IRON-BASED SUPERCONDUCTORS

Enigmatic nematic

Iron pnictide superconductors often feature nematic, symmetry-breaking electronic states. These phenomena are now found to persist into the tetragonal phase of NaFeAs — a new piece of information that may help settle the fundamental origin of nematic electronic states.

J. C. Davis and P. J. Hirschfeld

Spontaneously broken symmetry is a fundamental concept in modern physics. The ground state of a system can have, below a critical temperature, a lower symmetry than that of its total-energy function. A classic example is a ferromagnet, the energy of which can be invariant under rotations of the electronic spins but which nevertheless has all spins settling to a particular direction below its so-called Curie temperature. In recent years, new broken symmetries have been discussed in materials with mobile electrons, in which the total electronic wavefunction features a lower symmetry than that of the crystal hosting it. In particular, several different types of order that are analogous to those found in liquid crystals have been predicted and identified[1,2]. For nematic order, for example, the electronic state has the same translational periodicity as the underlying crystal, but a lower rotational symmetry.

Nematic states have been reported for many iron-based superconductors[3,4], and are characterized by a large 'nematic susceptibility', that is, the electronic ground state has a strong tendency to deform in response to a small structural symmetry-breaking perturbation. Take, for example, the famous iron-based superconducting compound $Ba(Fe_{1-x}Co_x)_2As_2$. Above the critical temperature T_N where the magnetization vanishes, but below the temperature T_S where the system's crystal structure changes from tetragonal to orthorhombic (Fig. 1), the *a* and *b* lattice constants differ by only a few tenths of a per cent, yet the fractional difference in the resistivities measured in the two directions can be as large as 30% (ref. 5). By contrast, on entering the high-temperature tetragonal phase ($T > T_S$), the nematic signal disappears rapidly in the resistivity anisotropy measurements.

Now, writing in *Nature Physics*, Ethan Rosenthal and colleagues[6] present another wrinkle in this physical picture, based on scanning tunnelling microscopy and real-space differential conductance data for a sample of NaFeAs.

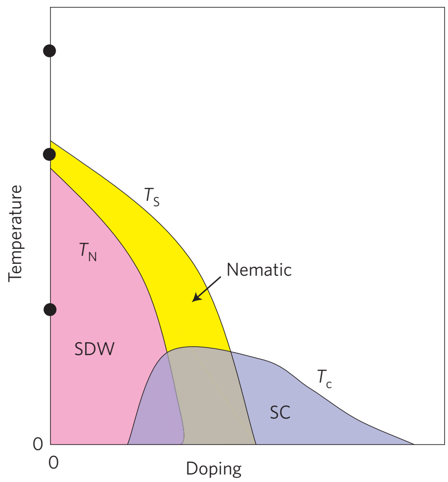

Figure 1 | Schematic temperature versus chemical-doping phase diagram of an iron-based superconductor displaying a crystal structure transition from tetragonal to orthorhombic. For temperatures below T_N, there is antiferromagnetic order (spin-density wave state). Below T_S, the crystal structure is orthorhombic whereas, for $T > T_S$, the crystal structure is tetragonal. T_c is the critical temperature for superconductivity. Normally, the symmetry of the electronic ground state follows that of the underlying crystal lattice. However, for NaFeAs Rosenthal *et al.*[6] (measuring for no chemical doping; black dots) now find that the symmetry of the electronic wavefunctions surrounding impurity atoms is orthorhombic well above T_S (persistent nematicity), adding a new piece to the complicated puzzle of iron-based superconductivity.

