ISSN 1674-1056
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http://iopscience.iop.org/cpb
中国物理 Chinese Physics B

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Citation: Chin. Phys. B . 2018, 27(8): 087402. **doi:** 10.1088/1674-1056/27/8/087402

Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

Chin. Phys. B Vol. 27, No. 8 (2018) 087402

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(Received 16 April 2018; revised manuscript received 24 May 2018; published online 25 July 2018)

Nematic order and its fluctuations have been widely found in iron-based superconductors. Above the nematic order transition temperature, the resistivity shows a linear relationship with the uniaxial pressure or strain along the nematic direction and the normalized slope is thought to be associated with nematic susceptibility. Here we systematically studied the uniaxial pressure dependence of the resistivity in $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$, where nonlinear behaviors are observed near the nematic transition temperature. We show that it can be well explained by the Landau theory for the second-order phase transitions considering that the external field is not zero. The effect of the coupling between the isotropic and nematic channels is shown to be negligible. Moreover, our results suggest that the nature of the magnetic and nematic transitions in $Sr_{1-x}Ba_xFe_2As_2$ is determined by the strength of the magnetic-elastic coupling.

Keywords: iron-based superconductors, nematic order, uniaxial pressure, resistivity

PACS: 74.70.Xa, 74.25.F– **DOI:** 10.1088/1674-1056/27/8/087402

1. Introduction

One of the basic building blocks of iron-based superconductors is the Fe–As or Fe–Se layers, where Fe ions form a square lattice.[1] In many systems, the electronic system shows in-plane anisotropic properties that are believed to be associated with the nematic order,[2–6] which breaks the C_4 rotational symmetry of the square lattice.[7] The onset of the nematic order is always coupled to a tetragonal-to-orthorhombic structural transition due to the electronic–lattice coupling,[7] i.e., the nematic transition temperature is equivalent to the structural transition temperature T_s. Therefore, from the symmetry point of view, the rotational symmetries of the nematic order and lattice are actually the same, which makes it hard to conclude whether the rotational symmetry breaking at T_s is driven by the electronic system or comes from the structural change. It is later found that the former picture should be appropriate,[8] where the nematic susceptibility is assumed to be proportional to the normalized slope of the strain dependence of elastoresistivity. This assumption has since been widely used in studying nematic susceptibility of iron-based superconductors.[9–14]

According to Ref. [8], the free energy of the nematic system under the uniaxial pressure p along the nematic direction can be written as follows:

$$F = F_0 + \frac{a}{2}\varphi^2 + \frac{b}{4}\varphi^4 + \frac{c}{2}\varepsilon^2 + \frac{d}{4}\varepsilon^4 + \lambda\varphi\varepsilon + p\varepsilon, \quad (1)$$

where F_0 is the free energy in the paranematic state, and φ and ε are the nematic order parameter and the strain, respectively. A linear coupling between φ and ε is required by the symmetry and λ is the magneto–elastic coupling. a, b, c, and d are the typical parameters in the Landau theory. Near the nematic transition, $a = a_0(T - T_0)$, where a_0 is a constant and T_0 is the mean-field nematic transition temperature without coupling to the strain. The nematic susceptibility $\mathrm{d}\chi/\mathrm{d}p$ or $\mathrm{d}\chi/\mathrm{d}\varepsilon$ is thus

$$\frac{\mathrm{d}\chi}{\mathrm{d}p} = \frac{-\lambda/a_0c}{T-(T_0+\lambda^2/a_0c)}, \quad (2)$$

$$\frac{\mathrm{d}\chi}{\mathrm{d}\varepsilon} = \frac{-\lambda/a_0}{T-T_0}, \quad (3)$$

which is valid when $p \to 0$. Experimentally, the resistance changes linearly with the uniaxial pressure or strain at high temperature along the nematic direction, so $\mathrm{d}\chi/\mathrm{d}p$ or $\mathrm{d}\chi/\mathrm{d}\varepsilon$ is treated as proportional to $\mathrm{d}(\Delta R/R_0)/\mathrm{d}p$ or $\mathrm{d}(\Delta R/R_0)/\mathrm{d}\varepsilon$, where R_0 is the resistance at zero pressure and $\Delta R = R(p) - R_0$.[8–13] Since R is normalized by R_0, the relative resistivity change $\Delta\rho/\rho_0$ is equivalent to $\Delta R/R_0$.

