Ultrafast above-transition-temperature resurrection of spin density wave driven by coherent phonon generation in BaFe$_2$As$_2$

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Abstract
A model incorporating the time-dependent Ginzburg–Landau theory of ultrafast cooperative interplay among charge, spin, and lattice is presented for the pnictide superconductor BaFe$_2$As$_2$. Under the ultrafast optical pumping, a pronounced spin–phonon coupling is found to drive the reconstruction of spin density wave (SDW) at $T > T_s$ ($T_s$: SDW transition temperature) through the coherent phonon generation. First-principles electronic structure calculation confirms that the macroscopically coherent $A_{1g}$ oscillation of As over a new equilibrium displacement offers a route to the antiferromagnetic SDW state. Our finding explains the recent experimental observation.

Keywords: BaFe$_2$As$_2$, spin density wave, coherent phonon, time-dependent Ginzburg–Landau theory, first-principles calculation

1. Introduction

In the last decade, substantial progress of laser technologies and measurement methodologies have opened a new era of the ultrafast nonequilibrium phenomena of materials, which mainly

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concerns physics of the femtosecond (fs) time range \([1, 2]\). Nonequilibrium dynamics following the ultrafast optical pumping usually cause the cooperative interplay among microscopic degrees of freedom. Cooperativity enhances the number of accessible phases and the richness of their physical nature. This generates thermally inaccessible hidden phases, for example, coherent charge transport \([3]\), melting of low-dimensional charge orders \([4–6]\), insulator-metal transition \([7, 8]\), charge-orbital-lattice or charge-lattice cooperative phase \([9–12]\), high-temperature regeneration of low-temperature phase \([13, 14]\), and so on.

The Fe pnictide has been a new class of unconventional high-temperature superconductor since it was discovered in 2008 \([15]\). As in cuprates, as the doping proceeds, the superconductivity of the Fe pnictide emerges from the magnetic ground state \([16]\). Therefore, as a common observation in both cuprates and pnictides, the competition between underlying magnetic order and superconductivity has been a key essence of discussion concerning the origin of high-temperature superconductivity \([17, 18]\). The antiferromagnetic (AFM) spin density wave (SDW) ground state is obtained in the undoped BaFe\(_2\)As\(_2\) of the series of BaFe\(_{2−x}\)Co\(_x\)As\(_2\), the most studied Fe pnictide superconductors. Further, the ground state of Fe pnictides may be controlled between magnetic and superconducting ones in terms of external pressure in a way similar to chemical doping, which implies a strong cooperative interplay among magnetism, superconductivity and lattice distortion \([19]\). In fact, giant magneto-elastic coupling and magnetic phonons were pointed out in Fe pnictides \([20]\).

Recent time-resolved terahertz spectroscopy has traced the ultrafast response of BaFe\(_2\)As\(_2\) after the near-infrared (NIR) optical pumping by measuring the mid-infrared (MIR) conductivity \([13]\). Optical pumping in the AFM-SDW (simply, SDW) state \((T < T_s; T_s = 120 \text{ K, where } T_s \text{ is the SDW transition temperature})\) led to the nonmagnetic (NM) metallic state together with melting of the SDW order as is often seen in cases of various low-dimensional ordered states \([4–7]\). In contrast, above the SDW transition temperature \((T > T_s)\), the SDW order was regenerated by the intensified optical pumping in the NM metallic state, which accompanied the macroscopically coherent lattice oscillation (i.e., coherent phonon) of a specific mode. This is remarkable in the sense that the low-temperature phase could be manufactured at high temperature by means of the optical method, being free from thermodynamic limitations.

In this paper, we propose a model implementing the ultrafast photoinduced dynamics of charge, spin, and lattice for BaFe\(_2\)As\(_2\) incorporating the time-dependent Ginzburg–Landau (TDGL) theory. We find that the coherent phonon generated by the photoexcited charges couples to the SDW order parameter due to a strong spin–phonon coupling anticipated in BaFe\(_2\)As\(_2\), which should be a driving force of resurrection of the SDW order at \(T > T_s\). Moreover, a change in the potential landscape between the NM state and the SDW state is calculated with respect to the fractional coordinate of As ion, \(z_{As}\), employing the first-principles electronic structure calculation. This confirms that the SDW state could be approached by making a macroscopic shift of As ion to smaller \(z_{As}\) in the NM state (i.e., \(T > T_s\)), which is, we point out, actually realized by the generation of coherent phonon under the optical pumping in the ultrafast time span.
2. Coherent phonon generation and reconstruction of SDW

2.1. Time-dependent Ginzburg–Landau theory

An original form of the equilibrium Ginzburg–Landau (GL) theory describes a fundamental equation for the macroscopic superconductivity in terms of the superconducting order parameter by regarding a given superconductor as a charged superfluid [21]. In the frame of GL without the optical pumping, the free energy $F_0$ of an undoped Fe pnictide is assumed to be written with respect to the SDW order parameter $\Delta_s$ as

$$F_0 = \frac{1}{2} \alpha (T - T_s) \Delta_s^2 + \frac{1}{4} \beta \Delta_s^4$$

(1)

with the usual positive GL constants $\alpha$ and $\beta$. Standard equilibrium thermodynamics governing the phase transition of SDW are readily understood from $\partial F_0 / \partial \Delta_s = 0$, i.e., $\Delta_s = \sqrt{\alpha (T_s - T)/\beta}$ is obtained when $T < T_s$, while $\Delta_s = 0$ when $T > T_s$.

