

Microscopic Study of the Role of Structural Distortion in Oxypnictide Superconductors: A Two Band Approach

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Abstract. The doped oxypnictides of type 1111 exhibit verities of lattice distortions. We propose here a tight-binding two band model to explain the temperature dependent lattice strain in this system. The two band tight-binding model consists of nearest neighbor and next-nearest-neighbor electron hoppings. The lattice distortion arising due to lattice strain is proposed to be investigated by incorporating JT type distortion in which the d_{xz} band is raised by Jahn-Teller (JT) energy, Ge and the d_{yz} band is suppressed by JT energy, $-Ge$, so that there exists a JT gap of energy, $2Ge$. This provides a strong interplay between the lattice energy and the electronic energy to stabilize the system. The lattice strain and hence the JT energy are calculated by using Zubarev's Green's function technique. Finally the lattice strain is computed self-consistently. The temperature dependent lattice strain exhibits a mean-field behavior exhibiting a tailing nature near the lattice distortion temperature. This indicates that the lattice strain is not robust but gradual near the transition temperature. The temperature dependent lattice strain is investigated by varying the physical parameters like JT coupling, elastic constant, different hopping integrals and chemical potential. The results are discussed in the text.

Keywords: Iron-based superconductors, Jahn-Teller effect.

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1. Introduction

The discovery of superconductivity in F doped iron based compound LaFeAsO with transition temperature $T_C = 26$ K by Kamhira et.al. [1] led the further discovery of even higher T_C materials with highest $T_C \approx 56$ K observed in

Gd_{0.8}Th_{0.2}FeAsO [2], St_{0.5}Sm_{0.5}FeAsF [3] and Ca_{0.4}Nd_{0.6}FeAsF [4]. There are both structural phase transition, T_S (tetragonal to orthorhombic) and spin density wave (SDW) transition, T_{SDW} for undoped 1111 class of compounds like LaFeAsO. For undoped CeFeAsO, two transitions occur at different temperatures i.e, T_S = 155 K and T_{SDW} = 140 K [5]. The two transition temperatures occur in the range 134 K to 175 K in other undoped 1111 materials [6, 7]. The T_S and T_{SDW} in LaFeAsO are suppressed by intermediate doping so that T_S remains greater than T_{SDW} [1].

2. Formalism and calculation of Green's functions

The band structure calculation of oxypnictide superconductor LaFeAsO by Mazin et.al [8] shows that all the 5d orbitals of Fe ion contribute to the electron density of states. However, the three iron orbitals d_{xz}, d_{yz} and d_{xy} contribute to the density of states near the Fermi level. Hence, different authors [9, 10, 11] have proposed a two band model with two degenerate d_{xz} and d_{yz} orbitals. The Hamiltonian is written as,

$$\begin{aligned} \mathbf{H}_0 = & \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{kx}} - \mu) \mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{kx}\sigma} + \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{ky}} - \mu) \mathbf{d}_{\mathbf{ky}\sigma}^+ \mathbf{d}_{\mathbf{ky}\sigma} \\ & + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{kxy}} (\mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{ky}\sigma} + \mathbf{d}_{\mathbf{kx}\sigma}) \end{aligned} \quad (1)$$

Here first and second terms in \mathbf{H}_0 represent the kinetic energies of d_{xz} and d_{yz} orbitals with energies $\epsilon_{\mathbf{kx}}$ and $\epsilon_{\mathbf{ky}}$ and chemical potential μ . The third term represents the hybridization between next nearest neighbors d_{xz} and d_{yz} orbitals. Here $\mathbf{d}_{\mathbf{kx}\sigma}^+$ ($\mathbf{d}_{\mathbf{ky}\sigma}^+$) is the creation operator for d_{xz} (d_{yz}) orbitals. The impurities in the system remove the degeneracy between d_{xz} and d_{yz} orbitals by producing the JT distortion. The Hamiltonian is written as,

$$\mathbf{H}_{\text{JT}} = \mathbf{Ge} \sum_{\mathbf{k},\sigma} \mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{kx}\sigma} - \mathbf{Ge} \sum_{\mathbf{k},\sigma} \mathbf{d}_{\mathbf{ky}\sigma}^+ \mathbf{d}_{\mathbf{ky}\sigma} \quad (2)$$