In practice, the application of an external pressure along one lattice axis will inevitably induce strains along all direc-

*Project supported by the Science Fonds from the Ministry of Science and Technology of China (Grant Nos. 2017YFA0302903, 017YFA0303103, 2016YFA0300502, and 2015CB921302), the National Natural Science Foundation of China (Grant Nos. 11674406 and 11674372), the "Strategic Priority Research Program (B)" of the Chinese Academy of Sciences (Grant Nos. XDB07020300 and XDB07020200), and the Youth Innovation Promotion Association of the Chinese Academy of Sciences.

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tions. As pointed out in Refs. [15] and [14], the relative change of the resistivity $\Delta\rho/\rho_0$ to strain ε can be understood within the point group of D_{4h} in the tetragonal notation as follows:

$$\left(\frac{\Delta\rho}{\rho_0}\right)_\alpha = \sum_{\tilde{\alpha},\tilde{\alpha}',\cdots} (m_\alpha^{\tilde{\alpha}}\varepsilon_{\tilde{\alpha}} + m_\alpha^{\tilde{\alpha}\tilde{\alpha}'}\varepsilon_{\tilde{\alpha}}\varepsilon_{\tilde{\alpha}'} + \cdots), \tag{4}$$

where the α' represents a complete, orthogonal basis set for the system and ε_α is the component of the overall strain along a given basis vector. Considering the symmetry strain of iron-based superconductors, there are three components of the in-plane elastoresistivity are relevant to this study, i.e., $(\Delta\rho/\rho_0)_{B_{1g}}$, $(\Delta\rho/\rho_0)_{B_{2g}}$, and $(\Delta\rho/\rho_0)_{A_{1g}}$. For an external pressure within the ab-plane of the tetragonal lattice, the B_{1g} and B_{2g} channels are along the (100) and (110) directions, respectively, while the A_{1g} channel represents the isotropic response.

It has been found that the strain dependence of the elastoresistivity along the (110) direction shows a nonlinear term,[14] which is attributed to the isotropic (A_{1g}) channel. It is argued that this is due to high-order terms as follows:[14]

$$(\Delta\rho/\rho_0)_{A_{1g}} = m_{A_{1g}}^{A_{1g}}\varepsilon_{A_{1g}} + m_{A_{1g}}^{B_{2g},B_{2g}}(\varepsilon_{B_{2g}})^2. \tag{5}$$

Due to the bilinear coupling between nematic order and $\varepsilon_{B_{2g}}$ in Eq. (1), the quadratic term $m_{A_{1g}}^{B_{2g},B_{2g}}$ should show divergent behavior near T_s as follows:[14]

$$m_{A_{1g}}^{B_{2g},B_{2g}} \approx \frac{a}{(T-\Theta)^2} + \frac{b}{T-\Theta} + c, \tag{6}$$

where a, b, and c are constant coefficients and Θ is the Curie–Weiss temperature. Their results suggest that the isotropic properties of iron-based superconductors may be strongly affected by the nematic character.

However, we note that the above analysis is based on the assumption that the external field is small and the system is close to the zero-field state. In a paramagnetic system, when the magnetic field H is small, the magnetization M is proportional to H. However, when the field is large, M will show nonlinear behavior. In this work, we study the nonlinear behavior of the elastoresistivity in $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$ along the (110) direction.[13] Our results can be well described by the Landau theory for the second-order phase transition without the introduction of unusual strong coupling between the isotropic and nematic channels. Moreover, the magnetic and nematic transitions may be driven from first order to second order due to the enhancement of magneto-elastic coupling.

