Resistance measurements of $CaFe_2As_2$ with uniaxial pressure along the c-axis

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Without applied pressure $CaFe_2As_2$ undergoes a first order phase transition at 170 K from the high temperature tetragonal phase to the low temperature antiferromagnetic/orthorhombic phase. We studied the effect of uniaxial pressure along the c-axis on this transition by measuring sample resistance. We observed a clear transition in the sample with more than 12 kbar of pressure applied to the sample. We also found that the critical temperature shifted to higher temperatures for the range of pressures observed when T_C was defined using the onset of the transition or the temperature of minimum slope upon heating. The temperature when the transition ended upon heating was fairly constant. Our results were contrary to those of another group which performed a similar measurement on this material.

I. BACKGROUND

$CaFe_2As_2$ exhibits superconducting properties when doped with sodium [1] and when certain amounts of non-hydrostatic pressure are applied [2]. Superconducting materials are currently an area of interest largely because of the potential for applications. A room temperature superconductor would obviously be very useful. $CaFe_2As_2$ is not a high temperature superconductor but if the factors which affect superconductivity in this material were better understood then perhaps superconductors with higher superconducting transition temperatures could be designed.

$CaFe_2As_2$ has a complex phase diagram with four known phases. One of them, the antiferromagnetic orthorhombic phase, is shown in Fig. 1. In an antiferromagnet the spins of the electrons align anti-parallel in the absence of an applied field. The fact that one of the phases has magnetic order may be a factor that affects superconductivity. Another factor may be the two-dimensional character that results from the atoms being arranged in a series of plains perpendicular to the c-axis.

When no pressure is applied, undoped $CaFe_2As_2$ undergoes a structural and magnetic phase transition at 170 K. Above this temperature the material has no magnetic order and a tetragonal crystal structure; below this temperature it is anti-ferromagnetic and the crystal structure is orthorhombic.

The stable crystal structure at zero temperature is the one with the lowest accessible internal energy, which in this case is orthorhombic[3]. A different structure is favored at higher temperatures if for the same temperature it allows greater thermal vibrations thus achieving a higher entropy. The transition between these two structures occurs at the critical temperature when their entropy is equal. Similarly magnetic order disappears at the critical temperature when thermal energy is on the same order as the energy associated with the alignment of the spins. Bulk transport properties (i.e. macroscopically measurable quantities which depend on electron configuration, such as specific heat, magnetic susceptibility, and resistivity) exhibit unusual behavior at the critical temperature [4].

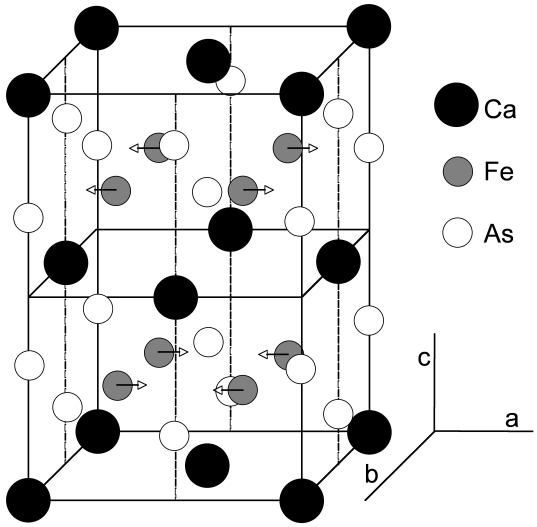

FIG. 1: $CaFe_2As_2$'s anti-ferromagnetic orthorhombic crystal structure. The direction of the magnetic moment is indicated by arrows on the Fe atoms.

A graph of resistivity versus temperature for $CaFe_2As_2$ obligingly shows a sharp feature at 170 K as shown in Fig. 3. The resistance of a metal in this temperature range could be expected to increase with temperature because increasing thermal motion increases electron scattering. The sample shows this behavior on either side of 170 K but something clearly different occurs in a narrow range around this temperature. These data also show the hysteresis characteristic of first order phase transitions i.e. transitions which require energy. The top curve results when heating the sample and the bottom curve when cooling it.

