

High pressure study of BaFe_2As_2 —the role of hydrostaticity and uniaxial stress

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys.: Condens. Matter 22 052201

(<http://iopscience.iop.org/0953-8984/22/5/052201>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 07:00

Please note that [terms and conditions apply](#).

FAST TRACK COMMUNICATION

High pressure study of BaFe_2As_2 —the role of hydrostaticity and uniaxial stress

W J Duncan¹, O P Welzel², C Harrison¹, X F Wang³, X H Chen³,
F M Grosche² and P G Niklowitz¹

¹ Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK

² Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

³ Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

E-mail: w.j.duncan@rhul.ac.uk and philipp.niklowitz@rhul.ac.uk

Received 22 October 2009

Published 5 January 2010

Online at stacks.iop.org/JPhysCM/22/052201

Abstract

We investigate the evolution of the electrical resistivity of BaFe_2As_2 single crystals with pressure. The samples used were from the same batch, grown using a self-flux method, and showed properties that were highly reproducible. Samples were pressurized using three different pressure media: pentane–isopentane (in a piston–cylinder cell), Daphne oil (in an alumina anvil cell) and steatite (in a Bridgman cell). Each pressure medium has its own intrinsic level of hydrostaticity, which dramatically affects the phase diagram. An increasing uniaxial pressure component in this system quickly reduces the spin density wave order and favours the appearance of superconductivity, which is similar to what is seen in SrFe_2As_2 .

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

The recent discovery of superconductivity in transition metal pnictides at temperatures as high as 55 K has ignited an industry of research. A number of structure families are being investigated: the '1-1-1-1 compounds', such as LaOFeAs , the '1-1-1 compounds', such as LiFeAs , the '1-1 compounds', such as FeSe , and the '1-2-2 compounds', such as SrFe_2As_2 . Among these, the oxygen-free compounds stand out for being comparatively easy to grow as high quality, homogeneous and stoichiometric, large single crystals. We concentrate on a key member of the 1-2-2 iron arsenide family, BaFe_2As_2 , which, when doped with potassium [1–4], has the highest superconducting transition temperature, T_c , of all the oxygen-free iron arsenide compounds.

The 1-2-2 compounds CaFe_2As_2 [5], SrFe_2As_2 [6] and BaFe_2As_2 [7, 8] undergo a magnetostructural transition into a spin density wave state on cooling. Their low temperature state can be modified effectively by substituting iron with a number of other transition metal elements, by substituting the alkaline earth element with potassium or by substituting arsenic with phosphorus. All of these approaches can be

used to suppress the magnetostructural order of the parent compounds, giving rise—in most cases—to superconductivity at elevated temperatures of the order of 20–40 K. The resulting phase diagram is similar to that of numerous heavy fermion systems [9], organic superconductors [10] and, more recently, an alkali metal fulleride compound [11]. This generality points to a fundamental connection between magnetism and superconductivity in these strongly correlated electron systems.

Alternatively, the low temperature phase diagram of the 1-2-2 compounds can be investigated by applying pressure. Several high pressure studies have been published within a short time, beginning with the discovery of pressure-induced superconductivity in CaFe_2As_2 [12]. Usually, pressure tuning has important advantages. It does not vary the disorder level, it can be applied with great precision, allowing access to the closest proximity of a quantum phase transition, and it is highly reproducible. The pressure studies on the 1-2-2 compounds, by contrast, have led to a bewildering array of confusing and apparently contradictory results. At first,

Table 1. Pressure studies in BaFe₂As₂. The table summarizes work carried out using different pressure media and techniques (DAC: diamond anvil cell, CAP: cubic anvil press, BC: Bridgman cell, PCC: piston–cylinder cell, AAC: alumina anvil cell). T_c gives the maximum observed transition temperature in the superconducting dome. This is the onset of a drop in magnetization [21] or the onset of a resistance drop (other work). Zero resistance is only reported in two of the studies [23, 24]. p_{\max} gives the pressure at which T_c is maximal. (If no superconductivity has been observed, p_{\max} gives the maximum pressure of the experiment.) dT_{SDW}/dp denotes the drop of the spin density wave transition temperature in the zero pressure limit.

