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Electron–phonon coupling in $BaFe_2As_2$: A possible origin of nematic phase

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ABSTRACT

Iron-based superconductors have the second-highest superconducting transition temperature next to cuprate superconductors. There are many electronic phases such as superconducting, antiferromagnetic and nematic phases, coexisting in the family of iron pnictides. The charge/spin orders are the key factors for understanding the mechanism of high-temperature superconductivity. In this paper we have performed a Raman scattering study of parent compound $BaFe_2As_2$. A relatively strong electron–phonon coupling is observed for B_{1g} phonon mode and is weakened after the structural transition at ~140 K. Through a careful symmetry analysis, we revealed the possibility that B_{1g} mode can be effectively coupled with d_{xz} and d_{yz} orbits. The coupling can remove the degeneracy of the two orbits and further cause the fluctuations of electronic nematic phases. The study suggests that electron–phonon coupling can be a possible origin of nematic phase.

1. Introduction

The discovery of LaOFeAs in 2008 inspired a new wave of research on iron-pnictide superconductors, due to the high transition temperature up to 55 K in the family [1]. There are many similarities between iron-based and cuprate superconductors. For instance, antiferromagnetic long-range orders and electron–phonon coupling are observed in the insulating parent compounds of both families [2,3]. Recent studies revealed a new order in iron-pnictides, i.e., electronic nematic phase [4]. The anisotropic resistivities were first observed by many groups [5–8]. Neutron scattering probed anisotropic spin excitations [9,10] and scanning electron microscopy [11] and point-contact spectroscopy [12] also observed the similar anisotropy. Furthermore, angle-resolved photoemission spectroscopy (ARPES) suggested a splitting of the d_{xz}/d_{yz} orbital bands [13,14]. The experiments point to the presence of electronic nematic phase. Electronic Raman scattering provided a direct probe for the excitations of nematic phase [15–21]. On the other hand, basically there are structural and spin-density-wave (SDW) transitions in iron-pnictides. The transitions are accompanied by a symmetry reduction from tetragonal to orthorhombic structures. This immediately gives rise to a basic question that for the lattice, charge and spin degrees of freedom, which one is the initial driving force.

The existing studies have pointed out that the anisotropy observed in resistivity is much larger than that of lattice [5,6]. It implies that the electronic nematic phase may be irrelevant to lattice vibrations. Furthermore, there is no long-range antiferromagnetic order in FeSe. This indicates that spin fluctuations instead of spin ordering can be considered as a possible option for the driving force [22–25]. Thus, it seems that the most possible candidate comes from the charge degrees of freedom [4]. In this paper our Raman experiments reveal a strong coupling between B_{1g} phonon mode and d_{xz}/d_{yz} orbits, which can reduce the symmetry of electronic system and break the degeneracy of d_{xz}/d_{yz} orbits. Therefore, the coupling may drive the formation of electronic nematic phase.

2. Samples and experiments

The high-quality single crystals were grown through the conventional self-flux method [26]. At high temperatures, the crystal exhibits a tetragonal structure with space group I4/mmm and point group D_{4h}. Symmetry analysis indicates that there are four Raman-active modes in the high-temperature phase: A_{1g}(As), B_{1g}(Fe), E_g(As), and E_g(Fe) [27]. After the structural and magnetic transitions at 140 K [28], the structure changes to orthorhombic phase with point group D_{2h}. Consequently, A_{1g}(As) changes to A_g(As) and each E_g mode will be split into B_{2g} and B_{3g} symmetries. The resistivity was measured by a standard four-probe method, which was performed in a physical property measurement system (PPMS, Quantum Design). Raman measurements were performed in a backscattering configuration with a triple-grating monochromator (Jobin Yvon T64000), equipped with a liquid-nitrogen cooled back-illuminated CCD detector,

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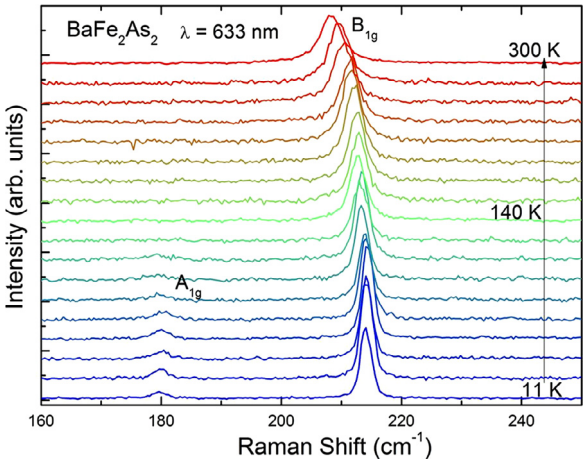

Fig. 1. Raman spectra collected at various temperatures. The structural and SDW transitions occur around 140 K.

delivering a spectral resolution better than 0.3 cm^{-1}. The light source was a 633 nm laser (Melles Griot) whose beam was focused into a spot of diameter approximately 10 μm on the sample surface.

