Thermo-mechanical analysis of a probe for electron paramagnetic resonance spectroscopy operating at cryogenic temperatures

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ABSTRACT

In this article, we present the thermo-mechanical analysis of an electron paramagnetic resonance (EPR) probe operating at cryogenic temperatures using finite element analysis. Thermo-mechanical analysis plays a key role in the mechanical design evaluation process as EPR probes are often subjected to large stresses under such extreme conditions. For simplification, we assume thermal conduction to be the dominant mode of heat transfer over convection and radiation. The simulation model consists of a cryostat-probe assembly with appropriate thermal and structural boundary conditions. The predicted temperature distributions from the steady-state thermal analysis is then used for the stress analysis of the EPR probe. The stress analysis indicated that stresses in the EPR probe are below the ultimate strengths of each component, and thus safe for running EPR experiments. Furthermore, the simulation results were confirmed experimentally, and we found that the predicted heat losses for the EPR probe assembly and the sample holder are in excellent agreement with the experimental measurements.

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I. INTRODUCTION

Electron Paramagnetic Resonance (EPR) spectroscopy is a versatile tool to study paramagnetic centers such as paramagnetic metal ions or clusters, or organic free radicals—species that occur in many areas of science, ranging from materials science to structural biology.^{1–4} EPR experiments are routinely performed at high and low magnetic fields. While many paramagnetic metal centers have very broad EPR spectra due to the metal center's large g-anisotropy, organic radicals, in contrast, often have relatively narrow EPR spectra due to their small g-anisotropy.¹ As a result, metal centers are often studied at low magnetic field strength (S-Band and below), while organic radicals can be studied at high magnetic field strength if the g-tensor anisotropy needs to be completely resolved. At low magnetic field strengths (X-band, Q-band) pulsed and continuous-wave (cw) EPR instruments are commercially available. However, at high magnetic fields/microwave frequencies (W-Band, >95 GHz) the research field is traditionally dominated by home-built instrumentation.^{5–9}

A key component of every EPR spectrometer is the EPR probe. The probe secures the sample in its specific place and ensures

efficient delivery of the microwave radiation to the sample. Often EPR experiments are performed at cryogenic temperatures to either take advantage of the increased relaxation times of the paramagnetic species at low temperatures or to trap a transient paramagnetic state, for example, when studying electron transport proteins. This makes the EPR probe one of the critical spectrometer components which must withstand drastic temperature cycles. The stresses induced by the thermal cycles can have devastating effects on the structural integrity of the probe.

Traditionally EPR probes, specifically probes for high-field EPR spectroscopy, are designed and built by highly skilled researchers, with tremendous experience and know-how in the field.^{10–12} However, since a good part of the design and fabrication process used to rely on trial-and-error, frequent repairs and maintenance are necessary.

With the advent of more powerful desktop computers and workstations, new powerful software tools have become more ubiquitous in mechanical design, spanning areas from the design of aircraft engines to semiconductor devices.^{13,14} These specialized analysis tools which are based on finite element analysis (FEA) and traditionally require fast processors and large amount of

memory are more recently attracting the interest of a broader group of researchers. Today, those working in the EPR community rely on high-frequency finite element simulations to evaluate novel resonator designs *in silico* prior to fabrication. This provides a rapid way to assess innovative microwave structures without having to go through the fabrication process and simulations have become an integral part of the overall resonator design process.^{15–18}

Finite element analysis (FEA) tools are also available to analyze structural and mechanical properties or fluid dynamic properties. In some recent examples, FEA was used to study the air flow paths in rotor/stator assemblies that are used in magic-angle spinning (MAS) solid-state NMR experiments. This analysis helps to gain insight into the fluid dynamics of the MAS stator, optimize turbine shapes and air delivery ducts to design MAS rotors and stators for higher MAS frequencies.^{19–22}

In this article, we focus on the thermo-mechanical analysis of a high-field EPR probe operating at cryogenic temperatures using FEA. The thermo-mechanical analysis plays a key role in the design process as EPR probes are often subjected to large stresses at low temperatures. From a theoretical analysis, we determined the thermal gradient across the probe, the thermal load introduced to the cryostat by the EPR probe, and the thermally induced mechanical stresses on all parts. Finally, we verified key outcomes of the simulation through experimentation and found that the simulation results are in excellent agreement with the experimentally obtained results.