Pressure medium	Technique	$T_{c,\max}$ (K)	p_{\max} (kbar)	dT_{SDW}/dp (K kbar ⁻¹)	Reference
Daphne oil 7373	DAC	29	40	NA	[21]
Fluorinert 70/77 1:1	CAP	30	~35	-1.35	[22]
Fluorinert 70/77 1:1	BC	30	53	-2.2	[23]
Steatite	BC	35.4	15	-2.43	[24]
Glycerine	CAP	—	(80)	-0.7	[25]
Daphne oil 7373	PCC	—	(24)	-0.76	[26]
Pentane–isopentane 1:1	PCC	—	(30.7)	-0.84	This study
Daphne oil 7373	AAC	≥24.5	≥55	-1.09	This study
Steatite	BC	32.5	10.6	—	This study

it seems quite straightforward to explain these discrepancies by the difference in sample quality; in the previous studies either polycrystals or single crystals were used and the residual resistivity ratio (RRR) was found to vary between 1.4 and 10. However, pressure results in the 1-2-2 iron arsenide compounds appear to scatter more wildly than the results of chemical substitution studies, suggesting an additional factor causing the discrepancies. This could be the difference in hydrostaticity caused by the usage of different pressure media in different pressure cells. The effect of the level of hydrostaticity has now been studied in both CaFe₂As₂ [12–14] and SrFe₂As₂ [15] but a comprehensive study for BaFe₂As₂ is still lacking.

At room temperature and ambient pressure, BaFe₂As₂ has the tetragonal ($I4/mmm$) ThCr₂Si₂ structure [6]. Below 135 K, it undergoes a magnetostructural transition to an orthorhombic spin density wave (SDW) phase [7]. In this phase, the Fe atoms acquire magnetic moments of 0.87(3) μ_B with an ordering wavevector $Q = (101)$ [8, 16]. Band structure calculations suggest that the spin density wave instability can be attributed to nesting between electron and hole Fermi surface sheets [17–20]. With increasing pressure or doping [17], this nesting degrades, leading to a gradual suppression of the spin density wave order.

A number of high pressure studies have been carried out on BaFe₂As₂ [21–26] (table 1). In all cases, pressure application suppresses the magnetostructural transition to lower temperatures. However, the rate of decrease of the spin density wave transition temperature, T_{SDW} with pressure differs greatly between these studies. Additionally, the extent to which indications for superconductivity are observed varies strongly. Whereas one study reports a diamagnetic signal indicating superconductivity in a large volume fraction of the sample [21], other studies show incompleteness [22] or even absence of superconducting transitions in the resistivity [25, 26]. In the studies showing signs of superconductivity the maximum transition temperature $T_{c,\max}$ and the pressure under which it occurs, p_{\max} , vary considerably, as does the pressure range, across which superconductivity has been observed. So far, it cannot be said, whether the observed variations are mainly due

to differences in the sample quality or rather due to differences in the employed pressure media.

To separate these issues, we present and compare high pressure data obtained from the *same* batch of high-quality single crystals of BaFe₂As₂ subject to three *different* pressure media: (i) pentane–isopentane (used in a piston cylinder cell up to 3 GPa), (ii) Daphne oil 7373 (used in an opposed alumina anvil cell up to 6 GPa) and (iii) steatite (used in a Bridgman cell up to 7 GPa). We expected nearly ideal hydrostatic conditions for method (i), and progressive deviation from hydrostaticity with methods (ii) and (iii). Due to the used pressure cell geometries, it is expected that deviations from hydrostaticity include significant uniaxial pressure components. Our results suggest that even very moderate amounts of uniaxial stress induce at least filamentary superconductivity in BaFe₂As₂. Stronger uniaxial stress fundamentally changes the phase diagram, leading to a fast suppression of the orthorhombic spin density wave phase.