The total tight-binding Hamiltonian becomes,

$$\begin{aligned} \mathbf{H}_{\text{TB}} = & \sum_{\mathbf{k},\sigma} \epsilon_{1\mathbf{x}}(\mathbf{k}) \mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{kx}\sigma} + \sum_{\mathbf{k},\sigma} \epsilon_{1\mathbf{y}}(\mathbf{k}) \mathbf{d}_{\mathbf{ky}\sigma}^+ \mathbf{d}_{\mathbf{ky}\sigma} + \\ & \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{kxy}} (\mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{ky}\sigma} + \mathbf{d}_{\mathbf{kx}\sigma}^+ \mathbf{d}_{\mathbf{kx}\sigma}) \end{aligned} \quad (3)$$

where d_{xz} orbital is raised by the energy, Ge and d_{yz} orbital is suppressed by the energy, -Ge. The modified dispersive energies are, $\epsilon_{1\mathbf{x}}(\mathbf{k}) = \epsilon_{\mathbf{kx}} + \mathbf{Ge} - \mu$ and $\epsilon_{1\mathbf{y}}(\mathbf{k}) = \epsilon_{\mathbf{ky}} - \mathbf{Ge} - \mu$. The dispersive energies are,

$$\begin{aligned} \epsilon_{\mathbf{kx}}(\mathbf{k}) &= -2\mathbf{t1} \cos \mathbf{kx} - 2\mathbf{t2} \cos \mathbf{ky} - 4\mathbf{t3}(\cos \mathbf{kx} \times \cos \mathbf{ky}) \\ \epsilon_{\mathbf{ky}}(\mathbf{k}) &= -2\mathbf{t2} \cos \mathbf{kx} - 2\mathbf{t1} \cos \mathbf{ky} - 4\mathbf{t3}(\cos \mathbf{kx} \times \cos \mathbf{ky}) \\ \epsilon_{\mathbf{kxy}}(\mathbf{k}) &= -4\mathbf{t4}(\sin \mathbf{kx} \times \sin \mathbf{ky}) \end{aligned} \quad (4)$$

where t_1, t_2, t_3 and t_4 are electron hopping integrals.

3. Calculation of lattice strain

In order to calculate the lattice strain, we have employed Zubarev's Green's function technique [12] for orbital electrons. The two Green's functions for d_{xz} orbitals are,

$$D_{1x}(k, \omega) = \langle\langle \mathbf{d}_{kx\sigma}; \mathbf{d}_{kx\sigma}^+ \rangle\rangle_{\omega}, \quad D_{1y}(k, \omega) = \langle\langle \mathbf{d}_{ky\sigma}; \mathbf{d}_{ky\sigma}^+ \rangle\rangle_{\omega} \quad (5)$$

Similarly, the two Green's functions for d_{yz} orbitals are,

$$D_{1y}(k, \omega) = \langle\langle \mathbf{d}_{ky\sigma}; \mathbf{d}_{ky\sigma}^+ \rangle\rangle_{\omega}, \quad D_{2y}(k, \omega) = \langle\langle \mathbf{d}_{kx\sigma}; \mathbf{d}_{kx\sigma}^+ \rangle\rangle_{\omega} \quad (6)$$

These Green's functions are calculated by Zubarev's technique. The lattice strain is calculated from the electron correlation functions derived from these Green's functions. Finally the lattice strain of the system appears as,

$$e = -\frac{g}{c_1} \sum_{k,\sigma} \left[\frac{\{\epsilon_{1x}(k) - \epsilon_{1y}(k)\}}{(\omega_{1k} - \omega_{2k})} \{f(\beta\omega_{1k}) - f(\beta\omega_{2k})\} \right] \quad (7)$$

where the quasiparticle band energies ω_{1k} and ω_{2k} are,

$$\omega_{1k}\omega_{2k} = \frac{\epsilon_{1x} + \epsilon_{1y}}{2} - \mu \pm \sqrt{\left[\left(\frac{\epsilon_{1x} - \epsilon_{1y}}{2} \right)^2 + \epsilon_{kxy}^2 \right]} \quad (8)$$

The physical parameters are scaled by the nearest neighbor hopping integral t_1 . They given by JT coupling $g = G/t_1$, elastic constant $c_1 = C_1/t_1$, chemical potential $\mu = \mu/t_1$, temperature $t = k_B T/t_1$ and the hopping integrals $t_1 = 1, t_2 = 1.3, t_3 = -0.85, t_4 = -0.85$.

