Symmetric and antisymmetric strain as continuous tuning parameters for electronic nematic order

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We report the separate response of the critical temperature of the nematic phase transition $T_S$ to symmetric and antisymmetric strains for the prototypical underdoped iron pnictide Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$. This decomposition is achieved by comparing the response of $T_S$ to in-plane uniaxial stress and hydrostatic pressure. In addition to quantifying the two distinct linear responses to symmetric strains, we find a quadratic variation of $T_S$ as a response to antisymmetric strains $\varepsilon_{B_{ij}} = \frac{i}{2}(\varepsilon_{xx} - \varepsilon_{yy})$, exceeding the nonlinear response to symmetric strains by at least two orders of magnitude. These observations establish orthogonal antisymmetric strain as a powerful tuning parameter for nematic order.

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I. INTRODUCTION

Electronic nematic order is found in several families of Fe-based superconductors [1–7] and also suggested to be an important aspect within the phase diagram of at least some cuprate high-temperature superconductors [8–14]. In order to assess the relevance of nematic fluctuations for superconductivity [15–22], new methods are required to continuously tune the critical temperature of the nematic phase transition, with the ultimate goal of potentially providing access to a nematic quantum phase transition with a smoothly adjustable external parameter. Here we show how symmetric and antisymmetric strains induced by external stresses can be used as separate tuning parameters for nematic order. We demonstrate this for a representative underdoped Fe pnictide, Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$, but emphasize that these ideas are quite general for nematic order. More broadly, the notions of symmetry decomposition that we employ can be applied to access strains as tuning parameters for other types of phase transitions, thus offering a road map to gain further insight into most existing stress based phase diagrams.

The irreducible representations of the crystallographic point group provide a natural basis in which to express strains experienced by a solid. Within the D$_{4h}$ point group, appropriate for the specific material discussed in this paper, the six independent components of the strain tensor can be decomposed into two components that are symmetric with respect to the primary (C$_4$) rotation of the point group $[\varepsilon_{A_{1u}}, 1 = \frac{i}{2}(\varepsilon_{xx} + \varepsilon_{yy})]$, $\varepsilon_{A_{1g},2} = \varepsilon_{xz}$, Fig. 1(c)(i)], two components that are antisymmetric $[\varepsilon_{B_{1g}} = \frac{i}{2}(\varepsilon_{xx} - \varepsilon_{yy})$ and $\varepsilon_{B_{2g}} = \varepsilon_{xy}$, Fig. 1(c)(ii) and 1(c)(iii)], and two components that belong to an $E_g$ representation, comprising vertical shear, $\varepsilon_{E_g} = (\varepsilon_{xx}, \varepsilon_{yy})$. The specific challenge is to separately determine the effects of each of these strain components on the critical temperature $T_c$ of a phase transition.

In this paper we demonstrate how this can be achieved by comparison of the response to two (or more) different stress conditions [illustrated in Figs. 1(a) and 1(b)]. This decomposition not only reveals the relative roles of in-plane and out-of-plane symmetric strains but also establishes orthogonal antisymmetric strain as a powerful new tuning parameter for nematic order.

As broken symmetries are the most fundamental organizing principle for (solids and) phase transitions, we start by reviewing the symmetry constraints for the nematic transition in underdoped Fe-pnictide superconductors, like Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ studied here. The nematic order parameter and associated lattice distortion that onset at the coupled nematic/structural phase transition at $T_S$ have a B$_{2g}$ (broken C$_4$ rotation and horizontal and vertical mirrors/rotations). Hence, an external stress that induces an antisymmetric strain with a B$_{2g}$ symmetry [Fig. 1(c)(iii)] necessarily induces a finite order parameter at all temperatures and therefore smears the phase transition [4,23–25]. Stresses that induce the orthogonal antisymmetric strain, $\varepsilon_{B_{1g}}$, however, preserve the horizontal and vertical mirrors/rotations [Fig. 1(c)(ii)]. Consequently, a nematic phase transition is still permitted and $\varepsilon_{B_{1g}}$ can therefore be used as a continuous tuning parameter for the phase transition. Since $T_S$ is an isotropic quantity (invariant under (C$_4$) rotation), antisymmetric strain $\varepsilon_{B_{1g}}$ can affect $T_S$ only in even powers, thus $\lambda_{B_{1g}} \equiv \partial T_S / \partial \varepsilon_{B_{1g}} = 0$ (\lambda_{B_{1g}}, A_{1g}, i) \equiv \partial^2 T_S / \partial \varepsilon_{B_{1g}} \partial \varepsilon_{A_{1g},i} = 0$. In contrast, the two symmetric strain components $\varepsilon_{A_{1g},1}$ and $\varepsilon_{A_{1g},2}$ do not lower the crystal symmetry [Fig. 1(c)(i)] and therefore do not affect $T_S$ linearly. Hence, considering both $A_{1g}$ and $B_{1g}$ symmetry strains, to second order the critical temperature $T_S$ is given by