The samples were grown using a self-flux method, which yielded single crystals that were typically 50 μm thick and weighed several mg. All measurements were conducted using a Quantum Design Physical Properties Measurement System (PPMS). The resistivity was measured using an AC four point technique with the current in the a – b plane and the magnetic field parallel to the c -axis. Contacts were made by spot welding 25 μm gold wire onto the sample, except in the case of the Bridgman cell measurements, in which the contacts consisted of 25 μm platinum wire pressed onto the sample. The pressure was determined from the superconducting transition temperature of a lead sample in the alumina anvil and Bridgman cells and of a tin sample in the piston cylinder cell. The pressure inhomogeneity was estimated from the width of the superconducting transition produced by the lead or tin sample. The BaFe₂As₂ crystals were characterized by resistivity and heat capacity measurements at ambient pressure. The samples showed properties similar to samples reported in the literature [2, 2, 27] including a spin density wave transition temperature $T_{\text{SDW}} = 131$ K.

The first set of measurements was conducted in a piston cylinder cell (figure 1), using a 1:1 mixture of pentane and isopentane as pressure medium. According to the width of

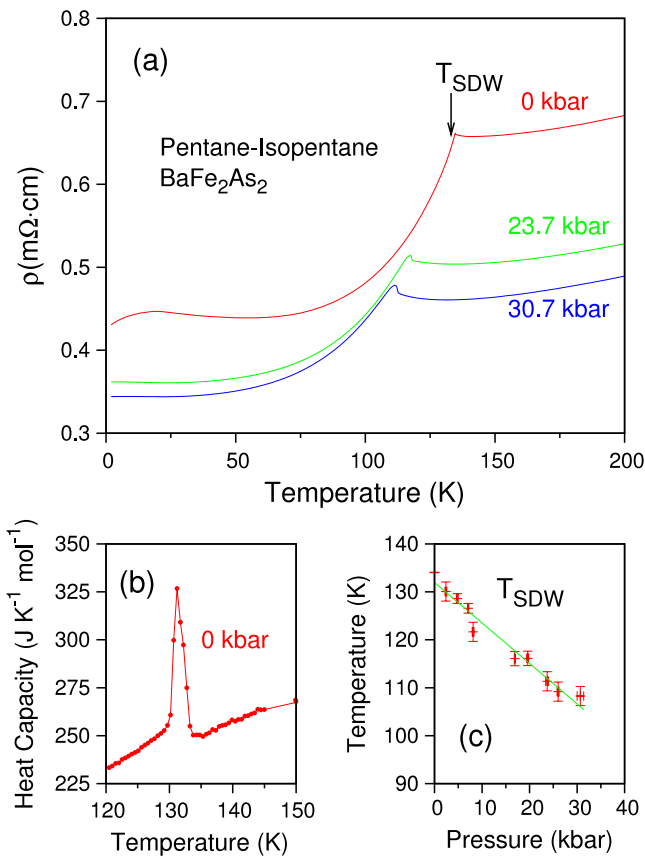


Figure 1. Measurements using pentane–isopentane as the pressure medium in a piston–cylinder cell. The magnetostructural transition (T_{SDW}) of $BaFe_2As_2$ is clearly visible (a) in the resistivity and (b) in the heat capacity at zero pressure. Under pressure (see (a) and (c)) the magnetostructural transition is suppressed at a rate of ~ -0.84 K kbar $^{-1}$.

the superconducting transition of the tin manometer, these measurements produced the most hydrostatic conditions of the three pressure methods employed in this study (figure 5). The resistivity was measured to a maximum pressure of 30.7 kbar. The magnetostructural transition, determined from the maximum of $d\rho/dT$, is slowly suppressed at a rate of approximately -0.84 K kbar $^{-1}$. At the maximum pressure, the spin density wave transition is still clearly visible with no signs of broadening, which indicates that the pressure remains hydrostatic. No anomaly suggestive of superconductivity was observed at low temperatures. At ambient pressure there is a broad maximum in the resistivity around 19 K, which disappears above 8 kbar, similar to what is seen by Matsubayashi *et al* [25]. The origin of this hump in the resistivity trace is unclear. It is not associated with any signature in the heat capacity.