2. Theoretical analysis

We first consider the effect when the external pressure is large. By minimizing the free energy of Eq. (1) with respect to variations in the nematic order parameter and strain, we have

$$\frac{\partial F}{\partial\varphi} = a\varphi + b\varphi^3 + \lambda\varepsilon = 0, \tag{7}$$

and

$$\frac{\partial F}{\partial\varepsilon} = c\varepsilon + d\varepsilon^3 + \lambda\varphi + p = 0. \tag{8}$$

From Eq. (7),

$$\varepsilon = -\frac{a\varphi + b\varphi^3}{\lambda}. \tag{9}$$

Putting Eq. (9) into Eq. (8) and neglecting higher-order φ terms,

$$\begin{aligned} p = &-\frac{a_0 c}{\lambda}\left[T - \left(T_0 + \frac{\lambda^2}{a_0 c}\right)\right]\varphi \\ &- \frac{bc + d a_0^3 (T-T_0)^3}{\lambda}\varphi^3, \end{aligned} \tag{10}$$

which will give rise to Eq. (3) when p is small. Accordingly, we can fit the pressure dependence of resistance as follows:

$$p = p_{c3} + \alpha\left(\frac{R}{R_0} - 1\right) + \beta\left(\frac{R}{R_0} - 1\right)^3, \tag{11}$$

where p_c, α, β, and R_0 are all constants. Here α^{-1} is equivalent to ζ defined previously when β is small.[11] The term p_{c3} is to account for the residual pressure in the uniaxial pressure device that causes the actual zero pressure deviating from the nominal one for zero voltage applied in the piezobender.[11] Equation (11) can also be approximately written as

$$\begin{aligned} R &\approx R_0 + \frac{\kappa(p-p_{c3})}{1+\sigma(p-p_{c3})^2} \\ &\approx R_0 + \kappa(p-p_{c3}) - \kappa\sigma(p-p_{c3})^3, \end{aligned} \tag{12}$$

where C_0, κ, σ, and p_{c3} are constants.

While the above analysis is for the uniaxial pressure dependence of the resistance, similar conclusions can be obtained for the strain dependence of the resistance since the pressure and strain are linearly coupled. The system we studied here is $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$, where the nematic and antiferromagnetic (AF) transitions change from first order to second order.[13] There is an intermediate doping range from 0.42 to 0.52, within which the nematic transition is first-order but the AF transition is second-order. All the data are obtained from Ref. [13].

3. Results and discussions

Figure 1 gives the uniaxial pressure dependence of the resistance for selected samples. All of them can be well fitted by Eq. (11). We notice that within the same pressure range, the nonlinear behavior becomes much weaker in the $x = 0.32$ sample, which makes the fitting unreliable. This is probably because both its magnetic and nematic transitions are strongly first-order.[13] Therefore, we will only discuss the data for $x \geq 0.39$ samples.