$$T_S = T_S(0) + \sum_{i=1}^2 \lambda_{(A_{1g},i)} \varepsilon_{A_{1g},i} + \sum_{i<j=1}^2 \lambda_{(A_{1g},i,A_{1g},j)} \varepsilon_{A_{1g},i} \varepsilon_{A_{1g},j} + \lambda_{(B_{1g}, B_{1g})} \varepsilon_{B_{1g}}^2,$$ (1)

defining the coefficients $\lambda_i$ that are to be measured. This is achieved by comparing measurements of $T_S(\varepsilon)$ obtained from uniaxial stress and hydrostatic pressure experiments.
II. EXPERIMENTAL METHODS

For both hydrostatic and uniaxial stress experiments, the transition temperatures are determined from resistivity data [Figs. 2(a) and 3(a)]. The longitudinal resistivity $\rho_{xx}$ as a function of temperature was determined during slow temperature sweeps (down and up for each $\varepsilon_{xx}$) using a standard four probe technique (see Appendix B) on a crystal contacted by PbSn reflow solder (for more details see Appendix A). The coupled structural/nematic transition temperature $T_S$ was determined from the center of a Gaussian function fit to a local maximum in the second derivative [Figs. 2(c) and 3(c)], the magnetic transition temperature $T_N$ from a minimum in the first derivative [Figs. 2(b) and 3(b)]. An upper bound for the error bar around $T_S$ is estimated by half the standard deviation of the Gaussian function [26].

Uniaxial stress experiments were performed using a commercially available strain apparatus (CS100, Razorbill instruments). Uniaxial stress was applied along a bar shaped sample of Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ (with typical dimension $2000 \times 400 \times 35 \, \mu m$) by affixing it in between two mounting plates that are pushed together/pulled apart using voltage controlled lead zirconate titanate (PZT) stacks. The cell is designed to compensate for the thermal expansion of the PZT stacks [27]. Furthermore, due to matching of the thermal expansion of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ [28] and the sample mounting plates (titanium) (see Appendix B1, Fig. 7), the strain on the sample is almost perfectly independent of temperature for a fixed voltage applied to the PZT stacks. Stress was applied along the tetragonal [100] axis resulting in a combination of $\varepsilon_{A1g}^{\text{disp}}$, $\varepsilon_{A2g}^{\text{disp}}$, and $\varepsilon_{B1g}^{\text{disp}}$ [see Fig. 1(b)]. The misalignment of the [100] crystal and the stress axis was estimated to be smaller than 2.5° by comparing to a uniaxial stress experiment on a crystal oriented such that stress was applied along the tetragonal [110] axis (see Appendix B1a). The nominal strain along the tetragonal [100] axis ($\varepsilon_{xx}^{\text{disp}}$) was determined by the zero strain length of the sample between the mounting plates and

FIG. 1. Schematic representation of strains experienced by a tetragonal material while held under (a) hydrostatic pressure, and (b) uniaxial stress applied along the [100] direction. Black arrows indicate stress. The strain tensor [right side of symbolic equations (a) and (b)] is derived by multiplying the stiffness and the stress tensor (left side). White arrows in panel (a) and (b) indicate the orientation of the tetragonal crystal axes. In each case, the strain tensor experienced by the material is decomposed into irreducible representations of the crystal symmetry. For materials with regular mechanical properties (i.e., a positive out-of-plane Poisson ratio and an in-plane Poisson ratio smaller than 1), the symmetric strain modes $\varepsilon_{A1g}$, $\varepsilon_{A2g}$, and $\varepsilon_{B1g}$ strains lower the primary rotational symmetry to $C_2$ and break diagonal and vertical mirror planes, respectively.