At low temperatures, elongated electronic impurity-states with two-fold rotational symmetry (C_2) are observed around impurity-atom sites, consistent with similar impurity-states observed in the equivalent phase of another iron-based compound[7,8]. This is not a surprising situation, as this is a magnetic phase exhibiting a stripe-like ordering of spins, which itself already breaks the four-fold rotational symmetry (C_4) of the crystal lattice. Rosenthal *et al.* find that these anisotropic impurity-states persist into the nematic phase between T_N = 39 K and T_S = 54 K, but here too the C_4 symmetry is broken by the crystal structure. Above T_S, however, the crystal structure is tetragonal ($a = b$, C_4) and there should be no small symmetry-breaking field to drive a nematic response. Nevertheless, the authors discovered the persistence of the C_2-symmetric anisotropic impurity-states for temperatures up to nearly twice T_S, which is perhaps related to the high-temperature persistence of symmetry breaking also reported in torque magnetometry experiments[9].

What is the origin of this tetragonal symmetry breaking of the electronic structure at high temperatures ($T > T_S$) in these systems? A possible explanation, proposed by Rosenthal and colleagues, is that nematic susceptibilities are so large, even at high temperatures, that residual strains present in the sample create small nematic regions with orthorhombic crystal symmetry ($a \neq b$, C_2). However, the origin of this tendency remains unclear. Theories have been put forward suggesting that either the magnetic moments of the iron atoms (ordering below T_N) or the iron *d*-orbital degrees of freedom (assumed to order below T_S) provide the driving mechanism for nematicity. Rosenthal and colleagues consider several further analyses to answer this fundamental question[6]. They performed an impressive temperature-dependent quasiparticle scattering interference (QPI) analysis of the anisotropic impurity-states in NaFeAs. Visualizing QPI enables the measurement of the characteristic wavelengths of the electronic ripples (Friedel oscillations) caused by local perturbations like impurity atoms. The QPI patterns have C_2 symmetry for temperatures up to nearly 90 K, and feature two characteristic dispersing wavevectors. The authors' explanation for this remarkable symmetry-breaking effect is a softening of electronic fluctuations along one crystal axis.

Do such fluctuations have magnetic or orbital character? Rosenthal *et al.* point out that the size of the anisotropy signal at high temperatures is strongly peaked at an energy close to the magnitude of the spin density wave (SDW) gap — the typical splitting of the metallic bands in the magnetic state observed in the tunnelling spectrum at low temperatures. Based on this concurrence, they propose that the fluctuations must have spin character, and occur on a scale typical of magnetic energies.

Although the results of Rosenthal *et al.* are definitely exciting, several questions remain. First, what is the basic mechanism for the creation of these highly anisotropic electronic states that form around simple defects in NaFeAs? It was recently shown that, theoretically[10], similar magnetic states can form and grow surprisingly large in the SDW state, and tend to have a dimer-like structure similar to that observed in $CaFe_2As_2$ (ref. 8). It remains to be seen, however, whether such states can survive in the nematic phase and at higher temperatures. In particular, it would be very interesting to find out whether such dimer-like electronic structures could do a better job of reproducing the NaFeAs QPI data than the impurity potentials considered by Rosenthal and colleagues and rejected as an explanation of their data.

Second, how airtight is the identification of spin degrees of freedom as the driving mechanism for nematicity? In the Lee–Rice–Anderson approach[11] used by Rosenthal and colleagues, the low-temperature SDW gap does not appear explicitly, so the only connection with the energy of the nematic response to impurity atoms occurs through its coincidence with the typical energy scale of a spin fluctuation. Because orbital ordering occurs at very similar temperatures, could it be that the energy peak of the nematic signal lying within the SDW energy gap is fortuitous? A resolution of this question requires a thorough theoretical calculation of the QPI signal in the fluctuating regime, including both spin and orbital degrees of freedom.