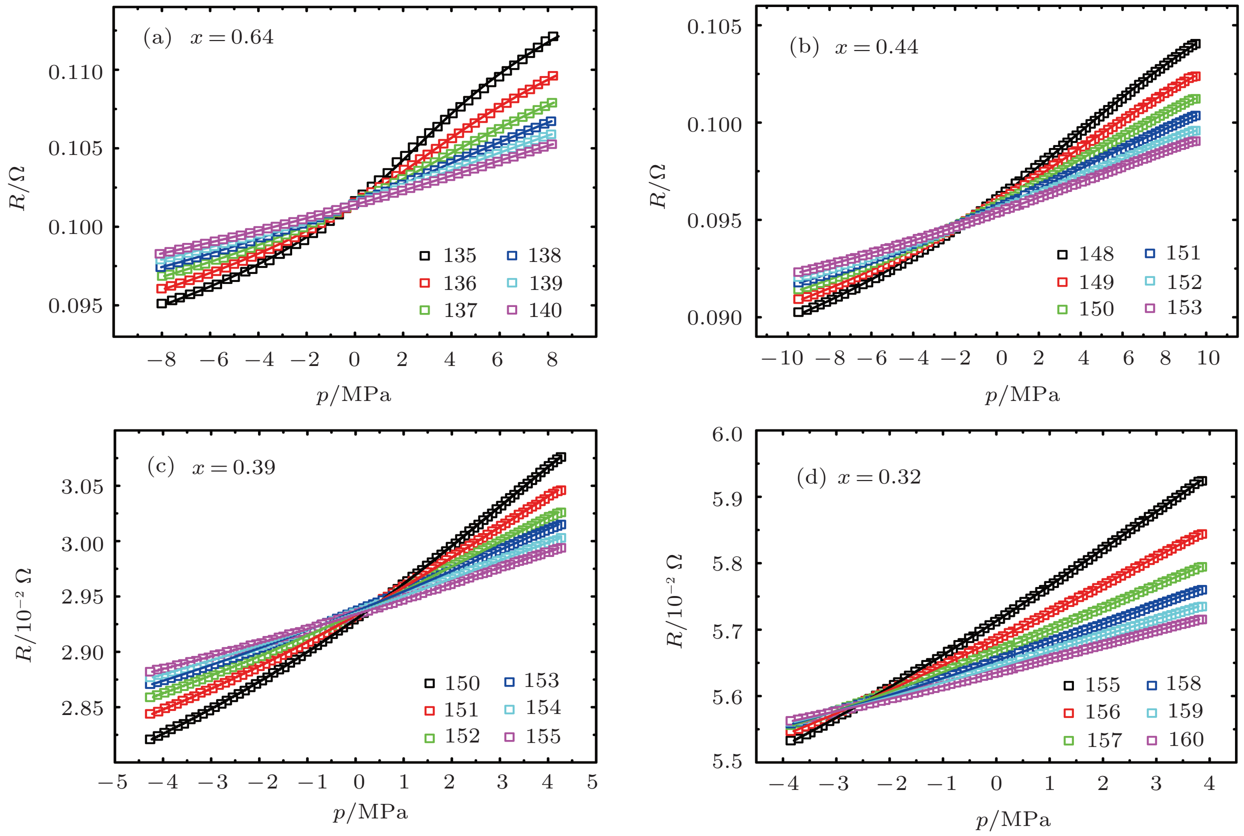

Fig. 1. (color online) Uniaxial pressure dependence of resistance for (a) $x = 0.64$, (b) $x = 0.44$, (c) $x = 0.39$, and (d) $x = 0.32$. The numbers in the labels are temperatures with the unit in Kelvin. The solid lines are fitted by Eq. (11). The legends for different symbols are for different temperatures.

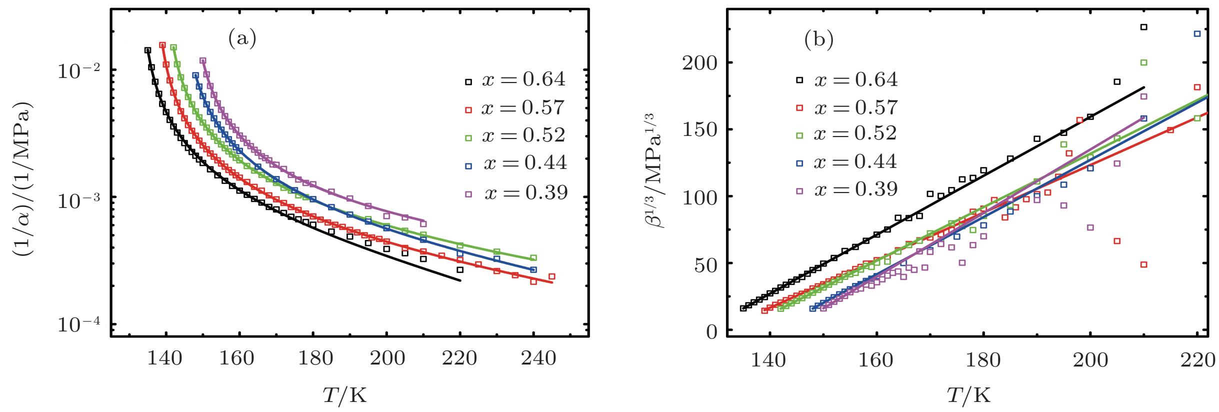

Fig. 2. (color online) (a) Temperature dependence of α^{-1}. The solid lines are fitted by Eq. (13). (b) Temperature dependence of $\beta^{1/3}$. The solid lines are fitted by Eq. (14).