FIG. 2. (a) Electrical resistivity of Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ as a function of temperature determined during a uniaxial stress experiment. For each temperature sweep (warming) shown here, the sample is held at a constant strain, $\varepsilon_{xx}^{\text{disp}}$, indicated by the color scale (blue data points indicate compressive strain, beige points tensile strain, and cyan colored data small strain around the strain neutral point). Panel (b) and (c) show the first and second derivative of the resistivity with respect to temperature. Panel (d) shows $T_S$ and $T_N$ versus nominal strain $\varepsilon_{xx}^{\text{disp}}$. The red lines are fits using a second order polynomial resulting $T_S(\varepsilon_{xx}) = 100 - (521 \pm 4)\varepsilon_{xx} - (28300 \pm 1100)\varepsilon_{xx}^2$, and $T_N(\varepsilon_{xx}) = 94.5 - (629 \pm 2)\varepsilon_{xx} - (24700 \pm 500)\varepsilon_{xx}^2$. 

(a) hydrostatic pressure

(b) in-plane uniaxial stress

(c) (i) $\varepsilon_{A1g}$ (ii) $\varepsilon_{A2g}$ (iii) $\varepsilon_{B1g}$
SYMmetric AND ANTISYMmetric STRain AS … PHYSICAL REVIEW B 98, 245133 (2018)

the length change measured by sampling a capacitance sensor using an Andeen-Hagerling AH2550A capacitance bridge. Due to strain relaxation effects in the mounting plates and the mounting glue, the actual strain $\varepsilon_{xx}$ experienced by the sample is smaller than $\varepsilon_{xx}^{\text{disp}}$. Using finite element simulations (see Appendix C), we estimate $\varepsilon_{xx} = (0.7 \pm 0.07)\varepsilon_{xx}^{\text{disp}}$. The extracted critical temperature can be well fit by $T_S(\varepsilon_{xx}) = T_S(\varepsilon_{xx} = 0) + \alpha \varepsilon_{xx} + \beta \varepsilon_{xx}^2$ (red line, [29]), with $\alpha = -521 \pm 4$ K and $\beta = -28300 \pm 1100$ K. As we will show later, the surprisingly large quadratic response is due solely to antisymmetric strain, $\varepsilon_{B1g}$.  

The second experiment reported here is electrical resistivity on a bar shaped ($1000 \times 600 \times 30 \mu m$) crystal of Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ as a function of temperature under hydrostatic pressure (Fig. 3). The measurements were performed using a HPC-30 pressure cell within a PPMS from Quantum Design using Daphne oil 7373 as pressure medium. The hydrostatic pressure was determined by measuring the superconducting transition temperature of a lead manometer. Under perfectly hydrostatic conditions (for details see Appendix B) the strain is purely symmetric, and both $\varepsilon_{A1g,1}$ and $\varepsilon_{A1g,2}$ are compressive (Fig. 1(a)). Both transitions are found to vary almost perfectly linearly under hydrostatic pressure, though with a slightly different slope [see Fig. 3(d)], thus merging for pressures greater than approximately 1.75 GPa. A linear fit results in $T_S(P) = T_S(P = 0) + \tilde{\alpha} P$, where $\tilde{\alpha} = -9.38 \pm 0.08$ K/GPa.