4. Results and Discussion

The lattice strain given in equation (7) is solved self-consistently taking 100×100 grid points of the electron momentum in the Brillouin zone. The temperature dependent lattice strains are plotted in figure -1 to figure -7. For a given set of parameters $c_1 = 1.3, \mu = 1.4$, the plotted lattice strain (e) vs. temperature (t) is shown in figure -1 for different values of JT couplings $g = 1.38, 1.4, 1.42$. For a given JT coupling $g = 1.38$, the lattice strain exhibits mean-field behavior at low temperatures and gradually decreases towards high temperatures exhibiting the tailing behavior. The lattice distortion temperature occurs near the temperature $t_s \approx 0.12$ ($T_s \approx 150$ K for $t_1 \approx 0.125$ eV ≈ 1250 K). The tailing behavior of lattice strain near t_s appears due to the effect of hybridization between two bands.

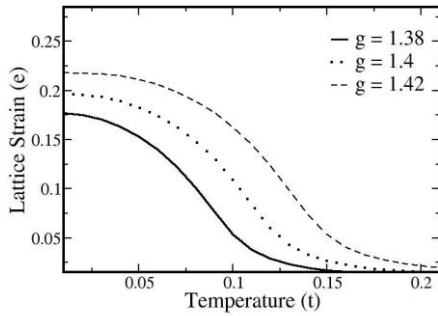


Figure-1

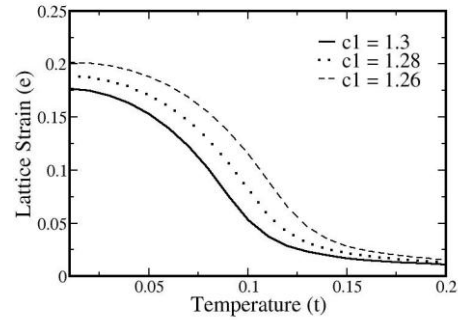


Figure-2

Fig. 1 shows the plot of lattice strain (e) vs. temperature (t) for different values of JT couplings $g = 1.38, 1.4, 1.42$ for fixed values of elastic constant $c1 = 1.3$ and chemical potential $um = 1.4$. **Fig. 2** shows the plot of lattice strain (e) vs. temperature (t) for different values of elastic constants $c1 = 1.3, 1.28, 1.26$ for fixed values of JT couplings $g = 1.38$ and chemical potential $um = 1.4$.

It indicates that the JT distortion in oxypnictide systems is not robust but gradual. Further, the lattice strain is enhanced with increase of JT coupling throughout the temperature range with the enhancement of the lattice distortion temperature. Our results agree qualitatively with the experimentally observed structural distortion temperatures in oxypnictide systems. The structural transition temperatures for different systems are $T_S = 158$ K for LaFeAsO [13], $T_S = 154$ K for PrFeAsO [14], $T_S = 155$ K for CeFeAsO [5], $T_S = 151$ K for CeFeAsO [15], $T_S = 150$ K for NdFeAsO [16], $T_S = 143$ K for NdFeAsO [17], $T_S = 175$ K for SmFeAsO [6] and $T_S = 135$ K for GdFeAsO [18]. Our model calculation with JT coupling from $g = 1.38$ to 1.42 can explain the range of structural transition temperatures observed experimentally. Figure – 2 shows the effect of elastic constant ($c1$) on lattice strain (e). It is observed that the lattice strain is enhanced with the decrease of elastic constant accompanied the enhancement of the gradual change in structural distortion temperature. The elastic constant for the system lies in a range of $c1 = 1.26$ to 1.30 . The increase of lattice strain with the decrease of elastic constant and increase of JT coupling indicates that there is strong competition between the lattice energy $1/2C1e^2$ and the electronic energy $2Ge$ arising due to JT distortion in the conduction band of the system. The decrease in lattice energy appears as the increase in electronic energy and vice versa. As a result, the electronic and magnetic and thermal

properties of the oxypnictide superconductors will be appreciably affected by JT distortion.

