Nature of charge density waves in the cuprate high-T_c superconductors

In conventional metals, the valence electrons are spread uniformly throughout the material. But in some substances, such as high-temperature superconductors (HTSCs), the electrons can form periodic modulations known as charge density waves (CDWs) which deform the underlying atomic crystal lattice of the metal. In 2012, researchers discovered this electronic state in the HTSC $YBa_2Cu_3O_{6+\delta}$, triggering intense debate about whether this behavior has the same origin as charge correlations discovered in another HTSC family, $La_{2-x}Ba_xCuO_4$, over twenty years ago [1,2]. Now, an international research team lead by Brookhaven National Laboratory has used state-of-the-art inelastic X-ray scattering (IXS) instrumentation at SPring-8 **BL43LXU** to examine the CDW correlations in $La_{2-x}Ba_xCuO_4$ through its interaction with collective lattice motions. The researcher found strong experimental evidence to support a unified CDW mechanism in high-temperature superconductors [3].

The research started by determining the collective lattice motions, also known as phonons, of $La_{1.875}Ba_{0.125}CuO_4$ at the room temperature. As shown in Fig. 1, two phonon modes, M1 and M2, are experimentally identified, and in agreement with the first principle calculations. From the calculations, the researchers ascertain that these modes are primarily associated with *z*- and *y*-direction motions of the La and Cu atoms. By gradually cooling the sample down, the researchers are able to track the temperature dependent changes of these phonons down to –265°C. Figure 2 shows representative experimental spectra at different temperature and different *K*. Strong temperature dependence is seen at the CDW wavevector $K = 0.23$ in reciprocal lattice units (r.l.u.), whereas the $K = 0.09$ and 0.35 r.l.u. show no obvious temperature dependence. By carefully analyzing and fitting the experimental data, the researcher discovered a large phonon softening associated with precursor CDW fluctuations. Significantly, as shown in Fig. 3, the phonon softening wavevector of the precursor CDW changes from 0.238 r.l.u. at –265°C to 0.3 r.l.u. at room temperature.

In cuprates, the origin of the CDW is under debate between reciprocal space pictures such as Fermi-surface nesting and real space pictures with strong magnetic and Coulomb interactions. In the first class of scenarios, the most important property of the

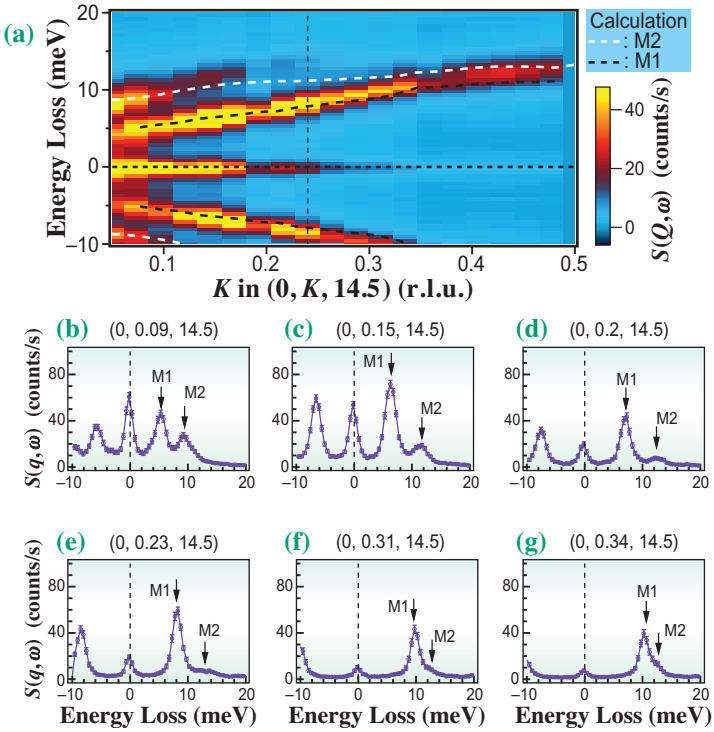

Fig. 1. **(a)** Color map around (0, *K*, 14.5) for $K = 0 \rightarrow 0.5$ r.l.u., showing two phonon modes labeled M1 and M2 that match theoretical predictions shown as dashed lines. **(b)-(g)** Representative experimental spectra at $K = 0.09, 0.15, 0.2, 0.23, 0.31$ and 0.34 r.l.u., respectively.