3. Results and discussions

The temperature evolution of Raman spectra is shown in Fig. 1. The two modes located at 180 cm^{-1} and 215 cm^{-1} are A_{1g} mode of As atoms and B_{1g} mode of Fe atoms, respectively. With increasing temperatures, phonon intensities of both modes decrease and the peaks become more broader. A_{1g} mode completely disappears at structural transition ~140 K. B_{1g} mode demonstrates a continuous softening with increasing temperatures. And it also exhibits a clear asymmetry in lineshape, indicating the existence of a coupling between B_{1g} mode and other excitations. Generally, the asymmetric lineshape originates from the coupling between discrete and continuous excitations and can be described by the following Fano formula [29]:

$$I(\omega) = I_0 \frac{(q + 2(\omega - \omega_c)/\Gamma)^2}{1 + 4(\omega - \omega_c)^2/\Gamma^2}. \quad (1)$$

where I_0 is a parameter proportional to peak intensity, the peak position ω_c is the excitation energy after taking into account the coupling, Γ is the full width at half maximum (FWHM) and inversely proportional to the excitation lifetime, q represents the degree of asymmetry and its reciprocal reflects the coupling strength. In other words, a small q corresponds to a large asymmetry and hence a strong coupling. The peak will go back to a completely symmetric Lorentizan type without coupling when q approaches infinity. There are no other continuous excitations in the sample, except for electronic excitations. The asymmetry of B_{1g} mode can be naturally attributed to electron–phonon coupling. We have made a careful fitting using the Fano formula.

The fitting results of low-temperature and high-temperature spectra have been depicted in Fig. 2. The Fano fitting works very well for the spectra. The fitting parameters indicate that the width at low temperatures is roughly a half of the width at high temperatures and the peak has a more symmetric lineshape at low temperatures. The fitting parameters and their temperature dependence are summarized in Fig. 3.

Fig. 3a shows the temperature dependence of FWHM. A jump in FWHM can be seen around the structural transition ~140 K. The intrinsic widths contributed by phonon–phonon scattering, can be given by an anharmonic fitting of the low-temperature data, as indicated by the black curve and squares in Fig. 3a. After subtracting the widths contributed by phonon–phonon scattering, the residual widths are displayed in Fig. 3b. The residual parts exhibit a jump of ~0.6 cm^{-1} at 140 K, which is ~26% of the total widths and suggest a strong coupling. The temperature evolution of $|1/q|$ shows the similar behavior as resistivity (Fig. 3c). This supports that the residual phonon widths of B_{1g} mode comes from electron–phonon coupling. A larger $|1/q|$ or stronger coupling above the transition reduces the phonon lifetime and enhances the electronic scattering rate. In contrast, $|1/q|$ has a quick decrease across the transition and the

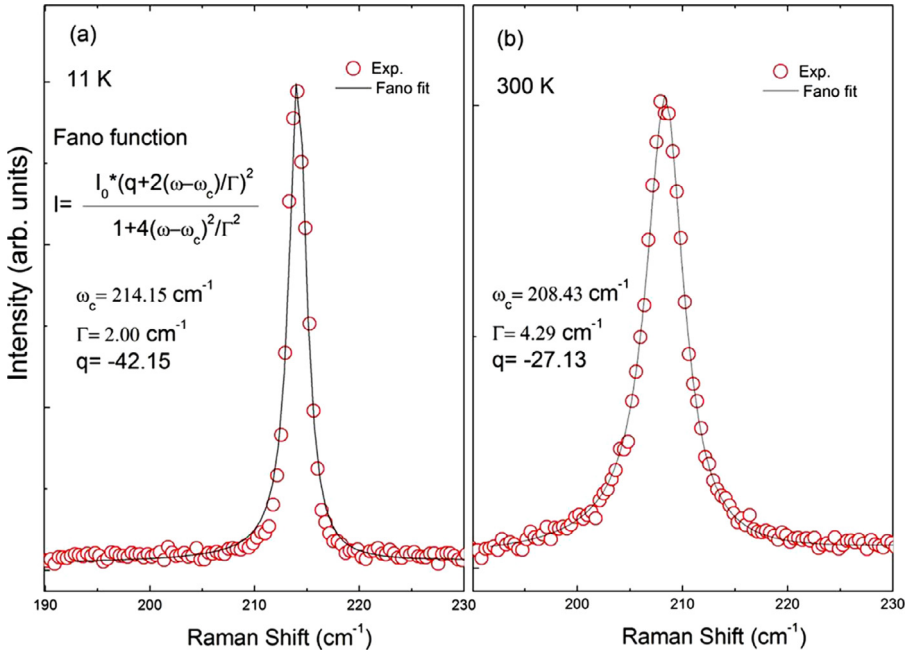

Fig. 2. Fano fitting for B_{1g} mode of $BaFe_2As_2$ at low (a) and high (b) temperatures. The red open circles and black solid lines are experimental data points and fitting curves, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)