The second set of measurements was conducted in an alumina anvil cell, in which the sample was aligned with the c -axis perpendicular to the anvil flats. The sample space was filled with Daphne oil 7373 as pressure medium. This appears to offer slightly less hydrostatic conditions than pentane–isopentane, possibly due to its increased viscosity (figure 5). In this case (figure 2) the magnetostructural transition is initially suppressed at a slightly higher rate of -1.09 K kbar $^{-1}$,

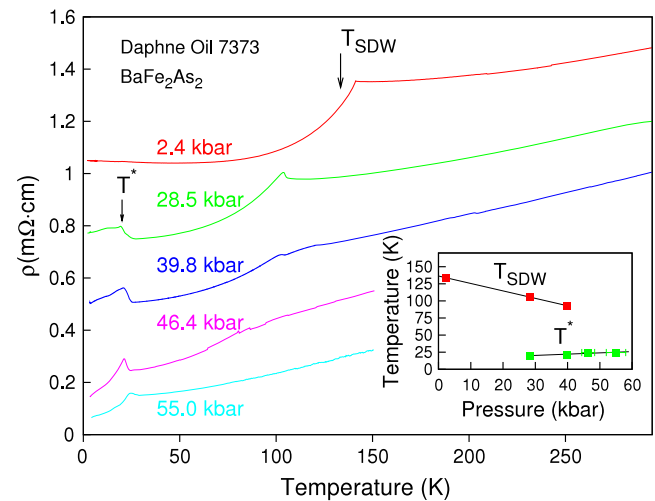


Figure 2. Resistivity measurements of $BaFe_2As_2$ using Daphne oil 7373 as the pressure medium in an opposed alumina anvil cell. Curves are shifted for clarity. In the inset, the pressure evolution of the superconducting onset (T^*) and of the magnetostructural (T_{SDW}) transition is shown. T_{SDW} is suppressed at a rate of ~ -1.09 K kbar $^{-1}$.

compared to the piston cylinder cell and is no longer visible at 46.4 kbar. At low temperatures, an anomaly (labelled T^*) appears at 28.5 kbar, where the resistivity has a maximum near 20 K. As the pressure is increased further, this feature grows into a sharp drop, which is largely pressure independent. Behaviour similar to the one at T^* has been associated with filamentary superconductivity in previous studies (e.g., [22]). It is also interesting to note that the pressure regimes where T^* and T_{SDW} are seen overlap in an interval, which is too large to be explained by pressure inhomogeneities.

The third set of pressure experiments was carried out using steatite as the pressure medium in a Bridgman cell, again with the c -axis of the sample normal to the anvil flats. This setup has been expected to provide the largest uniaxial pressure component. Already at the lowest pressure measured in this cell, 10.6 kbar (figure 3(a)), there is no sign of the magnetostructural transition. Because the jump in the resistivity at low temperatures is similar to the anomaly seen in the alumina anvil cell at 55 kbar, we also label this transition T^* . In this case T^* starts at a slightly higher temperature of ~ 32 K, which is comparable to the superconducting onset in other studies [17, 21–23]. With increasing pressure, the resistivity curves look similar to what is observed by Fukazawa *et al* [22]. T^* was found to be clearly field dependent: a magnetic field of 9 T applied at 53.6 kbar suppressed the transition by 0.80 K T $^{-1}$ (figure 4(b)). These observations and the fact that T^* is weakly pressure dependent suggest that T^* represents the onset temperature of partial or filamentary superconductivity. Our findings were reproduced in a second sample.

