent χ of the doped GaAs substrate (irrespective of the doping type). In the following we will try to get a quantitative estimate of the full temperature dependence of χ of GaAs in the entire temperature range from 2 to 300 K.

Within the tight binding approach, χ for a tetrahedral semiconductor with covalent bonding such as GaAs is the sum of three contributions: two diamagnetic contributions which originate from the valence (χ_L) and the core (χ_c) electrons and one van Vleck-type paramagnetic contribution (χ_p) due to the valence electrons [12, 13]. χ_L is essentially temperature independent except for a small effect due to the change in the number of atoms (or chemical bonds) per unit volume. This leads to a small change in the electron density N and thus it scales with α^3, where α is the linear thermal expansion coefficient. χ_L is analogous to χ_c involving bond states b_i and the electron density [13]:

$$\chi_L = \frac{-Ne^2}{3mc^2}\langle b_i|(r-r_i)^2|b_i\rangle \tag{1}$$

where N denotes the electron density. Due to its dependence on $(r-r_i)^2$ (in essence the spatial extent of the bond) and N, χ_L scales linearly with α, i.e. the diamagnetic contribution from the valence states increases with increasing temperature. However, since α is of the order of 10^{-6} K^{-1}, the temperature dependences of the diamagnetic contributions should both be very small; cf [12].

The van Vleck-type paramagnetic term χ_p is determined by the energy separation of bonding and anti-bonding states $E_a - E_b$ [13]:

$$\chi_p = \frac{Ne^2}{2m^2c^2(E_a - E_b)}\sum_j \langle a_j|l_{zi}|b_i\rangle^2 \tag{2}$$

where l_{zi} is the angular momentum operator. The leading temperature dependent quantity here is the energy separation $E_a - E_b$. Its temperature dependence is proportional to the temperature dependence of the band gap E_g which is of the order of 10^{-4} K^{-1}, suggesting that the overall temperature dependence of χ should be dominated by the paramagnetic contribution χ_p. A simplified version of (2) was suggested [12] which is useful for fitting our experimental results:

$$\chi_p = \frac{B}{\beta E_g} \tag{3}$$

where β is a proportionality factor of the order of unity and B is proportional to an average of the matrix elements in (2), which was experimentally determined to be 1.6×10^{-4} eV cm^3 mol^{-1} for GaAs [12]. Note that in [12] the temperature dependence of E_g was assumed to be linear and was estimated from the temperature dependence of the dielectric function ϵ. Using a more rigorous calculation based on (2) it was demonstrated that the polarity or ionicity of the chemical bond enters explicitly, providing an explanation for the observed material dependence of B [13].

More recent theoretical work used a Bloch representation and a finite temperature Green's function formalism to calculate the contributions to χ [14]. An all-electron calculation based on the linear density approximation was also carried out to calculate χ [15]. Reasonable agreement between theory and the experimental results could be achieved; however, we will use the more instructive tight binding approach since the inverse proportionality of χ_p with E_g remains the same in essence for all theories in question. This provides an intuitive explanation (neglecting the material dependence of B) as to why the measured temperature dependence of χ is much weaker for Si, which has a larger gap (3.4 eV) at the Γ point than GaAs (1.4 eV), and is irrelevant for sapphire (E_g of 9.9 eV).

To calculate the temperature dependence of χ of GaAs we refer to the experimental results of [12]. We extend the old work by using the respective explicit experimental findings for the linear thermal expansion coefficient α and the band gap E_g to determine the full temperature dependence of χ from 2 to 300 K. The temperature dependence of E_g between 60 and 5 K was recently determined with high precision [16]. In this temperature regime electron–phonon interactions play a dominant role. Earlier measurements of E_g covering the wider temperature range from 300 to 2 K reveal virtually the same temperature dependence [17]. These experimental data could be fitted with a semi-empirical model based on a Bose–Einstein statistical factor for phonon emission and absorption [18]:

$$E_g(T) = E_B - a_B\left(1 + \frac{2}{\exp(\Theta/T) - 1}\right) \tag{4}$$

where E_B and a_B are constants ($E_g(T = 0) = E_B - a_B$) and Θ is an average phonon frequency. Varshni's commonly used equation [19] slightly deviates from (4) at lower temperatures. We took (4) together with the experimental results measured in [17] ($E_B = 1562$ meV, $a_B = 43.3$ meV and $\Theta = 202$ K) since the experimental data are available for the entire temperature region in question. Figure 4(a) shows the resulting temperature dependence of the band gap of GaAs. The linear expansion coefficient α determines the temperature dependence of the diamagnetic contribution originating from the valence electrons. α for GaAs between 300 and 25 K shows a change in sign around 50 K [20]. Two more detailed investigations were performed later by [21] and [22]. A compilation of relevant results can be found in [23]. It is found that α goes to zero at three temperatures: 0, 12 and 56 K. To account for the two different temperature regimes measured by [20] and [21, 22], respectively, we fit a ninth order polynomial to the experimental data which is depicted in figure 4(b).

Combining the temperature dependences of E_g and α with the experimental findings from [12], i.e. the values for B, χ_L and χ_p, one can calculate the expected temperature dependence of χ shown in figure 5(a). First of all it is obvious that the overall temperature dependence is dominated by χ_p. The temperature dependence of χ_L would be of opposite sign but, as already pointed out, its temperature dependence is much weaker. Indeed, virtually the same temperature dependence as in figure 5(a) can be calculated if one neglects $\chi_L(T)$ due to the variation of α (not shown). The temperature dependence of χ of 1.8×10^{-9} cm^3 mol^{-1} K^{-1} between 55 and 300 K is slightly larger that the respective experimental value of 1.2×10^{-9} cm^3 mol^{-1} K^{-1} from [12]. This may be due to the fact that we use a different $E_g(T)$ than in [12] where the respective temperature dependence of the dielectric function ϵ was taken. Moreover, the temperature interval of the measurement is not specified in [12]. Thus the fitting parameter B in (3) could not be properly corrected. Nevertheless the measured temperature dependence of χ of undoped GaAs is in excellent agreement with the theoretical expectation over the entire temperature range from 2 to 300 K.