Figure 2 shows the temperature dependence of parameters α^{-1} and $\beta^{1/3}$ in Eq. (11). According to Eq. (10), α should be linear with T. However, as pointed out in Ref. [11], a constant term will appear in α^{-1}. Therefore, we fit α^{-1} as follows:

$$\alpha^{-1} = \frac{A}{T - T'} + y_0, \tag{13}$$

where A, T', and y_0 are temperature-independent parameters. For the parameter β, while it contains both the cubic term of temperature and the constant term, the temperature dependence of $\beta^{1/3}$ (Fig. 2(b)) shows linear behavior near T_s, suggesting the effect of the constant term can be effectively neglected at low temperature. Moreover, the nonlinear part in the pressure dependence of the resistance becomes much weaker at high temperature, which results in larger uncertainty. Therefore, we perform the linear regression for $\beta^{1/3}$ on the beginning linear region of the data (Fig.. 2(c)) as follows:

$$\beta^{1/3} = B(T - T_0), \tag{14}$$

where B and T_0 are temperature-independent parameters.

Figures 3(a)–3(c) shows the doping dependence of the fitting parameters A, B and $T' - T_0$ in Eqs. (13) and (14). The most significant change with doping is the value of $T' - T_0$.

According to Eq. (10), $T' - T_0 = \lambda^2/a_0c$, $A = -\lambda/a_0c$, so $(T' - T_0)/A$ = -λ. Therefore, $|\lambda|$ increases with increasing x, as shown in Fig. 4(d). We have shown that the magnetic and nematic transitions change from first order to second order with increasing x at $x = 0.52$ and 0.41, respectively.[13] Theoretical analysis has shown that these may be driven by the increasing of nematic coupling g,[16] which can be enhanced by the magneto-elastic coupling.[17] The enhancement of g is proportional to λ^2/C_s, where C_s is the shear modulus and effectively equivalent to c in Eq. (1). Previous measurements have shown that the bulk modulus changes from 46 GPa in $SrFe_2As_2$[18] to 59 GPa in $BaFe_2As_2$.[19] Therefore, one does not expect very significant change of shear modules in the $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$ system. On the other hand, the value of λ is doubled with increasing x, which suggests that the change of the magnetic–elastic coupling may play the most important role in determining the nature of the magnetic and nematic transitions in $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$.[13] In fact, there are many studies have addressed the importance of the magneto–elastic coupling in understanding the nematic order in iron-based superconductors.[20–22] The underlying mechanism for the enhancement of λ with Sr substituted by Ba needs to be further investigated.