The pressure–temperature phase diagrams obtained by the three different high pressure methods (figures 1(c), 2 (inset) and 3(b)) are dramatically different: no superconductivity is observed at all up to 30 kbar in the sample floating in pentane–isopentane, whereas the onset of at least filamentary

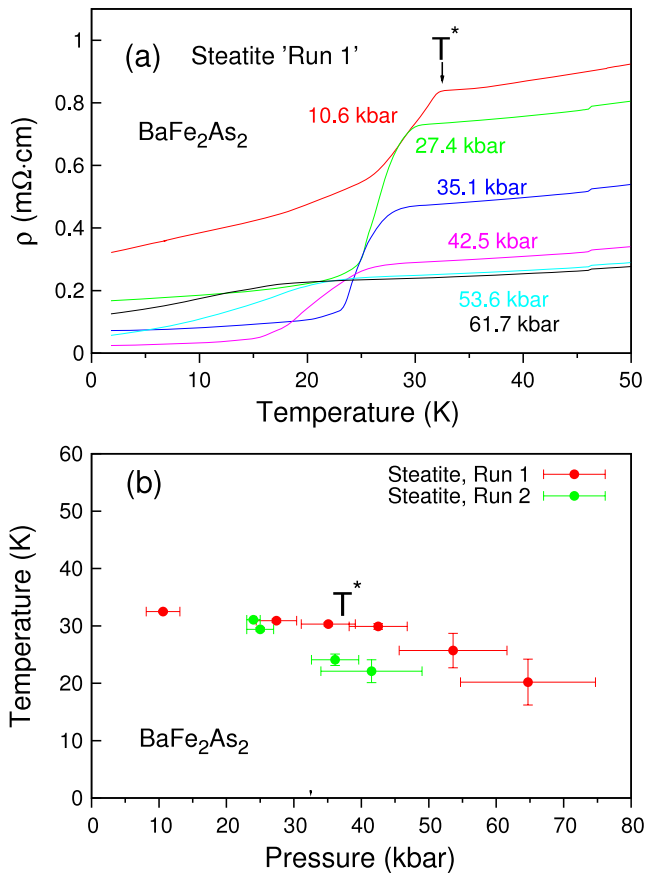


Figure 3. Resistivity measurements of BaFe_2As_2 using steatite as the pressure medium in a Bridgman cell. A representative data set ('Run 1') is shown in (a). The pressure evolution of the onset of the superconducting transition T^* is shown in (b).

superconductivity appears already at 10 kbar in a sample embedded in steatite. These results demonstrate that the precise pressure conditions strongly influence the high pressure

properties of BaFe_2As_2 . Since the minimal pressure for the onset of superconductivity or the critical pressure for the suppression of spin density wave order shifts by several tens of kbar in different pressure setups, simple pressure inhomogeneity (pressure gradients across the sample) does not explain the observed differences. Instead, non-hydrostaticity in opposed anvil setups is expected to arise in form of considerable uniaxial components leading to uniaxial stress on the sample. Therefore, our measurements show that increased uniaxial stress components along the c -axis suppress the spin density wave order at a faster rate. Uniaxial stress components also favour the appearance of a regime of at least filamentary superconductivity, which extends to lower nominal pressure in those pressure media, in which the uniaxial stress component is larger.

A comparison of our results with other high pressure data on BaFe_2As_2 (table 1) shows that the variations in previously observed phase diagrams can be explained by the differences in the pressure conditions alone. This follows from our result that we can reproduce a similar range of different phase diagrams using samples from the same batch with the same sample quality. It still remains to be seen, whether pressure-induced *bulk* superconductivity is intrinsic to BaFe_2As_2 . So far, one study reported evidence for bulk superconductivity in BaFe_2As_2 [21]. However, there are studies involving very high ([28]) and quite low (our measurements in steatite) levels of hydrostaticity, in which bulk superconductivity is absent up to high pressures.