Figure 5(b) shows measurements on nominally undoped GaAs(001) wafer pieces. Similar to the measurements on the doped samples, the data shown in figure 5(b) are representative for a number of pieces measured along different crystallographic directions. The value of χ measured at 300 K varies between -3.22 and -3.45×10^{-5} cm^3 mol^{-1} and thus agrees with the literature value. The temperature dependence of χ between around 55 and 300 K for all

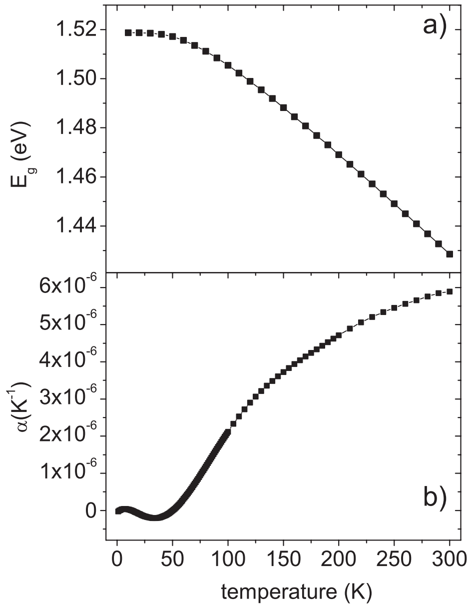

Figure 4. (a) Temperature dependence of the direct band gap of GaAs using equation (4) of [18] together with the experimental results of [17]. (b) Linear thermal expansion coefficient α according to [20]. The anomalous behaviour below 50 K was taken from [21] and [22]. The experimental data were fitted with a polynomial of ninth order.

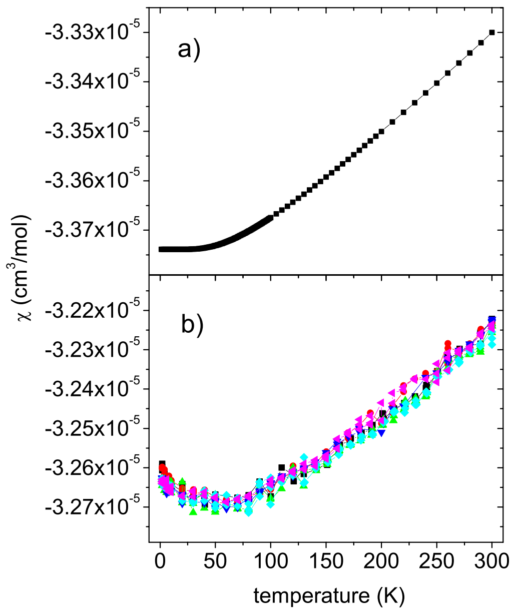

Figure 5. (a) Expected temperature dependence of χ according to our calculation (see the text). (b) Measured χ of nominally undoped GaAs(001) at external magnetic fields from 50 to 70 kOe.

measured samples is about $(1.8 \pm 2) \times 10^{-9}$ cm^3 mol^{-1} K^{-1} which is slightly higher than the value reported in the literature but significantly lower than for the n-doped GaAs(001) and the spin-LED p-doped GaAs(001) substrate. Since the temperature dependence of χ for the doped GaAs(001) is found to be about a factor of 2 to 3 larger, we conclude that the dopant must be held responsible for this discrepancy. A different intrinsic dopant concentration may also account for the discrepancy between the nominally undoped GaAs(001) wafer used here and the high purity single crystal GaAs used in [12]. For a quantitative determination of the correlation between the dopant level and the temperature dependence of χ further detailed experimental work, e.g., combined SQUID and Hall measurements, would be necessary. This may enable a determination of the doping level by a relatively fast magnetic measurement, which requires no processing of the wafer. Such a careful calibration is still lacking in the literature, however, it goes beyond the scope of the present paper.

4. Conclusion

Our studies show that the magnetic properties of the substrate of spin-LED devices cannot be ignored in studies of the magnetic properties of the spin-LED itself. This is particularly true in large magnetic fields due to the large substrate volume. The magnetization measurements have to be corrected by a temperature dependent background before comparing it to the optical data. In turn the temperature dependent background at high magnetic fields can be partially explained by the van Vleck paramagnetism in GaAs. Unfortunately there is no one to one correlation between the temperature dependence of the optical and the magnetic background, since in spin-LEDs spin relaxation effects and changes in the recombination time as a function of temperature play a role as well. However, the small net paramagnetic signal at high magnetic fields in the LED with a nonmagnetic Pt electrode [8] implies that the additional effects on the polarization of the emitted light are of the order of 1%.

Typical substrates for spin-LEDs formed from GaAs display both a temperature independent diamagnetic susceptibility and a temperature dependent paramagnetic susceptibility. The temperature dependence is dominated by the temperature dependence of the GaAs band gap. We show that over the entire temperature range from 2 to 300 K the functional behaviour of χ for undoped GaAs matches the theoretical expectation, i.e. it follows the temperature dependence of the band gap whereas the temperature dependence of the linear expansion coefficient plays a minor role. Moreover, the temperature dependence of χ becomes significantly larger with increasing doping level of the GaAs.

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