Canfield et al. found that the application of hydrostatic pressure affects the transition [2]. Hydrostatic pressure is applied evenly on all sides of the sample using a liquid medium, in this case helium. With increasing pressure the feature associated with the transition softens and shifts to lower temperatures until it is entirely suppressed at $\sim$3.5 kbar. At this pressure the transition is

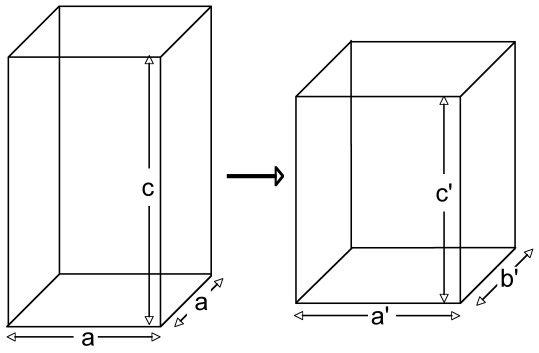

FIG. 2: The tetragonal to orthorhombic transition is characterized by an anisotropic change in unit cell dimensions and a loss of symmetry

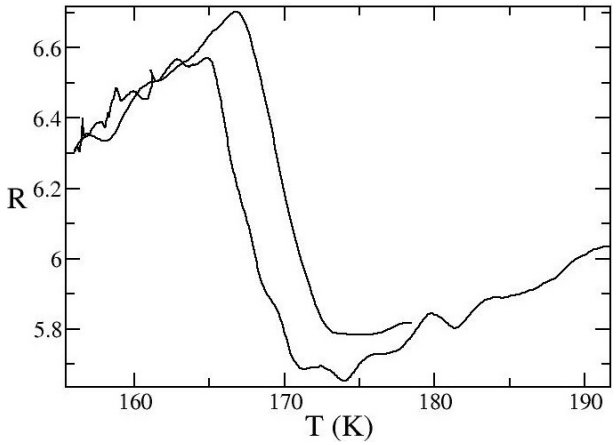

FIG. 3: Resistance vs. temperature in $CaFe_2As_2$ shows an anomaly at 170 K. Also notice the hysteresis. (The top curve is when warming and the bottom when cooling.)

replaced by a different structural transition from tetragonal to collapsed tetragonal at ∼120 K as shown in Fig. 4. (The stable structure at zero temperature can change with applied pressure because a more tightly packed crystal structure is favored [3].) Increasing pressure shifts this new transition to higher temperatures until it passes room temperature at ∼17 kbar.

Canfield et al. also used a different medium for applying pressure. However, unlike helium which is liquid for these pressures and temperatures this other medium froze well above the 120 K transition. Since materials do not always solidify uniformly in all directions this is problem when trying to apply hydrostatic pressure. Add to this the fact that the unit cell has a dramatic anisotropic change in dimensions and it is not surprising the non-hydrostatic components result. The sample expands in one direction and contracts in another while embedded in a solid. The phase diagram is very similar to the hydrostatic case with the addition of a superconducting dome for low temperatures and pressures ranging from ∼3 to ∼9 kbar.

Torikachvili et al. found that application of uni-

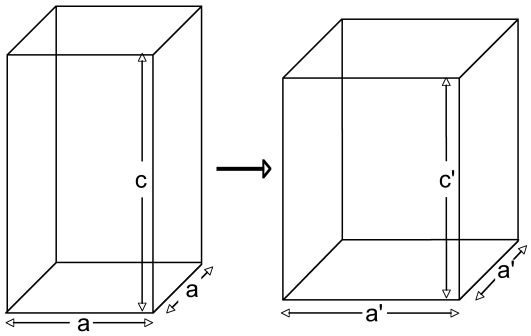

FIG. 4: The tetragonal to collapsed tetragonal transition also has a dramatically anisotropic change in unit cell dimensions. The a-axis expands by ∼ 2.5% and the c-axis contracts by ∼ 9%.

axial pressure along the c-axis resulted in a different response[5]. The 170 K transition was rapidly suppressed; it was completely gone by 3 kbar. The critical temperature increased up to ∼1.5 kbar and then decreased with additional pressure. No collapsed tetragonal phase was observed but this is possibly because the maximum pressure was relatively low (only 2.8 kbar). Also worth noting is that the material completed the superconducting transition at a significantly lower uniaxial pressure.