Finally, what ultimately drives the large nematic susceptibility responsible for the various remarkable phenomena (magnetism, orthorhombic-to-tetragonal structural transition and enhanced nematic fluctuations) observed for NaFeAs, but absent in LiFeAs, a structurally similar superconductor? As is now commonplace in the field of iron-based superconductors, the answer seems to depend on details, but an understanding of these details could prove crucial for uncovering the origin of superconductivity and finding a recipe to increase the critical temperature. ❐

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References

1. Kivelson, S. A., Fradkin, E. & Emery, V. J. *Nature* **393,** 550–553 (1998).
2. Fradkin, E., Kivelson, S. A., Lawler, M. J., Eisenstein, J. P. & Mackenzie, A. P. *Annu. Rev. Condens. Matter Phys.* **1,** 153–178 (2010).
3. Hu, J. P. & Xu, C. *Physica C* **481,** 215–222 (2012).
4. Fernandes, R. M. & Schmalian, J. *Supercond. Sci. Technol.* **25,** 084005 (2012).
5. Chu, J.-H. *et al. Science* **329,** 824–826 (2010).
6. Rosenthal, E. P. *et al. Nature Phys.* **10,** 225–232 (2014).
7. Chuang, T.-M. *et al. Science* **327,** 181–184 (2010).
8. Allan, M. P. *et al. Nature Phys.* **9,** 220–224 (2013).
9. Kasahara, S. *et al. Nature* **486,** 382–385 (2012).
10. Gastiasoro, M. N., Hirschfeld, P. J. & Andersen, B. M. Preprint at http://arxiv.org/abs/1307.4913 (2013).
11. Lee, P. A., Rice, T. M. & Anderson, P. W. *Phys. Rev. Lett.* **31,** 462–465 (1973).

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SOFT MATTER

A triangular affair

Disks interacting via particular potentials self-organize into triangles that stabilize mosaics with 10-, 12-, 18- and 24-fold symmetry, as revealed by computer simulations. Discoveries of further novel quasicrystals may now be within reach.

Michael Engel and Sharon C. Glotzer

Thirty years after their discovery, and after being celebrated by the 2011 Nobel Prize in Chemistry, quasicrystals are well recognized as thermodynamic equilibrium states of matter. We now know that long-range order does not require spatial periodicity. However, despite significant progress, why and how quasicrystals arise is still not fully resolved. Writing in *Nature*, Tomonari Dotera and colleagues address this problem by searching for a generic mechanism for quasicrystal formation in soft matter[1]. Unlike in alloys, where icosahedral and 10-fold quasicrystals are abundant, nearly all reported soft-matter quasicrystals[2] have 12-fold symmetry[3]. Working with a surprisingly simple model system, Dotera *et al.* now report old and new tilings, and discuss their relation to quasicrystals found in macromolecular and nanoparticle systems.

The team performed Monte Carlo computer simulations of identical disks in two dimensions that interact through hard-core/square-shoulder (HCSS) potentials. The simulations use three rules of interaction[4]: (1) particles may not approach closer than a distance σ, (2) particles do not interact at distances greater than $\lambda\sigma$ and (3) there is a modest energy penalty ε for each pair at distances between σ and $\lambda\sigma$. The behaviour of the system is determined by the ratio λ of the shoulder radius to the hard-core radius, the density and the temperature.

It is illustrative to discuss previous findings concerning the HCSS model. Two limits of the parameter λ have been studied extensively. For $\lambda = 1$, the hard-disk model is recovered. Hard disks exhibit a fluid phase, a long-debated hexatic phase[5] and a hexagonal crystal phase — all stabilized by entropy. In the opposite limit, when λ is large, the hard core disappears. Particles then resemble ultrasoft colloids[6] and form stripes[7] and micellar cluster crystals[8] — both are mesophases typical for block copolymers and other systems with competing interactions. In between these limits, when $1 < \lambda < 2$, the system exhibits re-entrant melting[4], which means that compression of the solid induces melting. Re-entrant melting is an example of anomalous thermodynamic behaviour observed for water and other network-forming liquids. The observation of re-entrant melting explains why the HCSS system and related soft-core systems are test beds for the study of liquid–liquid phase transitions[9].

Despite intensive previous work, and the simplicity of the HCSS model, little is known about the ordered phases occurring in the intermediate λ regime. This is surprising, because the existence of