Interpreting the magnetic moment data

Is the reported moment meaningful?

Before doing any anaylsis on the magnetic moment data, we must first determine if the reported magnetic moment is meaningful. The SQUID measures a modulation in voltage and interprets this as arising from the motion of a magnetic sample (or, in the case of AC susceptibility, the response of a magnetic sample to AC magnetic fields).

Reliability of DC Scan moment: this is the goodness of fit of the model to real data. This is shown in the Graph tab of measurements or in the .rw file for your measurements (if you selected "save raw data" when setting up DC Scan), and is quantified in the columns "DC Free fit" and "DC fixed fit" in the .DAT file (these correspond to the "DC Moment Free/Fixed Ctr" reported moments). These give regression values for the fit, where a perfect fit = 1.0, anything >0.9 is generally good, and <0.8 is unreliable. If the fit value is acceptable, use the "DC Moment Err" as an estimate of the error bar on the measurement. This is of course an oversimplification of a complex curve fitting optimization, so please consult with Neil if you have questions. The "free" and "fixed" refer to the analysis algorithm which varies the model's sample center location to optimize the fit ("free") or keeps it fixed based on the location entered when centering the sample ("fixed"), but will move the center as temperature changes (to account for thermal expansion) if Autotracking is selected. The MPMS-3 user manual has more detail.

Reliability of VSM moment: this is a simpler measurement that does not involve curve fitting but rather a simple multiplication of the Voltage(time) data over one period of oscillation of the motor, i.e., it is a digital lock-in technique. As such, it measures all the magnetic signals and the resulting voltage is a superposition of the sample signal and any other backgrounds. If the sample is not centered then there will be a multiplicative error. The VSM technique relies on making "blank" measurements (see below) for establishing the sample's magnetic moment.

Once you have established that the reported magnetic moments are meaningful, you can now think about accuracy. There are several factors to consider in order to obtain accurate reports of the magnetic moment of the sample in an ***m(H)*** measurement. We list here the factors to consider, and the operations that must be performed, IN THE ORDER IN WHICH THEY MUST BE DONE. This is crucial, since some of these operations do not commute (i.e., give different answers if done in wrong order).

First do corrections of the magnetic field

1. ***H* - magnetic field axis:**
    a. correction for *magnet remanence* – see the MPMS-3 **base system training** doc which describes the field and slope correction algorithm used the script:
    `HighFieldSlope and HRemanence Correction.BAS`
    and read below for details on using the script.
        i. run the script within MultiVu under:
        Utilities > Tools > Highfield Slope and HRemanence Correction
        ii. read the first page carefully to make sure this script is right for you!
        iii. make sure to check the box next to "correct for magnet remanence?"

iv. Make sure you select column with your magnetic moment data ("Y-axis data"): this will be "Moment(emu)" , "DC Moment Free Ctr(emu)", or "DC Moment Fixed Ctr(emu)"
v. The script creates a new data file (default name is to simply add "_ss" to your original file name) which has three new columns:
[HFSS] m - H * slope (emu) : slope corrected magnetic moment
[HFSS] Lin. Reg. Fit (emu) : straight line fit to the high field moment data
[HFSS] H_corr (Oe) : remanence corrected magnetic field, written only if you choose to correct magnet remanence.
vi. To get a slope and remanence corrected M(H) loop, you then plot
Y = **m-H*slope** vs. X = **H_corr**
vii. keep in mind the accuracy limits of the magnetic field correction which I estimate at +/- 1 Oe, and the caveats mentioned in first page of script.