II. MATERIALS AND METHODS

A. Finite element analysis

All simulations were performed using the finite element analysis (FEA) software ANSYS Mechanical (Canonsburg, PA, USA). The EPR probe was designed using Autodesk Inventor (San Rafael, CA, USA) and a simplified 3D computer aided design (CAD) model of the EPR probe was generated and imported into ANSYS Mechanical for mechanical and thermal analysis. Materials used in the simulation are given throughout the text. The sample is 4.3 mm in diameter and 2.6 mm long. We assumed the properties of ice for the sample material for all simulations. All other mechanical and thermal properties of materials used to fabricate the EPR probe are given in Table TI (see the [supplementary material](#)).

B. Experimental apparatus

The EPR probe was fabricated and assembled in-house, with some parts fabricated by external vendors. All low-temperature experiments were performed in a continuous flow cryostat (Janis, Research Company, Woburn, MA, USA, model STVP-200). The cryostat has a temperature range of 1.5–325 K with a nominal temperature stability of 50 mK. Liquid nitrogen was used for cooling in all experiments. The temperature inside the cryostat was regulated using the built-in heater element, controlled by a temperature controller (Stanford Research Systems, Sunnyvale, CA, USA, model CTC10-Cryogenic Temperature Controller). The temperature controller can supply a maximum power to the heater element of 100 W (max. 50 V, 2 A ± 1 mA). Temperature measurements were taken at a rate of 1 sample/min during the experiment.

III. BACKGROUND

In general, heat is transferred between components based upon a temperature gradient. In multi-material assemblies, each material can have a different coefficient of thermal expansions (CTE) and thermal stresses can occur for assemblies, made of parts machined from different materials, which are permanently attached to one another. To ensure these thermal stresses are below the ultimate tensile strength of each material, it is essential to include a thermo-mechanical analysis in the overall mechanical design process of EPR probes.

Conduction, convection, and radiation are the three basic modes of heat transfer mechanisms.²³ In the specific case of analyzing the EPR probe assembly, we assume thermal conduction to be the dominant mode of heat transfer. Modeling convection accurately would require a full 3D computational fluid dynamic (CFD) solver, which will be computationally more expensive. However, at the low cryogen flow rates that are typically required for maintaining a temperature of 10 or 90 K, we assume, that modeling the temperature distribution the EPR probe experiences under steady-state conditions are sufficiently mimicked by heat conduction. The generalized heat conduction equation for isotropic materials in Cartesian coordinates is given by²³

$$k \left[\frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial T}{\partial z} \right) \right] = \rho C_p \frac{\partial T}{\partial t} - \dot{q}, \quad (1)$$

$$k \left[\frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial T}{\partial z} \right) \right] = 0, \quad (2)$$

with k being the thermal conductivity, T the temperature, ρ the material density, C_p the specific heat capacity, and $\dot{q}$ the generated heat per unit volume of the medium. Under steady state assumptions, with the overall heat flow being zero, the rhs of Eq. (1) equates to zero and Eq. (2) becomes the generalized steady state heat conduction equation which is solved in the finite element analysis.

IV. RESULTS AND DISCUSSION

A. Description of the EPR probe

Figure 1 shows the 3D CAD model of the EPR probe [Fig. 1(a)] and a cross section of the EPR probe/cryostat assembly [Fig. 1(b)]. The probe is comprised of a combination of different subassemblies such as the sample holder, the probe support, the microwave waveguide, the top flange assembly, and the base plate. The sample holder is an assembly of several components such as the sample guide tube, made of stainless steel, and the sample holder made of polytetrafluoroethylene (PTFE). The top flange assembly made of stainless steel is used to hold the sample holder assembly inside the cryostat. The waveguide assembly consists of two parts: a straight section made from brass, and a tapered section fabricated from copper. The entire waveguide assembly spans from the top flange assembly to the base plate assembly. The base plate assembly consists of the RF coil former [optional for Electron Nuclear Double Resonance (ENDOR) and Dynamic Nuclear Polarization (DNP) experiments] fabricated from Kel-F (Polychlorotrifluoroethylene, a fluorocarbon-based polymer also known as PCTFE), and a base plate fabricated from brass. A miter-bend is attached to the base plate made of copper to guide the microwave radiation toward the sample. The

FIG. 1. 3D CAD model of the EPR probe. (a) Model of the entire EPR probe. (b) Cross section of the cryostat/EPR probe assembly and details. (c) Mesh density used in the simulation.

probe support tube assembly consists of a carbon reinforced fiber tube (CFRC), with additional support from a total of two plates made from G10 (Glass epoxy composite, garolite) equally spaced throughout the overall length of the EPR probe to guide the sample holder in and out of the EPR probe. In addition, a modulation coil former 3D printed from Acrylonitrile Butadiene Styrene (ABS) is attached to the base plate.