The dependence of the pressure–temperature phase diagram of BaFe_2As_2 on the level of hydrostaticity is reminiscent of what has been reported in the case of SrFe_2As_2 [15]. There, the phase diagram is influenced in a qualitatively similar way by uniaxial pressure components, although the effect is more dramatic in the case of BaFe_2As_2 . Similarly, in CaFe_2As_2 , superconductivity near the structural transition only appears when there is sufficient pressure inhomogeneity. The resulting shear stress gives rise to a

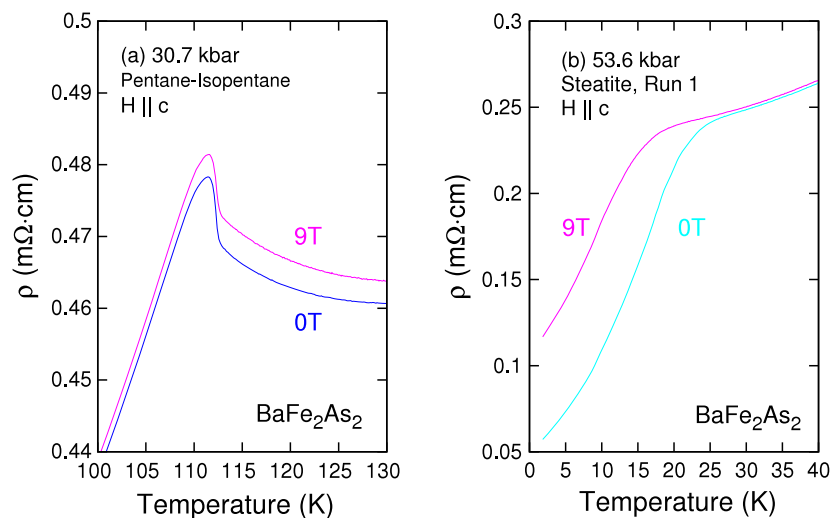


Figure 4. Effect of a magnetic field on the observed transitions. (a) The magnetosuperconducting transition (T_{SDW}) in the resistivity measurement at 30.7 kbar using pentane–isopentane as the pressure medium in a piston cylinder cell. This transition does not show any significant field dependence (b) The superconducting transition (T^*) in the resistivity measurement at 53.6 kbar using steatite as the pressure medium in a Bridgman cell. This transition has a clear field dependence.

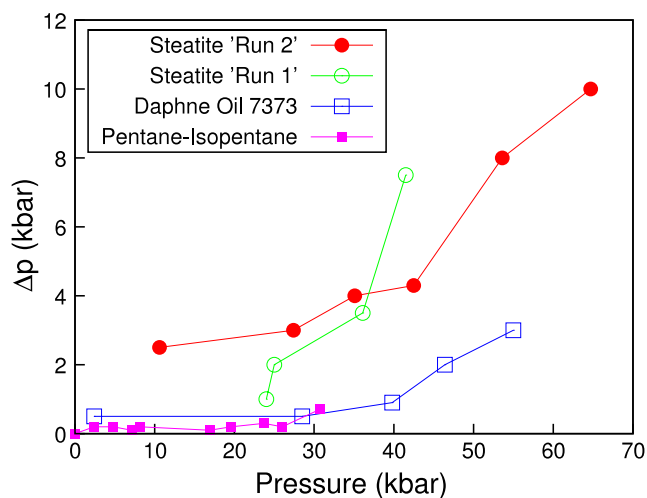


Figure 5. The pressure inhomogeneity (Δp) for each of the different pressure media as a function of pressure, as calculated from the width of the superconducting transition of the pressure gauge. The pressure media in order of highest hydrostaticity are pentane–isopentane, Daphne oil 7373, and steatite.

metastable phase and superconductivity is absent when a helium pressure medium is used [29]. An exception is the spin density wave order of CaFe_2As_2 , which is not more strongly suppressed by less hydrostatic [12] or even uniaxial pressure conditions [30]. The comparison of our and previous results on 1-2-2 compounds shows that sensitivity to the precise pressure conditions is a generic phenomenon of this material class.