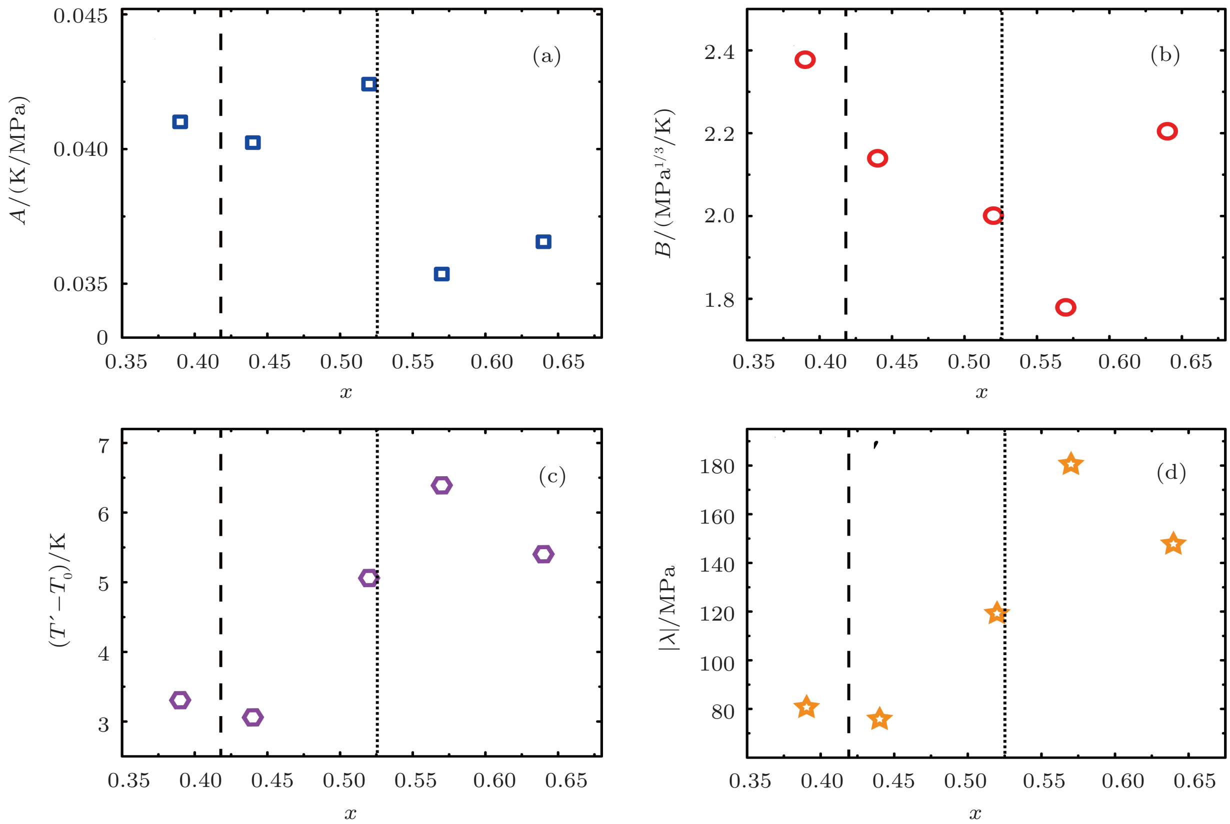

Fig. 3. (color online) Doping dependence of (a) A, (b) B, (c) $T' - T_0$, and (d) $|\lambda|$. Here $|\lambda| = |(T' - T_0)/A|$ as discussed in the main text. The dashed and dotted lines represent the crossovers from the first-order to second-order transition for the magnetic and nematic transitions, respectively.

As mentioned above, the nonlinear part of the resistivity may also come from the coupling between the isotropic (A_{1g}) and nematic (B_{2g}) channels.[14] In this case, the resistivity has a quadratic dependence on strain. However, according to Eq. (9), this may be simply resulted from the nonlinear effect when the strain is nonzero. To check the significance of the quadratic component in our data, we fit the pressure dependence of resistance of the $x = 0.64$ at 135 K by Eq. (12) plus a quadratic term. The contributions from the cubic and quadratic parts are shown in Fig. 4(a), where the latter is apparently negligible.

Here we propose that the reason that a quadratic component may be wrongly obtained is because in practice, the zero-point of the pressure is hard to determine and the strain or pressure range is rather limited. In Fig. 4(b), we plot the function of $x + x^3$ with the range close to $x = 0$. If we fit the data with a linear function, the slope is just 0.7811. Subtracting this liner component, a valley behavior can be found around $x = -0.4$ and can be fitted by the quadratic function. Following this idea, we re-plot the data of $x = 0.64$ with the linear component subtracted, as shown in Fig. 4(a). Around -3 MPa, the data can be fitted by a quadratic function as follows:

$$R_{\rm NL} = R_0 + \gamma(p - p_{c2})^2. \qquad (15)$$

The fitting range has been chosen as asymmetry to the center of the parabola function, since in Ref. [14], the range of the strain is asymmetric due to the constraint of piezostack. Here p_{c2} is about -3 MPa while p_{c3} obtained from the fitting by Eq. (12) is 2.7 MPa. It should be noted that the negative pressure here corresponds to the stretch of the sample, which will result in a negative strain, so the range chosen to fit by Eq. (15) is similar to that in Ref. [14]. Moreover, although we cannot determine the strain in our measurements and the samples are different, the resistivity change within the fitting range at 135 K is about 1.5%, which is larger than that in Ref. [14]. Figure 4(b) shows the temperature dependence of the parameter γ, which can be well fitted as follows:

$$\gamma = \frac{C}{(T-\Theta)^2}, \tag{16}$$

where C and Θ are temperature-independent constants.