b. field correction for *demagnetization effects* of the sample, which is a magnetostatic effect causing the internal field experienced by the sample to be different than the applied field. This is expressed in the equation $H_{in} = H_{applied} - 4\pi N*M$ where we are using cgs units here H[Oe], M[emu/cm^3] and the *demagnetizing factor* N [0…1] which is purely due to sample geometry. In the SI units one simply drops the 4π in the above equation.
i. helpful publications that tabulate demag factors for likely sample shapes are below. Note that you should use the *magnetometric* demag factor for these measurements which average over the volume of the sample.
1. overview from NIST : http://www.nist.gov/customcf/get_pdf.cfm?pub_id=30354
2. demag of cylinders (these next papers are at end of MPMS-3 Wiki if hyperlinks don't work)
3. demag of regular prisms and ellipsoids
4. when powders are packed, they are never at theoretical or "x-ray" density so the air gaps between particles changes the magnetostatics. This paper attempts to address that difficult issue using some assumptions.
ii. See figure below from Chikazumi's *Physics of Magnetism* textbook, showing how the M(H) loop for a ferromagnet is tilted to the right, or *sheared*, due to demag effects. Note that the coercivity Hc is reported correctly, since M=0 there (he uses letter "I" for magnetization).
iii. Demag effects are relevant when ALL these hold:
1. magnetization density M (emu/cm3) is very large like in ferromagnets and superconductors
2. sample has significant surface area that is perpendicular to the applied magnetic field (e.g., a film perpendicular to field, or a sphere)

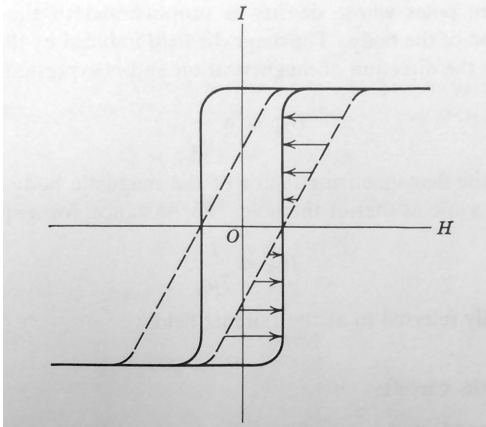


Fig. 2.10. Shearing correction of a magnetization curve.

c. Magnetic field gradients along the sample travel: while the uniformity of the field can be very good at high fields, remanent fields lead to unusual field variations on the order of a few oersted and they depend on HOW you get to low fields. This field variation over the travel of the sample can have drastic effects on hysteretic samples (superconductors, ferromagnets) whose properties can be affected by the small field variation. A lengthy primer about the physics of magnets and superconducting samples can be found at the Quantum Design website here, and an Excel spreadsheet with field profiles for our MPMS-3 magnet is located on the Wiki here. A uniform linear gradient of .05 gauss/mm is found after oscillating the field down from +3 tesla and this has been known to affect some samples.
d. "**Virgin" sample measurements not possible:** some materials require a measurement starting from zero applied field where the sample is in a virgin state (no history of magnetic field applied to it). Note that your sample will experience a vertical magnetic field, in both the positive and negative directions, of **+ and – 150 Oe** when inserting through the linear motor. If this is unacceptable, please consult Neil.

…then do corrections of the magnetic moment

2. ***m*** **- magnetic moment: relevant to all measurements – VSM, DC Scan and AC susceptibility**
   a. *SQUID drifts after changing the field:* mostly in region of |H|=1000-4000 Oe, see discussion in the "Setting up MPMS-3 measurements" section above.
   Additive artifact, Typically a few e-7 emu
   b. *sample holder background signal*:
   Additive artifact
      i. measure a "blank" with everything except your material of interest. For example, a blank substrate. Measure this using the IDENTICAL sequence you will use for your sample, so we make any other systematic errors as consistent as possible. This needs to be subtracted from the obtained data on your sample.
      ii. If you are measuring a ferromagnet, then one can often assume the high field slope is due to diamagnetism of substrate and sample holder. In this case, you can simply subtract that slope from the data using the script we mentioned above: `HighFieldSlope and HRemanence Correction.BAS` on MPMS-3.
   c. *sample geometry:*
   Multiplicative artifact, typically 5-20% estimated by the simulator or the table below, to apply to all the data
   the MPMS-3 is calibrated against a cylinder of palladium, so if your sample is not of this shape and size, then in principle the reported moment will be in error. The errors are multiplicative factors that are not dependent on moment, field, or temperature. They are usually of the order of a few percent, but can be up to 30% in some samples in certain measurement modes (VSM):
   see app note 1500-020 on quantifying the reported moment accuracy for various samples, and the associated sample geometry simulator. This app note supercedes a previous one (1500-015 on QDUSA website), from which this figure below is though a nice summary of the magnitude of the effect we deal with. Here is how to correct the data:

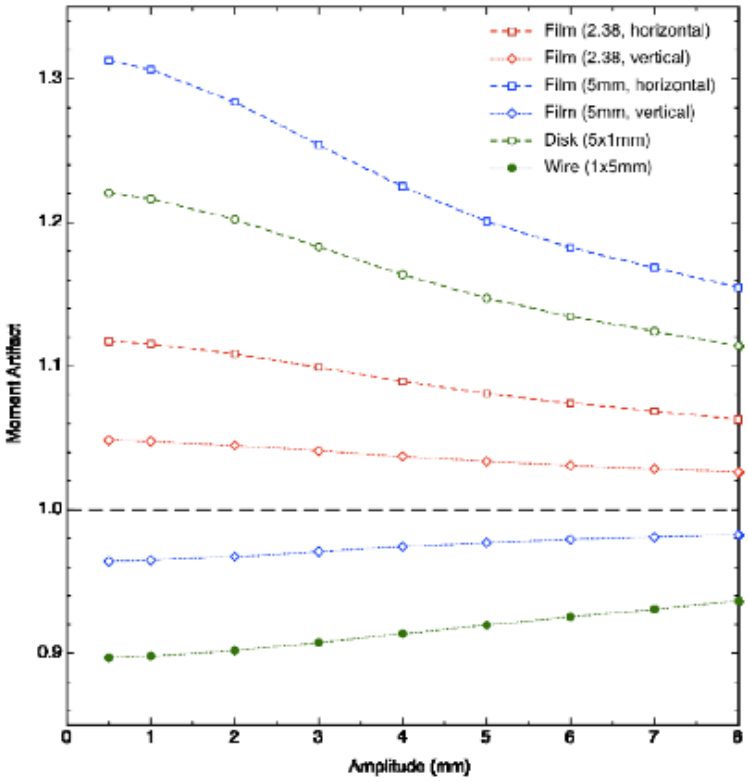
   corrected moment[emu] = reported moment[emu] / "moment artifact"

   Note that you DIVIDE by this factor. In the Sample Geometry Simulator program, the moment artifact is referred to as the "Estimated Correction Factor".

   For cases where getting best moment accuracy is critical, Here is a good trick: I have noticed using the sample geometry simulator that the correction needed for DC Scan measurements is almost exactly half as that which is needed for VSM at 5mm amplitude. That is:
   moment_artifact_DCScan – 1 = (moment_artifact_VSM5mm – 1) * 0.5

   So if you have the luxury of being able to do both the VSM(5mm) and DC Scan and you get a good quality fit for DC Scan (see discussion at start of this document), then you can

