Nematic correlation length in iron-based superconductors probed by inelastic X-ray scattering

Rod-shaped molecules in liquid crystals sometimes spontaneously align by "choosing" one of several equivalent orientations. This ordering is called nematic. Surprisingly, low temperature electronic nematic order was observed in iron (Fe)-based superconductors: Fluctuations of electronic spins and orbitals choose one of two equivalent orientations based on crystal symmetry. In many Fe-based superconductors, such as doped $BaFe_2As_2$, nematicity is believed to arise as a vestigial order of the stripe spin-density wave state that sets in at a lower temperature and selects one of two orthogonal wave-vectors related by a 90° rotation [1]. An exception may be FeSe, where nematic order sets in at 90 K, but magnetic order does not form at any temperature at ambient pressure [1], although antiferromagnetic (AFM) order appears under pressure. The origin of nematic order in FeSe remains a topic of intense debate.

The impact of the electron-phonon coupling on the nematic order in Fe-based superconductors has been investigated in different contexts.

Transverse acoustic (TA) phonons dispersing in the [100] direction exhibit the strongest experimentally observed electron-phonon coupling. They soften with temperature (T) on approaching the orthorhombic distortion at the structural transition temperature (T_S) of the atomic lattice in the nematic phase [2]. Quantitative analysis of this softening allows extracting the nematic correlation length ξ [2].

The new experiments [3] compared the T dependence of ξ in FeSe and underdoped $Ba_2(Fe_{1-x}Co_x)_2As_2$ (UD Ba-122), whose doping level (x = 0.03) was chosen such that its structural transition temperature T_S = 95 K was close to that of FeSe, which was T_S = 90 K. In addition, detailed measurements of an optimally doped $Ba(Fe_{0.94}Co_{0.06})_2As_2$ (OP Ba-122) sample with a superconducting transition temperature T_c = 25 K, reached larger wave vectors than in the previous study [3]. To achieve better wave vector resolution with larger scattering intensity, inelastic X-ray scattering instead of neutron scattering was used.

Measurements were carried out on the high-resolution inelastic X-ray scattering beamlines SPring-8 **BL43LXU** and APS Sector 30. The phonon softening is clearly seen in Fig. 1(a) as the separation between energy loss and energy gain peaks decreases and the intensity increases upon cooling toward T_S. The trend reverses upon further cooling. Figure 1(b), where the peaks are well separated, shows the individual contributions of the elastic peak plus the Stokes and anti- Stokes phonon peaks. The phonon energy at **Q** = (2, 0.05, 0) in FeSe as a function of temperature is similar to the expected behavior of the shear modulus C_{66} from mean-field theory (inset of Fig. 1(a)), which cannot otherwise be observed below T_S by three-point bending or resonant ultrasound experiments due to twinning in the sample.

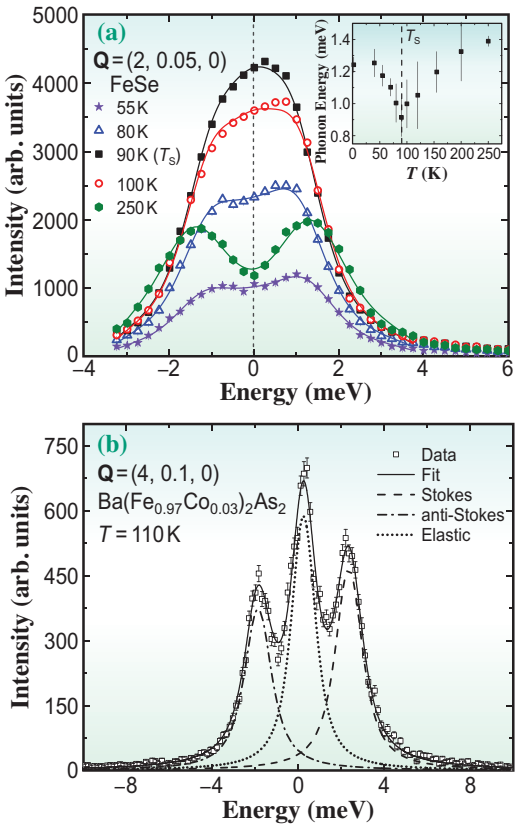

Fig. 1. Raw data with fits. **(a)** Energy scans on FeSe at **Q** = (2, 0.05, 0). Data taken at T_S = 90 K are represented by the black squares. Error bars are similar in size to the symbols. Inset: Phonon energy at **Q** = (2, 0.05, 0), with T_S marked by the dashed line. **(b)** An example fit for data on UD Ba-122 at **Q** = (4, 0.1, 0), T = 110 K. The raw data are represented by the empty symbols, the total fit by the solid black line, and then the elastic, Stokes, and anti-Stokes peaks by the dotted, dashed, and dash-dotted lines, respectively.