In FEA simulations, the model setup plays a vital role in determining the overall accuracy of the simulation's outcome. During this process, the geometric constraints, surface contacts and boundary conditions have to be identified. In addition, the coefficients of friction (COF) need to be assigned to the appropriate surfaces [Fig. 1(b), squared boxes]. In our case, exact COF values for the material pairs are not available in the literature and we decided to use values associated with smooth surface finishes. We assigned a moderate COF of 0.1 to the waveguide top flange and base-plate, respectively, and a COF of 0.03 to sample-holder [see Fig. 1(b)]. Bonded contacts were assigned to all other surfaces.

As heat conduction is the only mode of heat transfer, we prescribed temperature boundary conditions to the appropriate surfaces. We assigned low cryogenic temperatures to the surfaces adjacent to the cryostat inlet, as shown in Fig. 1(b). We also assumed that the elastomeric O-ring seals are efficient with minimum leakage. Thus, the top flanges and the adjacent components as

indicated in Fig. 1(b) are assigned room temperatures (RT). The outer surfaces of the cryostat are also assumed to be a perfect insulator.

In addition, to the model setup, the accuracy of FEA relies on the mesh density of the simulation domain. Figure 1(c) shows the mesh density used in the present FEA. We used a combination of 2 043 596 structured and unstructured elements to ensure uniform temperature and stress distribution throughout the EPR probe.

The simulation of a thread-bolt joint can be very challenging, since it requires a very high mesh density and the solution becomes computationally expensive. In addition, threads and bolts are modeled with frictional contacts and a non-linear model is required to solve the problem (see below). This is time consuming, as the simulation requires an iterative solver; in addition, it might have convergence issues. Since we are interested in the overall structural integrity of the probe assembly and not analyzing the stresses in the bolt-thread assembly, we can greatly simplify the analysis and use a modified bolt-thread configuration to attach the probe support tube and plates, as shown in Fig. 2. In this simplified model, the actual screw is replaced by a cylinder, which is attached to the G10 support plate [Fig. 2(b)]. Bonded contacts are applied across the surface in red. This is a standard FEA technique where the actual bolts are replaced by regular cylinders and bonded contacts are assigned across the interfaces.²⁴

FIG. 2. Schematic representation of the bolt-thread assembly. Left: Detailed bolt-thread assembly using a screw. Right: Simplified bolt-thread assembly used in the simulation.

B. Numerical simulations

1. Temperature distribution

EPR experiments are typically conducted over a wide range of temperatures. For the simulations, we chose two different temperatures, 10 and 90 K, respectively. In the FEA simulations, the inlet surfaces of the cryostat are held at these temperatures, which cover the lower and upper end of the typical operating temperatures.

Figure 3 shows the simulated temperature distribution across the EPR probe at 10 and 90 K. From the simulation, we observe that a temperature gradient develops along the entire length of the EPR probe. The profile of the temperature gradient at 10 and 90 K look identical, except the magnitudes are different and the temperature can be scaled as a function of the cryostat inlet temperature. From the simulated temperature profile of the EPR probe, it is also evident, that the major pathway for heat entering the system is through the sample stick.

In low-temperature EPR spectroscopy, it is imperative that the sample is maintained at an even temperature to avoid significant temperature gradient across the sample volume. Figure 4 shows the simulated axial and radial temperature gradient across the sample at 10 and 90 K, respectively. From the simulations, we can determine that the axial and radial temperature gradients are almost identical for 10 and 90 K. The axial temperature increases along the sample length and experiences a thermal gradient of $\nabla T_z = 0.08$ and 0.05 K/mm assuming a nominal sample temperature of 10 and 90 K, respectively. The radial temperature profile across the sample volume shows a typical temperature profile observed in many other applications, such as heat conduction of solid blocks and in pipe flows.²³ In general, we observe a very small temperature gradient

across the sample, thus it is safe to assume the sample is maintained at the desired nominal temperature.

EPR spectroscopy is performed by irradiating the sample with microwave radiation (pulsed or continuous wave) and detecting the reflected microwave signal while sweeping either the microwave frequency or the magnetic field strength through the EPR resonance condition. While the microwave radiation will cause sample heating, this effect is very small, even negligible, in high-field EPR spectroscopy (>140 GHz) since the available microwave power is in the milliwatt regime. In addition, our studies of the microwave induced magnetic and electric fields inside the non-resonant sample holder has shown that the fields are distributed evenly over the sample (data not shown). While the microwave radiation may cause a further increase of the sample temperature, albeit negligible, we do not expect an additional temperature gradient introduced by it.