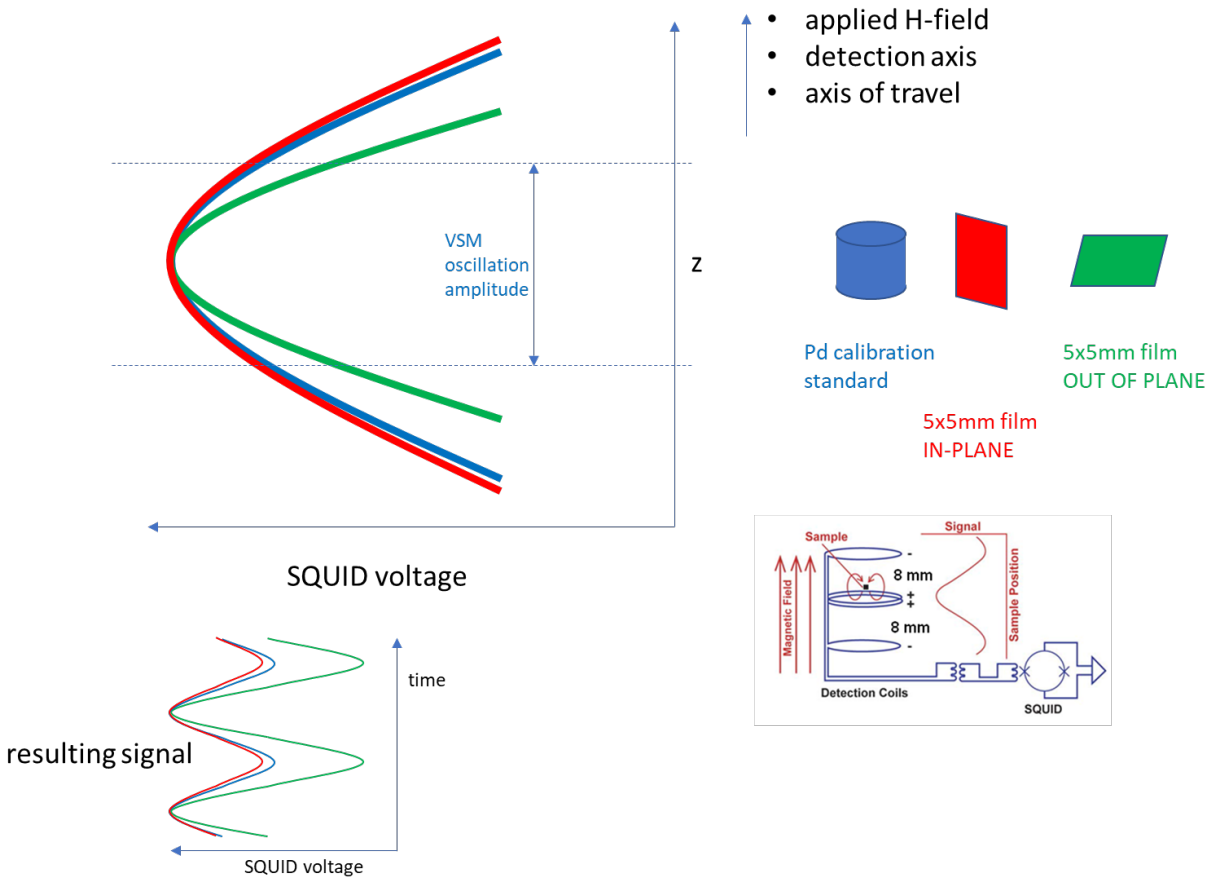
also estimate the corrected moment by extrapolating from DC Scan data as follows:
corrected moment = $m_{VSM\_5mm} - 2*(m_{VSM\_5mm} - m_{DC}) = 2*m_{DC} - m_{VSM\_5mm}$
This is a speculative comment that I have not tested, please use it with caution until we get some data to back this up! Due to the near universal relationship (2x) between DC and VSM corrections, this method has the potential advantage of being independent of the actual correction needed, and helps greatly in cases where sample geometry is complex or radial offset is unknown.