III. RESULTS AND DISCUSSION

To decompose the strain induced changes of $T_S$, the relative amount of strains within each of the different symmetry channels is first determined, based on the measured elastic stiffness tensor [30] (see Appendix C 1). The linear response (which, as described earlier, can only arise due to symmetric strain) can then be plotted as a function of the decomposed strains $\varepsilon_{A1g,1}$ and $\varepsilon_{A1g,2}$ (Fig. 4). For hydrostatic pressure (cyan plane in Fig. 4) the response is purely linear, so no subtraction is necessary. For uniaxial stress, the quadratic term ($\beta \varepsilon_{xx}^2$, defined earlier) is first subtracted using the fitted value of $\beta$, to leave the linear response: $T_S^{\text{lin}}(\varepsilon_{xx}) = T_S(\varepsilon_{xx}) - \beta \varepsilon_{xx}^2$ (purple stars in Fig. 4). Since the ratio of $\varepsilon_{A1g,1}$ and $\varepsilon_{A1g,2}$ is different for the two experiments, the purple and cyan planes in Fig. 4 are not parallel. Moreover, since two lines define a plane, the material’s response to symmetric strain (yellow plane in Fig. 4) is uniquely defined by these two sets of measurements. A full decomposition of the response to symmetric strains is now possible, and the associated partial derivatives are readily determined; $\lambda_{(A1g)} = -6.35 \pm 0.23$ K/%, and $\lambda_{(A1g)} = 16.70 \pm 0.32$ K/% [31] (for details see Appendix D). The ratio of these terms $\lambda_{(A1g,2)}/\lambda_{(A1g,1)} = -2.63 \pm 0.11$ demonstrates that $c$-axis strains have a considerably larger effect on $T_S$ than
symmetric in-plane strains. Considering the contributions of symmetric strain to a standard Landau free energy expansion of the nematic phase transition (discussed further below), we note that the finite values of $\lambda(A_{1g,1})$ and $\lambda(A_{1g,2})$ necessarily imply the formation of spontaneous symmetric strains $\varepsilon_{A_{1g,1}}$ and $\varepsilon_{A_{1g,2}}$ upon cooling below $T_S$. That $\lambda(A_{1g,1})$ and $\lambda(A_{1g,2})$ have opposite signs is consistent with the observation that the spontaneous strains as measured in recent thermal expansion experiments [33] have opposite signs.

Having decomposed the linear response, we turn to the quadratic response. Figure 5 shows the normalized nonlinear response of the coupled nematic/structural transition to strain during hydrostatic (cyan stars, top axes) and uniaxial stress (purple stars, bottom axes) experiments. The quadratic contribution evident in the uniaxial strain dominates the suppression of $\varepsilon_{B_{1g}}$. The origin of the kink near zero strain is currently unknown. The feature is, however, smaller than the error bars and has no statistically significant impact on the fit.

![FIG. 5. Normalized nonlinear response of the coupled nematic/structural transition to strain during hydrostatic (cyan stars, top axes) and uniaxial stress (purple stars, bottom axes) experiments. The quadratic contribution evident in the uniaxial strain dominates the suppression of $\varepsilon_{B_{1g}}$. The origin of the kink near zero strain is currently unknown. The feature is, however, smaller than the error bars and has no statistically significant impact on the fit.](image)

In-plane strains have previously been demonstrated as a suitable means to induce phase transitions [36]. Here we have shown how a complete symmetry decomposition, made possible by comparison to hydrostatic pressure, reveals the separate effects of symmetric and antisymmetric strains that are necessarily both present when a sample is held under in-plane uniaxial stress. We emphasize that antisymmetric strain is a powerful continuous tuning parameter for nematic phase transitions. While values of $\varepsilon_{B_{1g}}$ that would be necessary to completely suppress the coupled nematic/structural phase transition in Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ are slightly out of reach,
this is not necessarily the case for other materials, raising the distinct possibility that antisymmetric strain could be used to continuously tune a suitable material to a nematic quantum phase transition [35]. Finally, we report that symmetric $c$-axis strain has a significantly stronger effect on the nematic transition in Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ as compared to symmetric in-plane strain.

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APPENDIX A: SAMPLE PREPARATION