From the thermal analysis at 90 K, we determined a heat loss of the EPR probe of $\dot{Q}_p^S = 1.08$ W and for the sample stick $\dot{Q}_s^S = 0.11$ W.

In Sec. IV B 2, the simulated temperature gradient along the EPR probe is used to perform a stress analysis. The EPR probe is suspended from the top inside the cryostat where the EPR probe can freely move up and down inside the cryostat due to thermal contraction or expansion. Thus, the cryostat has no influence on the overall structural integrity of the EPR probe. To reduce the computational cost, only the temperature distribution of the EPR probe is considered in the stress analysis.

2. Nonlinear stress analysis

For a linear stress analysis using finite-element methods, the matrix equation, which needs to be solved during the simulation is called Hooke's Law^{25,26} and is given by

FIG. 3. Simulated temperature distribution of the EPR probe/cryostat assembly at 10 and 90 K.

FIG. 4. Simulated sample temperature distribution along the axial (left) and radial (right) directions of the sample at 10 K (top) and 90 K (bottom).

$$[K]\{x\} = \{F\} \quad (3)$$

with K being the stiffness matrix, x the displacement, and F the force of the system. Figure 5(a) shows schematically the case for a linear stress analysis, for which the stiffness matrix K is assumed to be constant.²⁵

In our analysis of the EPR probe, the linear theory breaks down due to abrupt changes in contact stiffnesses across the frictional surfaces, and the force-displacement relation follows a nonlinear trend as indicated in Fig. 5(b). As a result, we cannot assume K to be constant and the stress analysis has to be performed assuming nonlinear

conditions. In this case, the matrix equation solved during the FEA is given by

$$[K(x)]\{x\} = \{F\}. \quad (4)$$

A nonlinear analysis requires an iterative solution scheme as the relationship between the forces and displacements are not known in advance. As a result, a series of linear approximations are performed as shown in Fig. 5(c). This iterative scheme is typically referred to as the Newton-Raphson method.²⁷ In this method, the total force is applied during the first iteration, which results in a displacement.

FIG. 5. (a)–(c) Schematic description of the fundamental FEA equations. (a) Linear system. (b) Non-linear system. (c) Newton-Raphson Method. (d) Force convergence of the EPR Probe simulation.

FIG. 6. Axial displacement (left) and maximum principal stress (right) for the EPR probe at 10 and 90 K for a probe support structure fabricated from aluminum. Areas of high stress are marked with orange circles. The ultimate tensile strength for aluminum is indicated by arrows.

From this displacement, the internal force is calculated. If the system is not in equilibrium, the stiffness matrix is updated at every iteration based on the local slope until the residual forces are small enough for the solution to converge. For the case shown in Fig. 5(c), the system achieves equilibrium after the fourth iteration, at which point the solution is converged.

For complex systems, it may be necessary to apply the load incrementally in smaller substeps as the system may not reach equilibrium (converges) in a single step. This approach is very similar to the minimization using simulated annealing.²⁸ Although this approach is more time consuming, it enables the users to obtain converged solution for the intermediate load steps. Figure 5(d) shows the force convergence for the stress analysis of the EPR probe at a temperature of 10 K. The plot in Fig. 5(d) (top) shows the force convergence response (green) that tries to match the force criterion (blue) at each step. During the simulation, we observe that multiple substeps are applied due to complexity of the model (Fig. 5, dashed orange lines), but each substep converges before the load is increased. Each of the converged substeps enables us to analyze the

stresses building up in the EPR probe at intermediate temperatures before reaching the final temperature of 10 K. Because of the complexity of the EPR probe model, the analysis required a bisection step after 26 cumulative iterations [Fig. 5(d), red dotted line]. A bisectional step is an automatic adjustment of the load step to a lower time step to achieve a converged solution.^{26,27} While this is not the most efficient step, since the solutions from the previous load substeps are discarded, it is necessary to achieve overall convergence of the simulation. The bottom plot in Fig. 5(d) shows the intrinsic time plot to highlight the number of sub-steps and bisection steps used over the entire simulation.