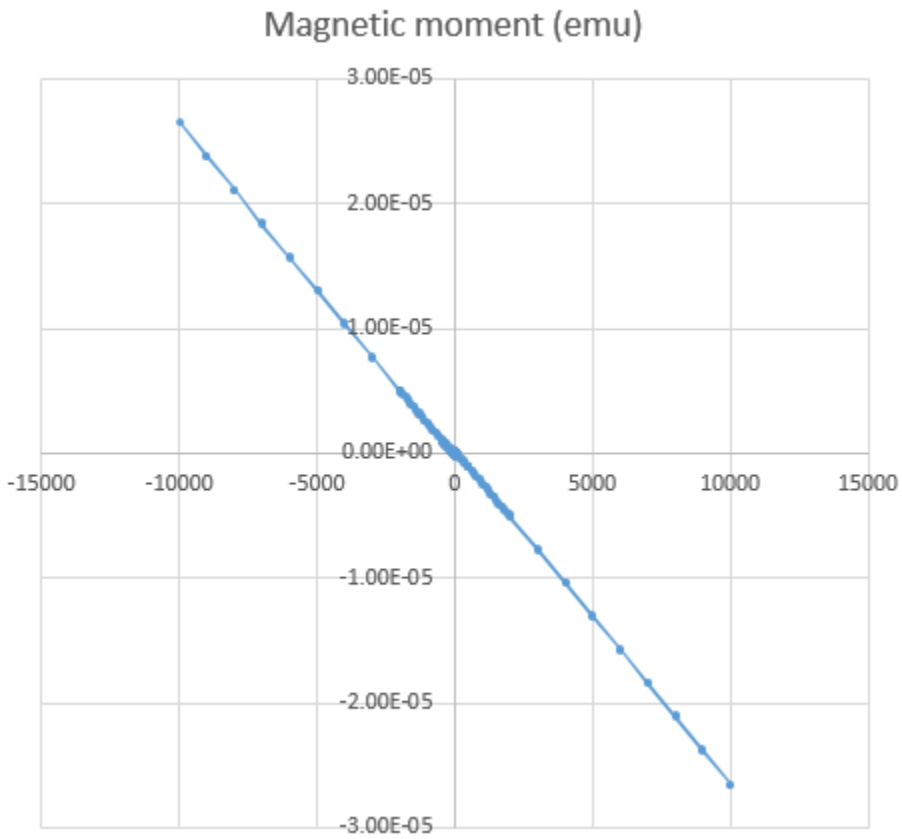
d. *radial and axial positioning error:*
Multiplicative artifact, hard to estimate (since we can't see the sample down in the chamber) but typically <5% if the error is less than 1mm. A sample which is axially (vertically) out of center will lead to an UNDERreported moment, while a sample which is radially out of center will lead to an OVERreported moment. Quantitatively, this relates to the above issue of sample geometry and the Simulator program allows for a radial offset so you can see how much this means. The radial offset is more important and can lead to 10-20% overreported moment if sample not mounted carefully. The quartz paddle sample holder will be the best way to minimize the radial error.

The figure below visually demonstrates the sample geometry effect on reported moment. The Pd standard sample is the model (blue curve), and an extreme case of the sample artifact is well demonstated by a 5x5mm film both with field in-plane (red) and out of plane (green). The SQUID voltage vs. position is more “compressed” for the green curve and results in a larger voltage for a given oscillation amplitude. Two take-home messages:

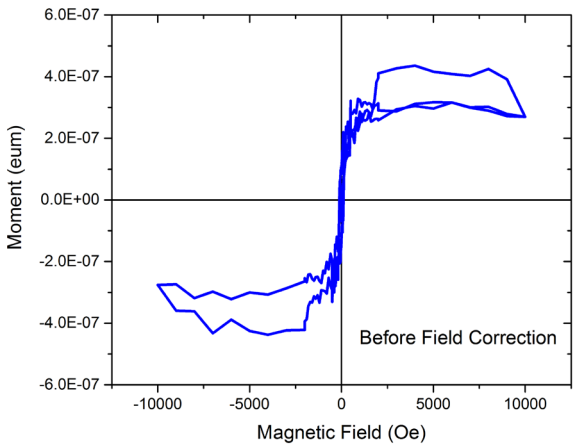
1) given that the Pd cylinder is the model for our analysis, samples that deviate from that will have an artifact in the magnitude of the moment. A good “rule of thumb” is that accuracy will be good when sample Z/R ~ 1, where Z is the height along the z-axis and R is the width of the sample (radius or width of film).
2) The DC Scan technique shows typically only half of the moment artifact as compared to VSM method (check this in the Sample Geometry Simulator tool), so you can estimate the real moment much better by measuring both with VSM and DC Scan, at least at a few points.

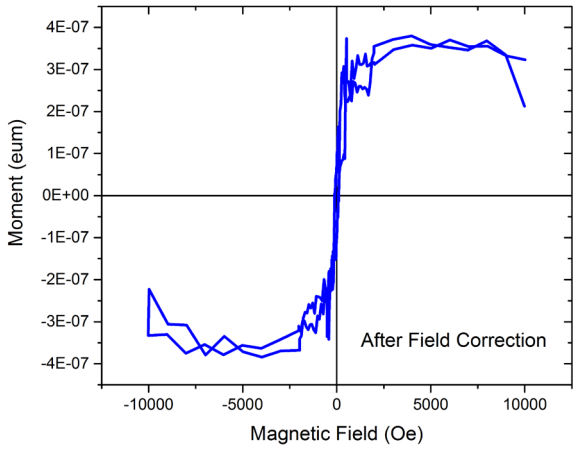


Below is an example of a measurement of a weak ferromagnetic signal on a diamagnetic substrate (Si):