The Ba(Fe$_{0.975}$Co$_{0.025}$)$_2$As$_2$ single crystals characterized here were grown using a FeAs self flux technique described elsewhere [37]. The crystals were cleaved into thin plates and cut into rectilinear bars. Typical samples dimensions for uniaxial stress and hydrostatic pressure experiments were $200 \times 400 \times 35 \, \mu m$ and $1000 \times 300 \times 35 \, \mu m$, respectively. Electrical contacts were made by a reflow soldering technique using a Sn63Pb37 solder paste with a solder particle size of 15–25 $\mu m$ (Chip Quick SMD291AX10T5). The initial steps of the contacting procedure using solder paste are similar to contacting methods using silver paint or silver epoxy. The ends of short (~10 mm) pieces of 25 $\mu m$ wide gold wire were dipped into the solder paste and positioned onto the freshly cleaved sample surface. The sample, resting on a 1 mm thick glass slide, is then placed on a hot plate preheated to 200°C to reflow the solder beads. To prevent oxidation of the contacts, the sample and glass slide are taken off the hot plate as soon as the solder particles melt. This can be easily seen as the contact appearance changes from matte to shiny. The typical contact resistance of such solder joints was estimated by a quasi-four-point measurement to be smaller than 20 mOhm per contact. While the contact resistance of soldered contacts is superior to silver paint and silver epoxy, it is important to note that the superconductivity of the solder ($T_c \sim 7.1 \, K$) [38] might be problematic for measurements at low temperatures. These solder joints are also significantly more mechanically robust and are better able to survive thermal cycling than silver paint contacts.

APPENDIX B: EXPERIMENTAL METHODS

Four point resistivity measurements during our uniaxial stress and hydrostatic pressure experiments were performed using a Stanford Research Lock In amplifier (SR830). The output of the lock-in amplifier was converted to a constant current source using a 1 kOhm series resistor. The voltage signal was amplified with a Stanford Research transformer preamplifier (SR554).

All resistivity measurements used the same cryostat, a PPMS from Quantum Design. The temperature was swept slowly at a rate of 0.5 K/min. The sample temperature was measured using a Cernox CX-1050 temperature sensor from Lakeshore mounted on the Ti body of the CS100 cell (for uniaxial stress experiments) and the Cu-Be body of the hydrostatic pressure cell, respectively. The temperature sensors were sampled using a Lakeshore 340 temperature controller. The thermal lag of the sample as compared to the measured cell temperature was estimated by taking resistivity measurements during cooling and warming runs. Thermal lags of about 0.1 K and 0.25 K were found for our uniaxial stress and hydrostatic pressure experiments, respectively.

1. Uniaxial stress experiments

Uniaxial stress experiments were performed using a commercially available CS100 cell from Razorbill Instruments. This cell uses piezo electric (PZT) stacks to separate two mounting plates. The exact working principle of such a cell is described in detail elsewhere [27]. Samples were affixed onto the mounting plates of the uniaxial stress cell (see Fig. 6) using Devcon 2-ton epoxy. The glue layer thickness between the sample and the bottom mounting plates was controlled using Nylon wire spacer with a diameter of 25 $\mu m$. The glue layer thickness between the sample and the top mounting plates was controlled by the thickness of spacer washers between the top and bottom mounting plates. Typically, the glue layer on top of the sample was approximately double the thickness of the bottom glue layer.

The zero-volt strain (zero volts across the PZT stacks results in zero piezoelectric extension or contraction of the stacks) experienced by the sample during uniaxial stress experiments is determined by the differential thermal expansion of the sample and the sample mounting plates and thus, in general, is not temperature independent. In this case however, the thermal expansion of the Ti mounting plates and the in-plane
expansion of Ba(Fe$_{0.92}$Co$_{0.08}$)$_2$As$_2$ are very similar (Fig. 7). Therefore we can approximate the strain as independent of temperature and fully controlled by the voltages applied to the piezoelectric stacks. Due to the hysteresis of the PZT stacks, zero volts across all three PZT stacks does not necessarily correspond to zero strain.

The nominal strain along the transport direction ($\epsilon_{xx}^{\text{disp}}$) was determined by measuring the displacement of the two sides of the cell (using a capacitive displacement sensor sampled by an Andeen Hagerling AH2550 capacitance bridge) with respect to the initial distance between the lower sample mounting plates. Since the zero-volt distance of the capacitor plates is not independent of temperature (due to the thermal expansion of the epoxy holding these plates), first a calibration of the zero volt capacitance has to be determined as a function of temperature. Ideally, this is done by affixing a relatively stiff bar of titanium (to match the thermal expansion of the cell made of titanium) across the two sides of the cell and measuring the capacitance as a function of temperature. Since the zero volt capacitance changes between each measurement run due to the hysteresis of the PZT stacks, it is important to record this value before the mounting procedure of each sample. The calibration can then be adjusted from measurement to measurement. The change of the capacitance with changing distance of the capacitor plates, on the other hand, is almost temperature independent (the thermal contraction of the plates as well as the change of the dielectric permittivity of helium gas within the experimental temperature range are small). The manufacturer supplied calibration is thus almost temperature independent.