In our case, the outer probe support structure is manufactured from light-weight CFRC, while traditionally aluminum is the material of choice. In Sec. IV B 2, we compare the mechanical properties of an EPR probe fabricated from these two materials. Figures 6 and 7 show the axial displacement and maximum principal stress of the EPR probe at a temperature of 10 and 90 K for a support structure made of aluminum and CFRC. Our results indicate that the stresses for an EPR probe support structure fabricated from aluminum are

FIG. 7. Axial displacement (left) and maximum principal stress (right) for the EPR probe at 10 and 90 K for a probe support structure fabricated from CFRC.

FIG. 8. Axial contraction of the waveguide at low temperatures.

significantly higher as compared to a support structure that is fabricated from CFRC. This is because of the higher CTE of aluminum as compared to CFRC, which results in larger contraction of the support structure. In addition, we observe areas of high stresses inside the waveguide and around the bolt-thread arrangement that eventually will exceed the ultimate tensile strength of aluminum [arrows shown Fig. 6(b)] and will result in a failure of the structure. By contrast, we observe very little stresses for an EPR probe using a CFRC support structure [Fig. 7(b)]. Also, the ultimate tensile strength of CFRC is much higher and falls outside the range of the stresses observed in Fig. 7(b).

From the simulation with CFRC support tube, we observe the waveguide experiences contraction of 1.02 and 1.44 mm at 90 and 10 K, respectively. This is in very good agreement, assuming a linear temperature gradient across the waveguide. The overall contraction of the waveguide can be approximated by

$$\Delta L = \text{CTE} \times \frac{1}{2}(T_{\text{top}} - T_{\text{in}}) \times L \quad (5)$$

with L being the overall length of the waveguide, CTE the coefficient of thermal expansion (see Table T1) and T_{top} and T_{in} the temperature of the top flange and at the cryogen inlet, respectively. Given a waveguide length of 558.8 mm, a temperature $T_{\text{top}} = 295$ K and an

inlet temperature T_{in} of 90 and 10 K, the overall contraction assuming this simplified model is 1.16 and 1.61 mm, respectively. These zero order values are in excellent agreement with the values obtained from the numerical simulation.

Figure 8 shows the simulated axial contraction of the waveguide at low temperatures. A small gap is intentionally maintained at the top between the waveguide and the flange to accommodate the contraction and expansion of the waveguide with temperature. We can add this gap because a small discontinuity will only introduce small microwave reflections and have no considerable influence on the overall microwave performance.^{29–31}

The thermal contraction can result in bending stresses at the bottom of the probe primarily due to the structural boundary condition where the EPR probe hangs freely from the top of the cryostat. In addition, the CTE mismatch across the EPR probe components will contribute to these stresses. This translates into tensile strain or expansion which we can observe around the bottom part of the probe.

Figure 7(b) shows the distribution of maximum principal stresses at 10 and 90 K, respectively. We observe that most of the high stress regions are in the metallic parts, but all stresses are well below the ultimate tensile or compressive strengths of the materials. The highest stress point resides on the probe support tube made of carbon fiber reinforced composites, adjacent to the simplified bolt-thread interfaces. However, even here, the stresses do not exceed the ultimate strengths of the material used to fabricate the section. Overall, we conclude from the simulation that the stress distributions across the EPR probe is acceptable and the EPR probe can be safely rated for operations at cryogenic temperatures.

3. Experimental verification

Verifying the theoretical results obtained from the simulations is no simple task. A direct measurement of the thermal stresses is not feasible in most cases. Even the relatively simple task of measuring the displacement of the waveguide is not straightforward given the complexity of the EPR probe. We therefore decided to experimentally confirm the simulated heat load introduced by the EPR probe.

Figure 9 shows a schematic overview of the experimental setup including a vacuum-jacketed cryogen transfer line, a diaphragm

FIG. 9. Schematic overview of the experimental setup.

pump, a manual flow regulator, and a vacuum gauge to measure the pressure inside the cryostat. The diaphragm pump creates a reduced pressure inside the cryostat, which will result in a constant flow of cryogenics (here liquid nitrogen) into the cryostat. During all experiments, the flow is kept constant at a rate of about 6 LPM (gas).

The temperature inside the cryostat is controlled by an electric heater element mounted directly at the cryogen inlet at the bottom of the cryostat.

During the experiments, the vacuum jacks of the transfer lines and the cryostat are constantly evacuated. This was necessary to maintain good vacuum insulation and to exclude further heat sources which could distort the results.

In Fig. 10, the heater output power for three different scenarios: (a) empty cryostat, (b) cryostat with EPR probe and sample holder, and (c) cryostat with EPR probe only. In contrast to the numerical simulations, the heat losses from the EPR probe cannot be measured directly but can be calculated from the measured heat losses.