II. METHOD

We also measured resistance as a function of temperature for increasing uniaxial pressure along the c-axis. We chose to perform this measurement despite its similarity to the work of Torikachvili et al. because our setup can achieve significantly higher pressures (our highest pressure was ∼16 kbar as opposed to ∼ 3 kbar) and we have a good deal of confidence in it having performed similar measurements in the past.

Samples were cut into regular rectangular shapes and polished to have flat surfaces and clean edges. Four leads were spot-welded to the sides of the sample (two for current and two for voltage) leaving the faces clear for application of pressure. Small amounts of silver epoxy were also used to make the connection more mechanically strong.

This was a difficult process since the samples are so thin and the wires so tiny. Usually the leads are attached to the relatively large faces of the sample but since this option was barred to us we had to contend with fragile attachments to the sides, which frequently snapped. There were also issues with polishing the samples because they are so soft.

The sample was mounted at the base of a Kelvinox 100 dilution refrigerator between two vertical posts. The bottom post is rigidly mounted with an adjustable screw. The top post is attached to a bellows mechanism with a piezocrystal sandwiched between. The distance be-

tween the two posts is controlled by the expansion and contraction of the bellows. The bellows expand when a controlled amount of helium 4 enters through a copper nickel fill line and contract when the helium is pumped out through the same line. The helium passes through a series of heat exchangers packed with copper sinter at each level of the fridge in order to minimize the additional heat load on the fridge. The force applied to the sample is measured by the intervening piezoelectric force transducer, which can be converted to pressure if the area of the sample is known.

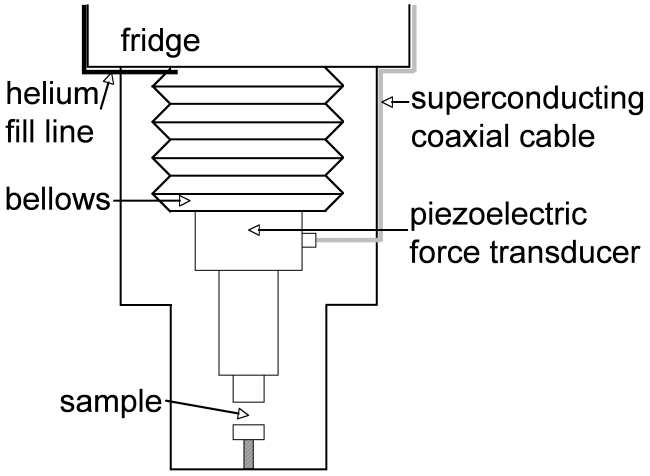

FIG. 5: mechanism for applying uniaxial pressure

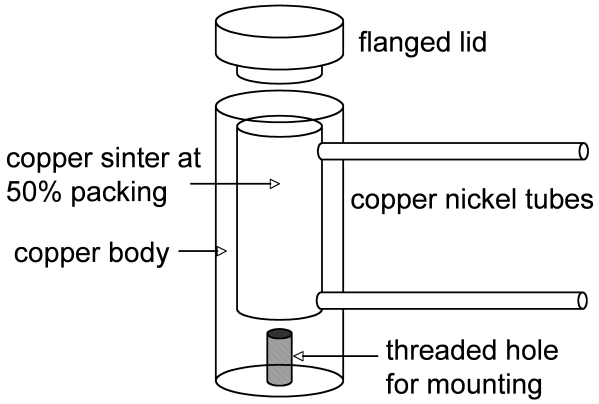

FIG. 6: heat exchanger

The dilution fridge where this apparatus is mounted is designed for temperatures which are much lower than the 170 K transition, so it was not used to control the temperature. The temperature of the sample was varied by raising and lowering a dewer of liquid nitrogen around the base of the fridge. This did not allow for careful control of the temperature, just whether it was increasing or decreasing. The temperature was monitored by a RuO_2 thermometer in close proximity to sample.

III. RESULTS

Like the other group who performed measurements on this material we found that the application of uniaxial pressure along the c-axis softens the feature associated with the structural transition. However, Torikachvili et al. observed a much more rapid suppression of the transition where we observed a clear transition past 12 kbar.