Due to strain relaxation effects within the glue layers and the Ti mounting plates, the actual strain on the sample differs from the nominal value. In this work, we estimated the strain relaxation effects using finite element simulations (more details given below). The strain experienced by the sample was calculated to be $\epsilon_{xx} = (0.7 \pm 0.07) \epsilon_{xx}^{\text{disp}}$. The difference in strain on the top and bottom surface of the sample was found to be less than 2%, despite the asymmetric glue layer thicknesses. The normal strains within the sample were found to be approximately constant in distances over 100 $\mu$m of the plates. The voltage contacts on our samples were placed so that only the section of the sample experiencing uniform strain was probed. To avoid shear strains introduced into the sample by asymmetric, point shaped contacts, the voltage (and the current) contacts were line shaped and spanned the entire width of the sample [see Fig. 6(b)].

\[ \text{a. Uniaxial stress along the tetragonal [110] axis} \]

$B_{2g}$ strain is known to turn the phase transition into a crossover and smear all the related features. This is indeed what we observe in our experiment applying uniaxial stress along the tetragonal [110] axis. Figure 8 shows the data for the $B_{2g}$ strain experiment. The feature corresponding to the nematic phase transition (step change in the derivative of the resistivity with respect to temperature) is quickly suppressed and replaced by a broad crossover. A relatively small strain $\epsilon_{xx}^{\text{disp}}$ of about $3 \times 10^{-3}$ is sufficient to fully suppress the feature associated with the nematic phase transition. Considering the evolution of the feature of the nematic phase transition in our $B_{1g}$ data presented in the paper (and the rotated compliance tensor), we estimate a misalignment of 2.25°. As the feature associated with the nematic phase transition stays sharp and clearly observable within the whole investigated strain range, the contamination (which to some extent might also originate from our voltage contacts) has no significance for our results.

\[ \text{2. Hydrostatic pressure experiments} \]

Hydrostatic pressure experiments were performed using a Quantum Design HPC-30 Cu-Be based self-clamping pressure cell. Although this version is no longer commercially available, information on the very similar updated version, HPC-33, can be found on the Quantum Design website. Hydrostatic pressure up to $\sim$3 Gpa is applied using a hydraulic press. Daphne Oil 7373 is used as a pressure transfer medium. Note that the freezing point of the Daphne oil is always below room temperature for pressures less than 2 GPa. This ensures a high degree of hydrostaticity throughout the experimental range [40]. Pressure measurements were performed...
by probing the superconducting transition temperature of a lead manometer [41]. In addition, the temperature dependence of the hydrostatic pressure within the HPC-30 pressure cell was determined by calibration measurements using both a lead and a manganin manometer [42]. Below 100 K the hydrostatic pressure was found to be almost independent of temperature.

APPENDIX C: FINITE ELEMENT SIMULATIONS

The goal of our finite element simulation was to estimate the strain relaxation effects in the glue layers as well as the Ti mounting plates. The mechanical properties used within our simulations are summarized in Table I below.

The elastic properties of Ba(Fe0.975Co0.025)2As2 were estimated using the elastic stiffness tensor for 3.7% Co doped BaFe2As2 at 100 K [30]. The mechanical properties of the epoxy were estimated to lie in between the properties of Devcon two-ton epoxy and unfilled Stycast 1260 [27]. To our knowledge, the actual mechanical properties of Devcon two-ton epoxy are not characterized down to 100 K. To justify the assumed mechanical properties we compared measurements on samples mounted using Devcon two-ton epoxy to those of filled Stycast 2850FT and unfilled Stycast 1260 [27]. Below 100 K the mechanical properties of the epoxy within our finite element simulations were estimated from varying the mechanical properties of the epoxy used within our finite element simulation shown on the cross section of our model. Since we focus on vertical shear-free deformations (as indicated by our finite element simulations), the elastic constants $C_{ij}$ with $i, j \leq 3$ (Voigt notation: $1 \equiv xx, 2 \equiv yy, 3 \equiv zz$) fully describe the stress-strain relations relevant for our experiments. Out of the four independent elastic constants top and bottom) is small, resulting in a difference of $\epsilon_{xx}$ on the top and bottom surface of the sample of only about 2% [Fig. 9(c)]. The strain transfer ratio $\epsilon_{xx}/\epsilon_{xx}^{\text{top}}$ used for analyzing our data was found to be $0.7 \pm 0.07$. The error bar was estimated from varying the mechanical properties of the epoxy within $\pm 50\%$ as well as the thickness of the bottom glue layer by $\pm 15\mu\text{m}$.