TDGL is a time-dependent extension of the equilibrium GL [22]. We need to extend $F_0$ to take into account the optical pumping by the ultrashort laser pulse $\tau$. Electronic part could be considered by putting $F^E_1(\tau) = \frac{1}{2} \mathcal{A}^2(\tau) \Delta_s^2$, which implies that the electronic state with a spin gap absorbs a major part of the applied optical energy. The lattice part, on the other hand, would respond to the optical pumping through the electron–phonon coupling. Optical excitation sometimes leads to an oscillating change of the macroscopic optical response of the material, like transmission or reflection. This indicates an excitation of the coherent phonon. Quantum mechanically, the equation of motion for the coherent phonon amplitude $\xi_q$ is given by [23]

$$\frac{\sigma^2}{\partial \xi_q^2} + \omega_0^2 \xi_q = -2 \omega_0 \sum_\sigma g_\sigma^\sigma n_\sigma^n,$$

(2)

where the right-hand side implicitly depends on the optical condition since $n_\sigma^n$ is the charge density excited by the optical pulse field $\mathcal{A}(\tau)$. $\sigma$ is the spin index, i.e., $\sigma = \uparrow$ or $\downarrow$. $\omega_0$ is the phonon frequency, corresponding to the $A_{1g}$ oscillation mode of As ion relative to the Fe layer in the present consideration, i.e., $5.5 \text{ THz}$ [13], and $g_\sigma^\sigma$ the spin-dependent electron–phonon coupling strength. A spin–phonon coupling expected in BaFe$_2$As$_2$ [20] signifies $g_\sigma^\uparrow \neq g_\sigma^\downarrow$, which lets us rewrite the right term of equation (2) as $2 \omega_0 \sum_\sigma g_\sigma^\sigma n_\sigma^n = \omega_0 g_\sigma^n (n_\sigma^\uparrow - n_\sigma^\downarrow) + \omega_0 \tilde{g}_q (n_\sigma^\uparrow + n_\sigma^\downarrow)$ with $\tilde{g}_q = g_\sigma^\uparrow - g_\sigma^\downarrow (\neq 0)$ and $\tilde{g}_q = g_\sigma^\uparrow + g_\sigma^\downarrow$. Here $\tilde{g}_q$ can be taken as the effective spin–phonon coupling strength. Now it is crucial to note $n_\sigma^\uparrow - n_\sigma^\downarrow = \Delta_s$ and $n_\sigma^\uparrow + n_\sigma^\downarrow = N(\tau)$. $N(\tau)$ is the photoexcited charge density. This completes a microscopic derivation of the free energy of the lattice part under the optical pumping, i.e., $F^L_1(\tau) = \frac{1}{2} \omega_0^2 \xi^2 - \omega_0 \tilde{g}_\sigma \Delta_s - \omega_0 \tilde{g}_s N(\tau)$. Hereafter we simply drop $q$ in $\xi_q$, $\tilde{g}_q$, and $\tilde{g}_s$ since it is redundant.
Therefore, the total free energy $\mathcal{F}(\tau)$ reads as

$$\mathcal{F} = \mathcal{F}_0 + \mathcal{F}^E(\tau) + \mathcal{F}^I(\tau),$$

from which the time-dependent equations within a frame of TDGL are

$$\frac{\partial}{\partial \tau} \Delta_s = -\kappa \left[ \alpha (T - T_s) \Delta_s + \beta \Delta_s^3 + \mathcal{A}(\tau) \Delta_s - \omega_0 \bar{g} \xi \right],$$

$$\frac{\partial^2}{\partial \tau^2} \xi = -\omega_0^2 \xi + \omega_0 \bar{g} \Delta_s + \omega_0 g \mathcal{N}(\tau).$$

Equation (4) is obtained from $\partial \mathcal{A}_s / \partial \tau = -\partial \mathcal{F} / \partial \Delta_s$ and $\partial^2 \xi / \partial \tau^2 = -\partial \mathcal{F} / \partial \xi$. $\kappa$ is a TDGL constant which is related to the relaxation of $\Delta_s$. In the lowest order approximation, we take a rate equation $\partial \mathcal{N} / \partial \tau = \eta \mathcal{A}(\tau)$ to determine $\mathcal{N}(\tau)$ within the linear response. By solving equation (4), it would then be possible to understand the ultrafast interplay among photoexcited charge density, coherent phonon and SDW order.

### 2.2. Coherent phonon and SDW

Figure 1 displays the dynamics of the SDW order for $T < T_s$ with respect to the full widths at half maximum (FWHM) of the optical pumping pulse, where the initial condition should be $\Delta_s(0) = \sqrt{\alpha (T_s - T) / \beta}$. Without much dependence on the width, according to figure 1, SDW is found to melt by an absorption of the optical energy and, after the optical pulse ends, recovers by the rapid energy transfer from electron to lattice. Such an energy transfer is often described by the two-temperature model [24].