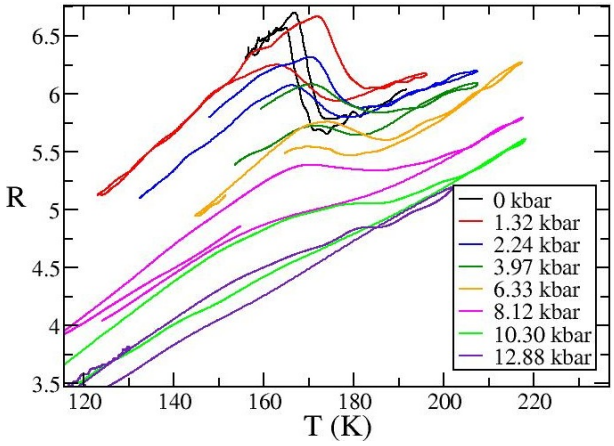

FIG. 7: Resistance vs. temperature in $CaFe_2As_2$ for increasing pressures

There are at least six points which could be sensibly selected to represent T_C, three on the heating curve and three on the cooling: the point when the transition starts, the point where the transition stops, and the point of minimum slope. For low pressures which point is selected does not matter but as the feature gets smeared out with addition pressure there is a greater difference between these points. The heating curve is better than the cooling curve for extracting T_C because the slope is steeper and the local extrema more pronounced, which makes it easier to select an accurate point even at high pressures.

When it is defined as the temperature of minimum slope in the heating curve, T_C increases with pressure over the entire range of observed pressures as shown in Fig. 8. When it is defined as the onset of the transition (local maximum) on heating there is a similar increase with pressure as shown in Fig. 9. However, the point where the transition stops (local minimum) remains fairly constant. Regardless of the method for choosing T_C we did not see the initial increase followed by a decrease observed by Torikachvili et al. However, since they saw the transition suppressed so much more rapidly they were extracting T_C from curves without very pronounced transitions.

IV. CONCLUSION

We observed a clear transition in the sample with more than 12 kbar of uniaxial pressure applied to the sample. We also found that the critical temperature shifted to

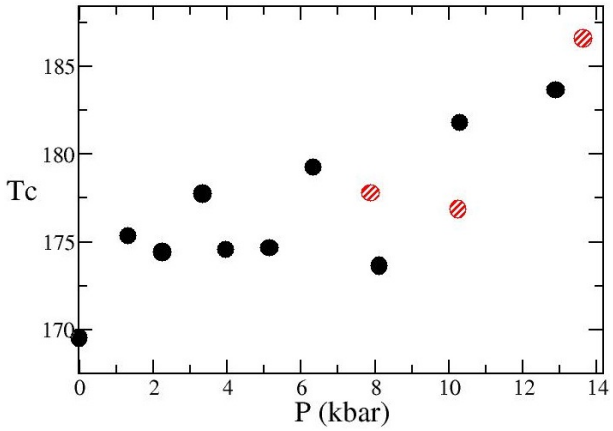

FIG. 8: The critical temperature, selected using the minimum slope criterion, increases with pressure. (Increasing pressure is solid black. Decreasing pressure is striped red.)

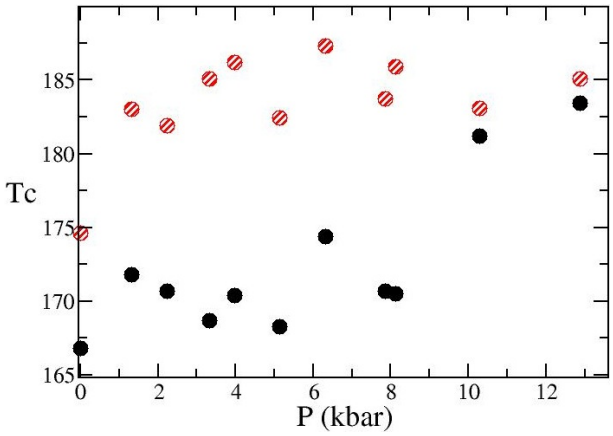

FIG. 9: The critical temperature selected using the beginning of the transition (solid black) shows an increase similar to the critical temperature selected using the minimum slope. The critical temperature selected using the end of the transition (striped red) is fairly constant.

higher temperatures for the range of pressures observed when T_C was defined using the onset of the transition or the temperature of minimum slope upon heating. The temperature when the transition ended upon heating was fairly constant. Our results were contrary to those found by the other group which performed similar measurements on this material. The measurement will be repeated using a different $CaFe_2As_2$ crystal to ensure our results are reproducible.

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