At a given cryogen flow, a heater power of $\dot{Q}_{H1}^E = 5.13 \text{ W}$ ($\pm 0.04 \text{ W}$) is necessary to maintain a temperature of 90 K inside the cryostat while using liquid nitrogen as the coolant (Fig. 10, blue). With the EPR probe inserted an additional heat source is present and consequently the temperature controller will drop the required output power to $\dot{Q}_{H2}^E = 4.31 \text{ W}$ ($\pm 0.02 \text{ W}$) or $\dot{Q}_{H3}^E = 3.5 \text{ W}$ ($\pm 0.06 \text{ W}$), depending if the sample holder is present or not (Fig. 10, red and yellow). Over a period of about 30 min, we observe a slight increase of the heater output power. Since the temperature inside the cryostat is kept constant by the temperature controller this could be the result of increased vacuum insulation due to constantly evacuating the heat shields of the transfer line or the cryostat. However, this effect is neglected in the further analysis of the data.

The heat loss of the probe and the sample stick can be calculated from the following three Eqs. (6)–(8), which correspond to the different experimental scenarios

FIG. 10. Heater output power required to maintain a sample temperature of 90 K for the empty cryostat (blue), cryostat with EPR probe and sample holder (red), and cryostat with EPR probe (yellow). The dashed lines are guides to the eye.

TABLE I. Comparison of the simulated and measured heat losses of the EPR probe.

$\dot{Q}_P^S \text{ (W)}$	$\dot{Q}_P^E \text{ (W)}$	$\dot{Q}_S^S \text{ (W)}$	$\dot{Q}_S^E \text{ (W)}$
1.08	0.82 ± 0.06	0.11	0.87 ± 0.08

$$\dot{Q}_{H1}^E = \dot{Q}_C^E, \quad (6)$$

$$\dot{Q}_{H2}^E = \dot{Q}_C^E + \dot{Q}_P^E + \dot{Q}_S^E, \quad (7)$$

$$\dot{Q}_{H2}^E = \dot{Q}_C^E + \dot{Q}_P^E, \quad (8)$$

with $\dot{Q}_H^E$ being the heater value, $\dot{Q}_C^E$ the heat load of the empty cryostat, and $\dot{Q}_P^E$ and $\dot{Q}_S^E$ the heat losses from the probe and the sample holder. The heat loss of the probe and the sample stick is calculated at each point. From the experimental data, we calculated a heat loss for the probe of $=0.82 \pm 0.06 \text{ W}$ and for the sample holder of $=0.87 \pm 0.08 \text{ W}$. The error is given by the standard deviation of the calculated values [the linear offset (dashed lines in Fig. 10) was subtracted prior to calculating the error]. The comparison between the simulated and measured heat losses for the EPR probe and the sample holder are summarized in Table I.

We observe that the absolute difference between the simulated and the measured heat losses for the EPR probe assembly is low as compared to that of the sample holder. These discrepancies between the simulated and measured data could be attributed to the simplified assumption of including thermal conduction as the dominant mode of heat transfer. Other modes of heat transfer such as convection and radiation, could have some effect on the system. Considering the fact that the thermal simulation predicts heat losses within the same orders of magnitude as the experimental data, the FEA simulation can be considered as a useful tool to predict the temperature distributions in probes at cryogenic temperatures.

V. CONCLUSION

In summary, we have presented a simplified thermo-mechanical analysis of an EPR probe operating at cryogenic temperatures using FEA. The simulation model consisted of a cryostat-probe assembly with the appropriate thermal and structural boundary conditions. Temperature distributions predicted from the steady-state thermal analysis were consecutively used for a stress analysis. Our results indicate that the stresses inside the probe are below the ultimate strengths of each component and safe for running EPR experiments at cryogenic temperatures. For validation of our simulation tool, we experimentally determined the heat load introduced by the EPR probe and the sample holder. The results show that the simulated heat losses for the probe assembly and the sample holder are in very good agreement with the experimental data. The presented workflow is not specific to the analysis of EPR probes and can be used to analyze any cryogenic probe. The general concept requires one to calculate the temperature distribution across the probe under study prior to performing the stress analysis. The stress analysis then gives a detailed insight into the temperature induced stresses and is used to make sure all stresses are well below the ultimate strength of each material. We believe that FEA is

a highly valuable tool and should be part of the general engineering toolbox when designing cryogenic EPR probes.

SUPPLEMENTARY MATERIAL

See [supplementary material](#) for a collection of mechanical and thermal material properties used in the simulations.

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