All of the above results are consistent with those in Ref. [14], which suggests that the quadratic dependence of the resistance on the strain is wrongly obtained due to the uncertainty in determining the zero strain and the limited strain range a piezostack can achieve. While the coupling between A_{1g} and B_{2g} should present from the symmetry point of view, its effect is actually negligible.

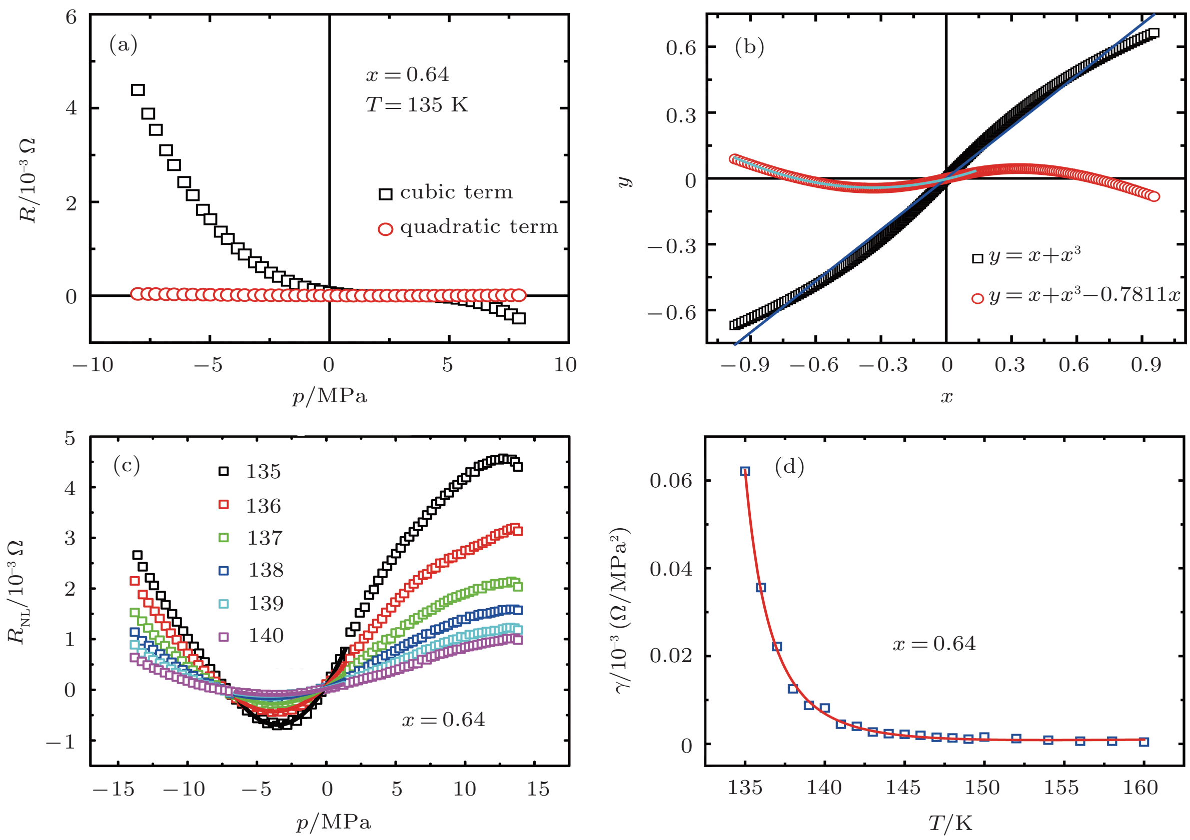

Fig. 4. (color online) (a) The cubic (black squares) and quadratic (red circles) components in the uniaxial pressure dependence of resistance of the $x = 0.64$ sample at 135 K. (b) Illustration on how the quadratic term may be wrongly. The blue line is a linear fit to the cubic function of $x+x^3$ (black squares). The red circles are subtracted results from the cubic function by the linear fit result. The cyan line is fitted by the quadratic function. (c) Uniaxial pressure dependence of the nonlinear part of the resistance for the $x = 0.64$ sample. The solid lines are fitted by Eq. (15). The numbers in the label are temperatures with the unit of Kelvin. (d) Temperature dependence of γ for the $x = 0.64$ sample. The solid line is fitted by Eq. (16).