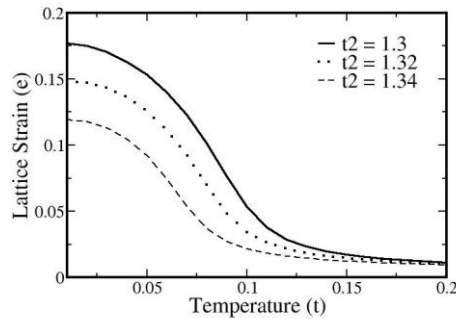


Figure-3

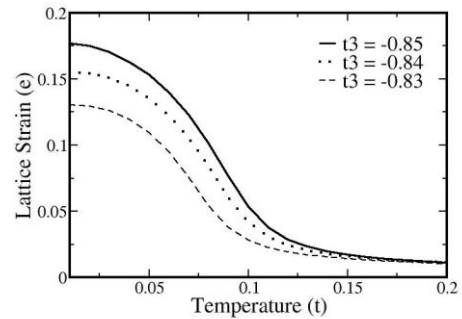


Figure-4

Fig. 3 shows the plot of lattice strain (ϵ) vs. temperature (t) for different values of second hopping integrals $t_2 = 1.3, 1.32, 1.34$ for fixed values of JT couplings $g = 1.38$, elastic constant $c_1 = 1.3$ and chemical potential $\mu = 1.4$. **Fig. 4** shows the plot of lattice strain (ϵ) vs. temperature (t) for different values of third nearest hopping integrals $t_3 = -0.85, -0.84, -0.83$ for fixed values of JT couplings $g = 1.38$, elastic constant $c_1 = 1.3$ and chemical potential $\mu = 1.4$.

In the present tight binding model calculation, we have considered the near neighbor hopping integral t_1 between σ - orbitals and near neighbor hopping between π - orbitals as t_2 . We include a second neighbor hopping integral t_3 between similar d-orbitals and second neighbor hopping integral t_4 between different d-orbitals. For a given t_1 , the effect of t_2 on temperature dependent lattice strain (ϵ), is shown in figure 3. The lattice strain is suppressed with increase of hopping integral t_2 , accompanied by the suppression of lattice distortion temperature. This indicates that the increase of electron hopping t_2 suppresses the lattice distortion. Hence the lattice energy indicates the dominant role played by the hopping (t_2) over the lattice distortion. The effect of hopping integral t_3 on lattice strain is shown in figure – 4. The lattice strain is suppressed with the decrease of hopping integral from $t_3 = -0.85$ to -0.83 throughout the temperature range. Correspondingly the lattice distortion temperature is also suppressed. This indicates that the decrease of electronic hopping energy is accompanied by corresponding decrease in lattice distortion exhibiting interesting interplay between lattice energy and kinetic energy of the system. This type of

suppression of kinetic energy as well as lattice energy occurs for electron hopping between similar d – orbitals of iron ion.

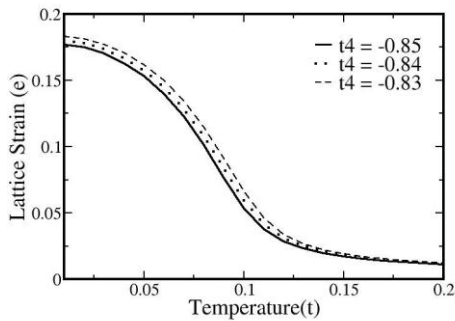


Figure-5

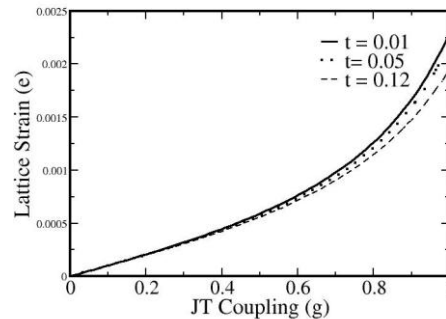


Figure-6

Fig. 5 shows the plot of lattice strain (e) vs. temperature (t) for different Values of fourth nearest hopping integrals $t_4 = -0.85, -0.84, -0.83$ for fixed values of JT couplings $g = 1.38$, elastic constant $c_1 = 1.3$ and chemical potential $\mu = 1.4$. **Fig. 6** shows the plot of lattice strain (e) vs. temperature (t) for different Values of temperatures $t = 0.01, 0.05, 0.12$ for fixed values of elastic constant $c_1 = 1.3$ and chemical potential $\mu = 1.4$.