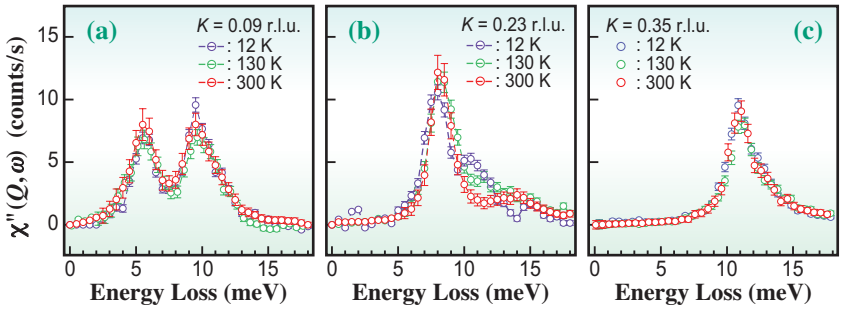

Fig. 2. Temperature dependence of the $La_{1.875}Ba_{0.125}CuO_4$ phonon spectra. **(a)–(c)** Elastic-line-subtracted and Bose-factor-corrected IXS spectra at K = 0.09, 0.23, and 0.35 r.l.u., respectively. Purple, green, and red circles correspond to data at 12, 130, and 300 K, respectively. Strong temperature dependence is seen at 0.23 r.l.u., whereas the K = 0.09 and 0.35 r.l.u. show no obvious temperature dependence.

ground state is the wave vector. Here, the temperature dependence of the incommensurability shown in Fig. 3 does not match theoretical expectations based on the Fermi surface. These scenarios would predict that the CDW wave vector should either decrease at higher temperatures or be temperature independent, neither of which is observed here. Instead, real space pictures are likely more important. These include those based on the competition between minimizing the number of broken magnetic bonds and kinetic energy and Coulomb repulsion between the doped holes. In such scenarios, the ordering wave vector arises from a balance between different ordering tendencies and is not a crucial defining parameter of the mechanism. These scenarios are more compatible with our observed variation of the CDW wave vector with temperature, which implies that the CDW wave vector is not solely defined by doping. It should be noted that a similar conclusion has been put forward based on STM studies of $Bi_2Sr_2CaCu_2O_{8+x}$, where the authors found that the local CDW wave vector is doping independent and that the change of the wave vector is due to "phase slips" in the CDW domain boundaries and hence not a fundamental property of the CDW [4].

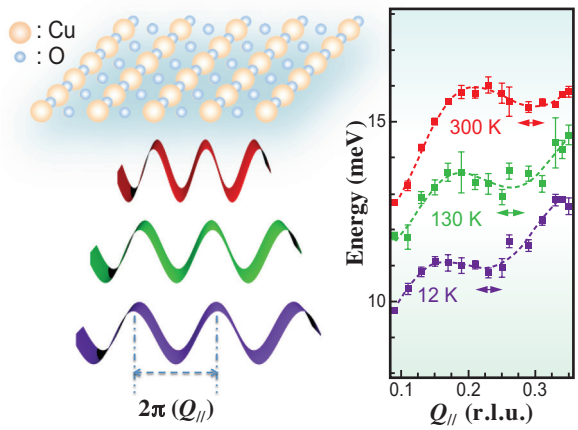

Fig. 3. Illustration of CDW periods associated with different wavevectors, $Q_{//}$. Phonon dispersions of M2 at 12, 130, and 300 K along (0 K 14.5) are shown as purple, green, and red squares. Dashed lines are guides to the eye, and arrows indicate the Q associated with the CDW-related phonon softening. Dispersions at 130 and 300 K are offset by 1.5 and 3 meV, respectively, for clarity.

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References

[1] R. Comin and A. Damascelli: Annu. Rev. Condens. Matter Phys **7** (2016) 369.
[2] H. Miao *et al.*: Proc. Natl. Acad. Sci. USA **114** (2017) 12430.
[3] *H. Miao, D. Ishikawa, R. Heid, M. Le Tacon, G. Fabbris, D. Meyers, G.D. Gu, A.Q. R. Baron and M.P.M. Dean: Phys. Rev. X* ***8*** *(2018) 011008.*
[4] A. Mesaros *et al.*: Proc. Natl. Acad. Sci. USA **113** (2016) 12661.