The stronger suppression of spin density wave order in BaFe_2As_2 by a uniaxial pressure component rather than by hydrostatic pressure alone might be a consequence of the effects of uniaxial stress on the Fermi surface. Stronger reduction of the c/a ratio will tend to increase interplane hopping and warping of originally cylinder-like Fermi surface sheets. As a consequence nesting will be reduced, which decreases the possibility for spin density wave order to form. To test this interpretation it is best to focus on studies, which provide the most direct link between lattice and electronic properties. This includes studies using pressure tuning or charge-neutral chemical substitution but excludes studies involving electron or hole doping. Examples for the suppression of spin density wave order being accompanied by a reduction of the c/a ratio are tuning BaFe_2As_2 by pressure [17] or substitution of As by P [31] or tuning SrFe_2As_2 by Ru substitution [32].

The ways to optimize any superconducting transition temperature (T_c) might be independent from the best way to suppress spin density wave order. For optimizing T_c several key factors have been proposed: the c/a ratio in connection with SrFe_2As_2 [15], the pnictogen height in connection with NdFeAsO and LaFePO (which is also supposed to influence the symmetry of the order parameter) [33], or the As–Fe–As bond angles in connection with $\text{CeFeAsO}_{1-x}\text{F}_x$ and BaFe_2As_2 (which should approach the value for an ideal tetrahedron) [17, 34]. Our and previous data on BaFe_2As_2 (table 1) suggests that the highest values for T_c are found in those experiments, in which the lowest hydrostatic pressure

was needed to suppress the spin density wave transition and thereby to induce superconductivity. This implies that, once spin density wave order has been suppressed, T_c is optimised by having a larger unit cell volume and a larger c/a ratio. However, before a final answer can be expected, the intrinsic nature of superconductivity in BaFe_2As_2 has to be better established.

In summary, our investigation in three different pressure environments demonstrates that the pressure–temperature phase diagram of BaFe_2As_2 is extremely sensitive to the precise pressure conditions and, in particular, to the level of resulting uniaxial stress. Reducing the c/a ratio of a magnetically ordered FeAs compound appears to suppress spin density wave order and favour superconductivity.

References

- [1] Hu W Z, Dong J, Li G, Li Z, Zheng P, Chen G F, Luo J L and Wang N L 2008 *Phys. Rev. Lett.* **101** 257005
- [2] Rotter M, Tegel M and Johrendt D 2008 *Phys. Rev. Lett.* **101** 107006
- [3] Sasmal K, Lv B, Lorenz B, Guloy A, Chen F, Xue Y Y and Chu C W 2008 *Phys. Rev. Lett.* **101** 107007
- [4] Jeevan H S, Hossain Z, Kasinathan D, Rosner H, Geibel C and Gegenwart P 2008 *Phys. Rev. B* **78** 092406
- [5] Ni N, Kreyssig A, Goldman A I, Mun E D, Bud'ko S L and Canfield P C 2008 *Phys. Rev. B* **78** 014523
- [6] Pfisterer M and Nagorsen G 1980 *Z. Naturf. b* **35** 703
- [7] Rotter M, Tegel M, Johrendt D, Schellenberg I, Hermes W and Pöttgen R 2008 *Phys. Rev. B* **78** 020503
- [8] Huang Q, Qiu Y, Bao W, Green M A, Lynn J W, Gasparovic Y C, Wu T, Wu G and Chen X H 2008 *Phys. Rev. Lett.* **101** 257003
- [9] Mathur N D, Grosche F M, Julian S R, Walker I R, Freye D M, Haselwimmer R K W and Lonzarich G G 1998 *Nature* **394** 39
- [10] Lefebvre S, Wzietek P, Brown S, Bourbonnais C, Jérôme D, Mézière C, Fourmigué M and Batail P 2000 *Phys. Rev. Lett.* **85** 5420
- [11] Takabayashi Y, Ganin A Y, Jeglic P, Arcon D, Takano T, Iwasa Y, Ohishi Y, Takata M, Takeshita N, Prassides K and Rosseinsky M J 2009 *Science* **323** 1585
- [12] Torikachvili M S, Bud'ko S L, Ni N and Canfield P C 2008 *Phys. Rev. Lett.* **101** 057006
- [13] Chu C W and Lorenz B 2009 *Physica C* **469** 385
- [14] Park T, Park E, Lee H, Klimczuk T, Bauer E D, Ronning F and Thompson J D 2008 *J. Phys.: Condens. Matter* **20** 322204
- [15] Kotegawa H, Kawazoe T, Sugawara H, Murata K and Tou H 2009 *J. Phys. Soc. Japan* **78** 083702
- [16] Kofu M, Qiu Y, Bao W, Lee S H, Chang S, Wu T, Wu G and Chen X H 2009 *New J. Phys.* **11** 055001
- [17] Kimber S A J, Kreyssig A, Zhang Y Z, Jeschke H, Valenti R, Yokaichiya F, Colombier E, Yan J, Hansen T C, Chatterji T, McQueeney R J, Canfield P C, Goldman A I and Argyriou D N 2009 *Nat. Mater.* **8** 471
- [18] Singh D J 2008 *Phys. Rev. B* **78** 094511
- [19] Shein I R and Ivanovskii A L 2008 *J. Exp. Theor. Phys. Lett.* **88** 107
- [20] Zhang Y-Z, Kandpal H C, Opahle I, Jeschke H O and Valenti R 2009 *Phys. Rev. B* **80** 094530
- [21] Alireza P L, Ko Y T C, Gillett J, Petrone C M, Cole J M, Lonzarich G G and Sebastian S E 2009 *J. Phys.: Condens. Matter* **21** 012208
- [22] Fukazawa H, Takeshita N, Yamazaki T, Kondo K, Hirayama K, Kohori Y, Miyazawa K, Kito H, Eisaki H and Iyo A 2008 *J. Phys. Soc. Japan* **77** 105004