1. Elastic properties of Ba(Fe0.975Co0.025)2As2

Since we focus on vertical shear-free deformations (as indicated by our finite element simulations), the elastic constants $C_{ij}$ with $i, j \leq 3$ (Voigt notation: $1 \equiv xx, 2 \equiv yy, 3 \equiv zz$) fully describe the stress-strain relations relevant for our experiments. Out of the four independent elastic constants

<table>
<thead>
<tr>
<th>Material</th>
<th>$E$ (GPa)</th>
<th>$E'$ (GPa)</th>
<th>$C_{66}$ (GPa)</th>
<th>$C_{44}$ (GPa)</th>
<th>$\nu$</th>
<th>$\nu'$</th>
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<td></td>
<td>39.5</td>
<td></td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>Epoxy</td>
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<td></td>
<td>3.8</td>
<td>0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ba(Fe0.975Co0.025)2As2</td>
<td>82</td>
<td>82</td>
<td>10</td>
<td>39</td>
<td>0.26</td>
<td>0.164</td>
</tr>
</tbody>
</table>

FIG. 9. (a) Model used for the finite element simulations presented here. The dashed-dotted blue lines on the top view show the mirror planes $m_1$ and $m_2$ used to reduce the model size. (b) Results of our finite element simulation shown on the cross section of our model. (c) Normal strain $\epsilon_{xx}$ along the center line in the $x$ direction on the top and bottom surface of the sample. The vertical black solid lines mark the position of the mounting plate edges. Nominally, a strain of $\epsilon_{xx} = 1\%$ was applied. The strain relaxation within the mounting plates and the glue result in a strain transfer ratio of 0.7.
for 3.7% Co doped BaFe₂As₂ at 100 K. Using this tensor as an estimation for the shear-free mechanical properties of 2.5% Co doped BaFe₂As₂ in the vicinity of its structural transition, it is straightforward to calculate the symmetry decomposed strain fields from the measured hydrostatic pressure and ε_xx for the two sets of experiments.

APPENDIX D: STRAIN DECOMPOSITION

The relation between ε_A1g,1 = 1/2(ε_xx + ε_yy) and ε_A1g,2 = ε_zz under the two stress conditions studied here is determined by the elastic properties (the elastic stiffness tensor) of the investigated material. For hydrostatic pressure (σ_xx = σ_yy = σ_zz), ε_A1g,2 = 1−2ν′/ν′ε_A1g,1, for uniaxial stress (σ_xx ≠ 0, σ_yy = σ_zz ≠ 0), ε_A1g,2 = 1−ν′/ν′ε_A1g,1, where ν and ν′ are the in- and out-of-plane Poisson ratio.

Using these relations the total response of T_S to ε_A1g,1 can be written as

$$
\frac{dT_S}{d\epsilon_{A1g,1}}^{hyd} = \frac{\partial T_S}{\partial \epsilon_{A1g,1}} \bigg( \frac{1}{1-\nu'} - \frac{1}{1-\nu} \bigg)
$$

$$
\frac{dT_S}{d\epsilon_{A1g,1}}^{uni} = \frac{\partial T_S}{\partial \epsilon_{A1g,1}} \bigg( \frac{1}{1-\nu} - \frac{1}{1-\nu'} \bigg)
$$

for the hydrostatic pressure and the uniaxial stress experiment, respectively. Using the in- and out-of-plane Poisson ratio determined from the elastic stiffness tensor C (ν = 0.26 and ν′ = 0.164) as well as the experimentally determined responses (d T_S/d ε_A1g,1)hyd and (d T_S/d ε_A1g,1)uni, the above equations can be solved for d T_S/d ε_A1g,1. We find d T_S/d ε_A1g,1 = −6.35 ± 0.23 K/GPa and d T_S/d ε_A1g,2 = +16.7 ± 1.45 K/GPa for the investigated Ba(Fe₀.₉₇₅Co₀.₀₂₅)₂As₂ confirming the largest linear contribution comes from ε_A1g,2.