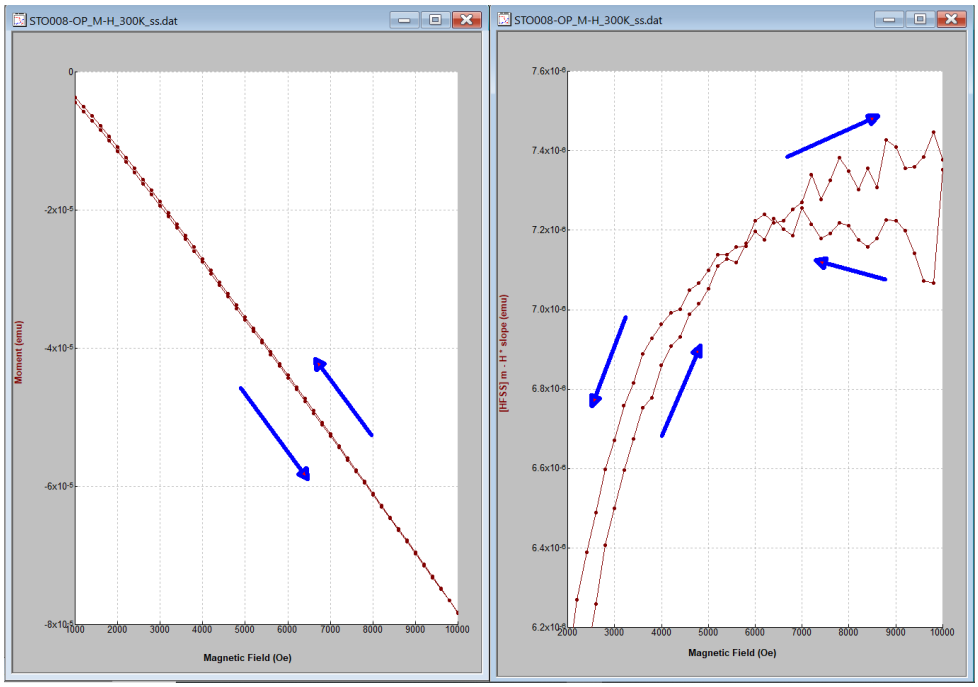


The high field slope was subtracted from data, and below we show the results when the field correction (see Sec. 1a above) was NOT applied (LEFT) or was applied before the slope subtraction (RIGHT). You see the apparent hysteresis at high fields when field correction is not applied, and that just comes from the field shift. By using the script `HighFieldSlope and HRemanence Correction.BAS` this remanence and slope is taken care of correctly.





The script is not perfect, and tends to overcorrect the magnet remanence at high fields (March 2021), while being better near zero field. See example below from a FM film on a diamagnetic substrate: the magnetic hysteresis looks as expected in the original data (left), but after the correction for magnet remanence and high field slope there is an apparent crossing around 6000 Oe which is an artifact (right). This happens because the y-axis is "m – H*slope" where there is a new systematic error in the value of H that is introduced by the script. One can also run the script without magnet remanence correction to see the difference. A more careful script would use a field-dependent magnet remanence value which goes to zero at high fields with a Lorentzian-like dependence. This brings up a general point: all corrections bring with them their artifacts! A more sophisticated script could correct better for this, but would potentially introduce even more subtle and non-intuitive artifacts. Reverting to the raw data is always important.



Example: Curie-Weiss Law Paramagnetism

The exercise below is helpful to give you an idea of the magnitude of signal you should expect from independent local paramagnetic spins such as found in rare earth metals at high temperature, or NiO above its Neel point of 525 K.