Figure- 5 shows the effect of hopping integral t_4 on lattice strain. It is observed that the lattice strain is suppressed slightly with the increase of hopping t_4 . This indicates that the increase of electronic kinetic energy is associated with corresponding small suppression in lattice strain. This occurs for electron hopping t_4 between the dissimilar d – orbitals of iron ion. The effect of hopping integrals t_3 and t_4 exhibit opposite effects on the lattice strain and also the lattice energy. The effect of hopping integral t_4 on lattice strain is much smaller compared to the effect of hopping integrals t_2 and t_3 on the lattice strain. Thus, we conclude that different types of electron hopping integrals have appreciable effect on the lattice strain. This type of conclusion was drawn from the band structure calculation which provides the indication that all the d – orbitals of the iron ion contribute the electronic density of states and hence the electronic properties of the oxypnictide superconductor calculation [8]. Figure – 6 shows how lattice strain changes with JT coupling (g). The lattice strain increases with coupling (g) linearly at the lower values of the coupling up to $g = 0$ to 0.5 . With further increase of JT coupling, the lattice strain enhances much more rapidly from $g \approx 0.5$ to 1.0 . This indicates that for higher JT coupling the lattice strain increase so rapidly that ultimately lattice melts. It is to note further that lattice

strain doesn't depend on temperatures for lower values of JT coupling. However, lattice strain is suppressed more and more with increase of temperature for higher values of JT coupling i.e, $g = 0.5$ to 1.0 . This exhibits the interplay between thermal energy and lattice strain energy for given values of kinetic energy of the d electrons.

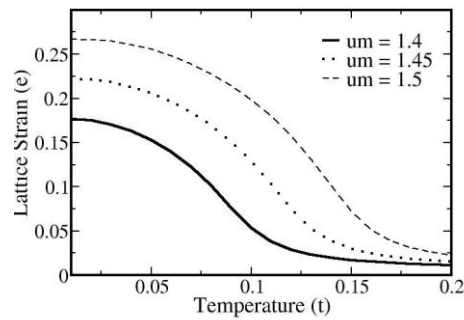


Figure-7

Fig. 7 shows the plot of lattice strain (e) vs. temperature (t) for different values of chemical potentials $um = 1.4, 1.45, 1.5$ for fixed values of JT couplings $g = 1.38$ and fixed values of elastic constant $c1 = 1.3$.

Figure 7 shows the effect of electron doping with chemical potential ($um = 1.40, 1.45, 1.50$) on lattice strain. When the system is doped with electrons, more number of electrons enter to the conduction band and participate in the lattice distortion. The lattice strain is enhanced throughout the temperature with the increase of electron doping (i.e, increase of chemical potential). Correspondingly the lattice distortion temperature is also enhanced with the increase of electron doping.

5. Conclusions

In the present report, we have considered a tight binding two band model in presence of hybridization between two bands. The degeneracy of the two bands is removed by the JT type structural distortion. The lattice strain for the oxypnictide system is calculated by the Green's function technique. The temperature dependent lattice strain is varied by changing JT coupling, elastic constant and different hopping integrals. It is observed that the lattice strain is enhanced with the increase of JT coupling and decrease of elastic constant. This indicates the interesting interplay between lattice energy and electronic energy displaying that

decrease of one energy is compensated by the increase of other type of energy. The lattice strain is suppressed with the increase of hopping integral between π – orbitals and hopping between similar d – orbitals of the iron ion. This indicates that there is a strong interplay between lattice energy and different types of kinetic energy arising due to electron hoppings. Further, lattice strain increases linearly for lower values of JT coupling and increases rapidly for higher values of JT coupling leading to the melting of the crystal. Jena and Rout et.al. [19-22] have reported a one band model study for 122 type iron based superconductors (for example AFe_2X_2 , $A \approx K, Na$ and $X = Te, Se, As$) describing the one electron pocket in the Fermi surface in absence of hole pocket suppressed by impurity atoms. They have reported the temperature dependent spin density wave (SDW) interaction, Jahn-Teller type lattice distortion to study the competition between kinetic energy and SDW and JT distortion in one band model approach [19, 20]. Jena. et. al. [21] have addressed the different pairing mechanisms like s-wave, d-wave and s_{\pm} -wave pairing symmetry for the 122 systems to explain the anomalous tunneling spectra within one band tight binding approach. More recently, Jena. et. al. [22] has reported the strong interplay between lattice distortion, superconductivity and kinetic energy of the 122 system taking s_{\pm} pairing symmetry.

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