- [23] Colombier E, Bud'ko S L, Ni N and Canfield P C 2009 *Phys. Rev. B* **79** 224518
- [24] Mani A, Ghosh N, Paulraj S, Bharathi A and Sundar C S 2009 *Europhys. Lett.* **87** 17004
- [25] Matsubayashi K, Katayama N, Ohgushi K, Yamada A, Munakata K, Matsumoto T and Uwatoko Y 2009 *J. Phys. Soc. Japan* **78** 073706
- [26] Ahilan K, Ning F L, Imai T, Sefat A S, McGuire M A, Sales B C and Mandrus D 2009 *Phys. Rev. B* **79** 214520
- [27] Chu J H, Analytis J G, Kucharczyk C and Fisher I R 2009 *Phys. Rev. B* **79** 014506
- [28] Matan K, Morinaga R, Iida K and Sato T J 2009 Anisotropic itinerant magnetism and spin fluctuations in BaFe_2As_2 : a neutron scattering study *Phys. Rev. B* **79** 054526
- [29] Yu W, Aczel A A, Williams T J, Bud'ko S L, Ni N, Canfield P C and Luke G M 2009 *Phys. Rev. B* **79** 020511
- [30] Torikachvili M S, Bud'ko S L, Ni N, Canfield P C and Hannahs S T 2009 *Phys. Rev. B* **80** 014521
- [31] Jiang S, Xing H, Xuan G, Wang C, Ren Z, Feng C, Dai J, Xu Z and Cao G 2009 *J. Phys.: Condens. Matter* **21** 382203
- [32] Schnelle W, Leithe-Jasper A, Gumeniuk R, Burkhardt U, Kasinathan D and Rosner H 2009 *Phys. Rev. B* **79** 214516
- [33] Kuroki K, Usui H, Onari S, Arita R and Aoki H 2009 *Phys. Rev. B* **79** 224511
- [34] Zhao J, Huang Q, de La Cruz C, Li S, Lynn J W, Chen Y, Green M A, Chen G F, Li G, Li Z, Luo J L, Wang N L and Dai P 2008 *Nat. Mater.* **7** 953