As a practical matter, the paramagnetism will be accompanied by other signals which need to be quantified in order to separate the Curie-Weiss (CW) component. In general in an applied field the measured magnetic moment is:

$$m[emu] = (\chi_{CW} H + \chi_0 H) \cdot (\text{mass}) + m_{bg}$$

$\boldsymbol{\chi_0}$ is a temperature-independent background (para- or dia-magnetic) which is ubiquitous. Core electron diamagnetism for materials is tabulated as Pascal's constants. There can also be conduction electron paramagnetism (Pauli paramagnetism) which is roughly temperature independent. Both of these susceptibilities are small, typically ~10^{-7} in units of susceptibility we will use here [emu/g-Oe].

$\boldsymbol{m_{bg}}$ is remaining background signals from the sample holder or other T-dependent magnetism in the sample. This must be accounted for by measuring a suitable control sample like a sample without the CW magnetic component on an identical "blank" sample holder.

Curie-Weiss susceptibility $\chi_{CW} = \frac{M}{H} = \frac{C}{T-\theta}$

M[emu/g] = m[emu] / mass

H[Oe]: applied field

C = Curie constant = $\frac{N_A \mu^2}{3Ak_B}$

N_A = 6.02 x 10^{23} mol^{-1}

A = atomic weight [g/mol]

k_B = 1.38e-16 erg/K

μ = magnetic moment per atom, in units of Bohr magnetons ([μ_B]=[erg/Oe])

θ = Curie-Weiss temperature[K]

Since paramagnetism is a much weaker signal than ferromagnetism, I find it useful to write the equation in terms of the measured moment for a given amount of material at a given temperature:

$$m[emu] = \frac{H \cdot mass \cdot C}{T - \theta} \approx 0.127 \frac{H[Oe] \cdot mass_{mag}[g] \cdot s^2[dimensionless]}{A_{mag}[\frac{g}{mol}] \cdot T[K]}$$

Where $mass_{mag}$ is the mass of only the magnetic atom or molecule, $s = \mu/\mu_B$ is the atomic moment relative to μ_B, and A_{mag} is the molecular weight of the magnetic atom or molecule. I've dropped the θ since it is often small, is not usually known prior to any fitting, and does not change our ability to make an order of magnitude estimate at higher temperatures.

For a thin film of NiO, which is paramagnetic above T_N=525 K, let's take sample volume of
V = 5mm x 5mm x 120nm = 3e-6 cm3 of NiO, or mass = V*density = 2e-5 grams of NiO.
This corresponds to $mass_{mag}$ = 2e-5*(59 g/mol)/(59+16)=1.6e-5 grams of Ni
A_{mag} = 59 g/mol
s = 0.6
T = 525 K ; H = 1e4 Oe
➔ m = 2.4e-7 emu
which is small but not impossible to measure. The main challenge is to discern the sample from the magnetic background signal, in this case the oven sample holder.

Useful Conversions

1 emu = 1.08e20 μ_B

References for experimental magnetism

Tutorial: a beginner's guide to interpreting magnetic susceptibility data with the Curie-Weiss law (Nature Comm. Physics, 2022): this is a very good review of practical aspects of measuring magnetism, with focus on the Curie-Weiss analysis.
Abstract: Magnetic susceptibility measurements are often the first characterization tool that researchers turn to when beginning to assess the magnetic nature of a newly discovered material. Breakthroughs in instrumentation have made the collection of high quality magnetic susceptibility data more accessible than ever before. However, the analysis of susceptibility data remains a common challenge for newcomers to the field of magnetism. While a comprehensive treatment of the theoretical aspects of magnetism are found in numerous excellent textbooks, there is a gap at the point of practical application. We were inspired by this obstacle to put together this guide to the analysis and interpretation of magnetic susceptibility data, with an emphasis on materials that exhibit Curie-Weiss paramagnetism.

https://www.nature.com/articles/s42005-022-00853-y

Approximations to Brillouin functions for analytic descriptions of ferromagnetism, A. S. Arrott, JAP (2008): https://aip.scitation.org/doi/10.1063/1.2836337 :
Abstract The statistical theory of magnetism leads to the magnetic field appearing in the two terms of the Brillouin function, both of which are transcendental, making it impossible to solve explicitly for the argument of that function. The replacement of the Brillouin function BJ(x) by a square root function yields simple algebraic expressions for mean field treatments of cooperative magnetic phenomena. This is useful in the teaching of ferromagnetism.