Figure 2 shows the phonon dispersion (solid lines) in (a) UD Ba-122 at 290 and 98K (T_S = 95 K) and (b) in FeSe at 300 and 95 K (T_S = 90 K) fitted with Eq. 1 in Ref. 4, where ξ is the only free parameter. The fits accurately described the phonon behavior at all recorded temperatures, including the phonon softening effect near the structural transition temperature.

There was a striking similarity in the behaviors of the nematic correlation lengths between all three compounds, despite their rather different ground states, demonstrated in Fig. 3. Most importantly, the T dependence of ξ in FeSe and underdoped and optimally doped $Ba_2(Fe_{1-x}Co_x)_2As_2$ is very well described by $(T - T_0)^{-1/2}$. Combined with the Curie-Weiss behavior observed in nematic susceptibility, these results point to a mean-field behavior with fluctuations extending to rather high temperatures above the structural transition temperature T_S. This mean-field behavior may originate from the coupling to the lattice, which is known theoretically to change the universality class of the nematic transition from Ising-like to mean field due to the long-range nematic interactions mediated by strain fluctuations.

These observations highlight the key role played by the nematoelastic coupling, which not only changes the character of the nematic transition, but also extends the impact of the nematic fluctuations to rather high temperatures above T_S. Such a coupling has been proposed to be detrimental to the enhancement of T_c by quantum critical nematic fluctuations. Whether this explains the observed behavior of T_c across the phase diagram of chemically substituted $FeSe_{1-x}S_x$, is an interesting topic for future investigation. Moreover, the similar behavior of the nematic correlation length in FeSe and Ba-122 raises important questions about the interplay between nematicity and magnetism. Although FeSe displays no long-range magnetic order, it has a strong fluctuating magnetic moment, comparable to that of Ba-122. Whether this is enough to explain the similar behavior of ξ in both compounds is an issue that deserves further studies.

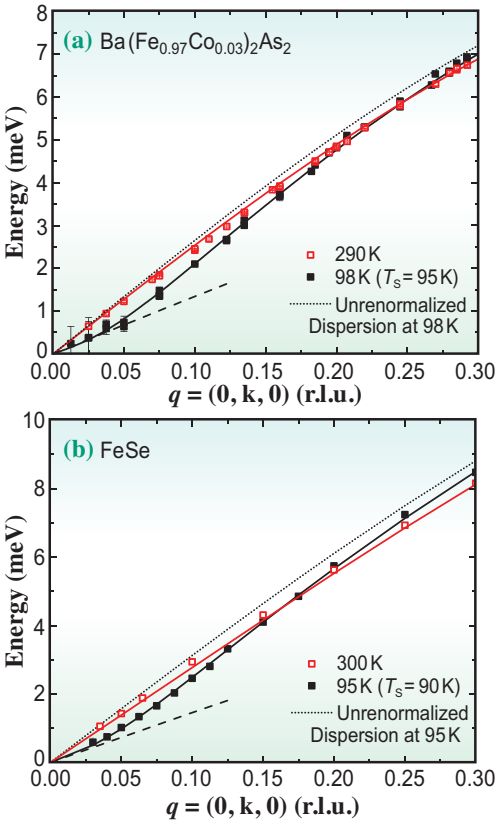

Fig. 2. Phonon dispersion fits for UD Ba-122 **(a)** and FeSe **(b)**. The dotted black line is the expected dispersion in the absence of nematic fluctuations. The data (solid black squares) and fit (solid black curve) show clearly visible softening that increases at low q. The dashed line shows the expected low q slope if the nematic correlation length was very small; it matches the phonon energies only at very low q. Hollow red squares (solid red line) show data (fit) at high temperature.

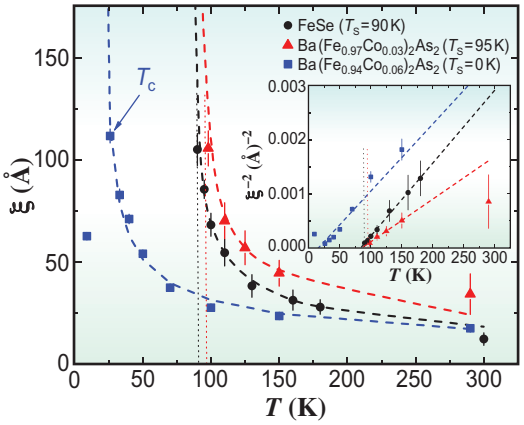

Fig. 3. Nematic correlation length as a function of temperature for FeSe (black circles), for UD Ba-122 (red triangles), and for OP Ba-122 (blue squares). The dashed lines are power-law fits of the form $\xi = \xi_0/(T - T_0)^{1/2}$. Note that only the data above T_c were fit for OP Ba-122, since the increase in nematic correlation length on cooling is reversed by superconductivity. Inset: ξ^{-2} for the materials as in the main panel, with linear fits (dashed lines). It demonstrates the universal power-law behavior with the x intercepts at 84 ± 1 K for FeSe, 86 ± 2 K for UD Ba-122, and 16 ± 4 K for OP Ba-122.

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