4. Conclusions

We have systematically analyzed the uniaxial pressure dependence of the resistance in the $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$ system, which shows significant nonlinear behavior near the structural transition. By adopting the Landau theory for the second-order phase transition with a linear coupling between the strain and nematic order parameter, the data can be well described by considering the higher-order terms. Our results show that the coupling between the isotropic and nematic channels is negligible in iron-based superconductors. Moreover, the most significant factor in determining the nature of the magnetic and nematic transitions in $Sr_{1-x}Ba_xFe_{1.97}Ni_{0.03}As_2$ may be the strength of the magneto-elastic coupling.

References

[1] Dai P 2015 *Rev. Mod. Phys.* **87** 855
[2] Chu J H, Analytis J G, De Greve K, McMahon P L, Islam Z, Yamamoto Y and Fisher I M 2010 *Science* **329** 824
[3] Yi M, Lu D H, Chu, J H, *et al.* 2011 *Proc. Natl. Acad. Sci. USA* **113** 8139
[4] Lu X, Park J T, Zhang R, Luo H, Nevidomskyy A H, Si Q and Dai P 2014 *Science* **345** 657

[5] Gallais Y *et al.* 2013 *Phys. Rev. Lett.* **111** 267001
[6] Böhmer A E, Burger P, Hardy F, Wolf T, Schweiss P, Fromknecht R, Reinecker M, Schranz W and Meingast C 2014 *Phys. Rev. Lett.* **112** 047001
[7] Fernandes R M, Chubukov A V and Schmalian J 2014 *Nat. Phys.* **10** 97
[8] Chu J H, Kuo H H, Analytis J G and Fisher I R 2012 *Science* **337** 710
[9] Hosoi S, Matsuura K, Ishida K, Wang H, Mizukami Y, Watashige T, Kasahara S, Matsuda Y and Shibauchi T 2016 *Natl. Acad. Sci. USA* **113** 8139
[10] Kuo H H, Chu J H, Palmstrom J C, Kivelson S A and Fisher I R 2016 *Science* **352** 958
[11] Liu Z Gu Y, Zhang W, *et al.* 2016 *Phys. Rev. Lett.* **117** 157002
[12] Gu Y, Liu Z, Xie T, *et al.* 2017 *Phys. Rev. Lett.* **119** 157001
[13] Gong D, Liu Z, Gu Y, Xie T, Ma X, Luo H, Yang Y and Li S 2017 *Phys. Rev. B* **96** 104514
[14] Palmstrom J C, Hristov A T, Kivelson S A, Chu J H and Fisher I R 2017 *Phys. Rev. B* **96** 205133
[15] Shapiro M C, Hlobil P, Hristov A T, Maharaj A V and Fisher I R 2015 *Phys. Rev. B* **92** 235147
[16] Fernandes R M, Chubukov A V, Knolle J, Eremin I and Schmalian J 2012 *Phys. Rev. B* **85** 024534
[17] Fernandes R M, Schmalian J 2012 *Supercond. Sci. Technol.* **25** 084005
[18] Uhoya W O, Montgomery J M, Tsoi G M, Vohra Y K, McGuire M A, Sefat A S, Sales B C and Weir S T 2011 *J. Phys.: Condens. Matter* **23** 122201
[19] Jϕrgensen J E, Hansen T C 2010 *Eur. Phys. J. B* **78** 411
[20] Dhital C, Yamani Z, Tian W, Zeretsky J, Sefat A S, Wang Z, Birgeneau R J and Wilson S D 2012 *Phys. Rev. Lett.* **108** 087001
[21] Dhital C, Hogan T, Yamani Z, Birgeneau R J, Tian W, Matsuda M, Sefat A S, Wang Z and Wilson S D 2014 *Phys. Rev. B* **89** 214404
[22] Hu Y, Ren X, Zhang R, *et al.* 2016 *Phys. Rev. B* **93** 064504(R)