Errors reported in the paper represent statistical uncertainty. A full error analysis considering also systematic uncertainty yields d T_S/d ε_A1g,1 = −6.35 ± (0.23 ± 1.45)% statistical ± (2.28 ± 0.32)% systematic and d T_S/d ε_A1g,2 = 16.7 ± (0.32 ± 1.45)% statistical ± (1.45 ± 0.32)% systematic. The main systematic errors considered are a 5% uncertainty in the elastic constants as well as the measured hydrostatic pressure and a 10% uncertainty in the strain relaxation factor. All errors were assumed to be uncorrelated. As the size of our measured responses is robust within the error bars, our main results and discussion are unaffected by the systematic errors mentioned here.

Note that Fig. 2(d) shows the fits on the original data, before the correction for strain relaxation effects using \( \lambda_{(A1g \leftrightarrow A1g)} = 0.06 \pm 0.07 \text{K}/\%^2 \) and \( \lambda_{(B1g \leftrightarrow A1g)} = 0.05 \pm 0.05 \text{K}/\%^2 \). The quadratic response of \( T_\delta \) to \( \varepsilon_{B1g} \) is thus found to be at least two orders of magnitude larger. Since the uncertainty in \( \lambda(\varepsilon_{B1g}, \varepsilon_{A1g}) \) is so large, this is essentially a lower bound on the ratios \( \lambda(\varepsilon_{B1g}, \varepsilon_{A1g})/\lambda(\varepsilon_{A1g}, \varepsilon_{A1g}) \), which could therefore be considerably larger.

1. The 95% confidence interval of the center of the Gaussian function is smaller than \( \pm 50 \text{mK} \) in each case. To also take into account systematic uncertainty introduced by data smoothing or the potentially asymmetric shape of the peak around \( T_\delta \), we empirically determined half the standard deviation as an upper bound for the experimental uncertainty.

2. The sign of \( \varepsilon_{A1g,1}/\varepsilon_{A1g,2} \) is expected to match the sign of \( \lambda_{(A1g,1)}/\lambda_{(A1g,2)} \) in case \( \lambda_{A1g,1} > 0 \) and \( \lambda_{A1g,2} > 0 \), where

\[
\lambda_{A1g,1} = \frac{\partial F}{\partial \varepsilon_{A1g,1}},
\]

\[
\lambda_{A1g,2} = \frac{\partial F}{\partial \varepsilon_{A1g,2}}.
\]

3. The 95% confidence interval of the center of the Gaussian function is smaller than \( \pm 50 \text{mK} \) in each case. To also take into account systematic uncertainty introduced by data smoothing or the potentially asymmetric shape of the peak around \( T_\delta \), we empirically determined half the standard deviation as an upper bound for the experimental uncertainty.

4. The sign of \( \varepsilon_{A1g,1}/\varepsilon_{A1g,2} \) is expected to match the sign of \( \lambda_{(A1g,1)}/\lambda_{(A1g,2)} \) in case \( \lambda_{A1g,1} > 0 \) and \( \lambda_{A1g,2} > 0 \), where

\[
\lambda_{A1g,1} = \frac{\partial F}{\partial \varepsilon_{A1g,1}},
\]

\[
\lambda_{A1g,2} = \frac{\partial F}{\partial \varepsilon_{A1g,2}}.
\]

5. The 95% confidence interval of the center of the Gaussian function is smaller than \( \pm 50 \text{mK} \) in each case. To also take into account systematic uncertainty introduced by data smoothing or the potentially asymmetric shape of the peak around \( T_\delta \), we empirically determined half the standard deviation as an upper bound for the experimental uncertainty.