The situation for $T > T_s$ is very different from $T < T_s$. In figure 2(a), the relevant phonon mode shows a shifted oscillation over a new equilibrium position $\bar{\xi}$. In an approximation neglecting $\omega_0 \bar{g} \Delta_s$ in equation (4), we can get an analytic solution for $\xi(\tau)$ in the long time limit.
where a shifted equilibrium position is given by \( \bar{\xi} = \bar{\eta} \). For instance, it gives \( \bar{\xi} = 0.00058 \) Å for FWHM = 4.88 fs. An equilibrium shift \( \bar{\xi} \) and an oscillation amplitude vanish rapidly following \( e^{-\omega_0^2 \tau^2 / 4} \), \( e^{-(\omega-a_0)^2 \tau^2 / 4} \), and \( e^{-(\omega+a_0)^2 \tau^2 / 4} \) with an increase of \( \tau \) (i.e., \( \propto \) FWHM), as is observed in figure 2(a). This indicates a criterion for the creation of coherent phonon. As a matter of fact, for FWHM of 10.82 fs, the oscillation does not shift and its amplitude essentially vanishes after the termination of the optical pumping (note that the oscillation for 10.82 fs is demonstrated as multiplied by \( 10^6 \) in figure 2(a)). Simultaneously with the coherent phonon oscillation, reconstructing dynamics of the SDW order starting from

5 In this study, in order to have a nonzero amplitude of the coherent phonon, one should adopt much shorter pulse duration than the phonon period (\( \sim 180 \) fs), which is rather conflicting with the well-known physics of the coherent phonon (i.e., the laser pulse shorter than (or similar to) the phonon period should work). This is because we used too simple an equation (i.e., a rate equation below equation (4)) to evaluate the photoexcited charge density \( N(\tau) \) quantitatively. An analytic solution for \( \xi(\tau) \), equation (5), confirms this point. Nevertheless, the result is consistent qualitatively in that the shorter laser pulse favors the more robust production of coherent phonon.
the initial condition $\Delta_i(0) = 0$ are presented in figure 2(b). Naturally, $\Delta_i(\tau)$ becomes zero for the vanishing coherent phonon amplitude. This finding reproduces a recent experimental observation that the regeneration of SDW was made above the transition temperature through a creation of the coherent lattice oscillation [13]. It is worth noting that the detailed electronic structure of BaFe$_2$As$_2$, like the Fermi surface topology or multiband structure was not considered in the present TDGL theory. This may imply a quantitative limitation of our present theory. To be beyond the limitation, a microscopic understanding of the spin–phonon coupling incorporating the multiband electronic structure of BaFe$_2$As$_2$ should be required.

3. First-principles calculation and its implication

3.1. Energetics

Coherent phonon induces a macroscopic ionic shift toward a new equilibrium position in a unit cell (see the inset of figure 2(a)). First-principles electronic structure calculation could give an important insight of energetics between NM and SDW states of BaFe$_2$As$_2$ with respect to the relevant shift in figure 3. First-principles calculation was carried out using the Vienna ab-initio simulation package (VASP) code [25] and a density functional theory (DFT) approach with the projector augmented wave (PAW) method [26]. The exchange-correlation functional was expressed using the generalized gradient approximation (GGA) proposed by Perdew et al [27]. An energy cutoff of 450 eV was used for the plane-wave expansion. In this calculation, an integration over the Brillouin zone was performed by using a $\times 13 \times 13 \times 7$ Monkhorst-Pack k-point mesh for the orthorhombic structure (Fmmm) of SDW and $\times 13 \times 13 \times 13$ for the tetragonal structure (I4/mmm) of NM state, respectively. Lattice constants for the orthorhombic phase were determined to be $a = 5.708 \text{Å}$, $b = 5.599 \text{Å}$, and $c = 12.921 \text{Å}$, which are in good agreement with the experimental values within a difference of 2% [28], while $a = b = 3.973 \text{Å}$ and $c = 12.626 \text{Å}$ were obtained for the tetragonal phase. Besides, in the calculation for SDW, we considered the collinear spin structure. According to the calculation, the SDW state is found to be energetically favored by 128 meV/f.u. over the NM state. However, for NM state, the calculated fractional (internal) coordinate of As ion $z_{As}$ (i.e., $z_{As} = 0.3451$ (DFT)) to 0.3541 (at $T = 175 \text{K}$, experiment [28]) by about 3%. This discrepancy would be mainly attributed to the correlation effect of the Fe $3d$ orbital. DFT calculation of the NM phase usually underestimates the Fe-As bond length in all the Fe pnictide superconductors [29]. In figure 3(a), from NM state, we extrapolate the total energy of NM$_{T>T_c}$ (NM$_{T>T_c}$ means the NM state at $T > T_c$; we actually assume $T = 175 \text{K}$) by shifting $z_{As}$ ($=0.3451$ (DFT)) to 0.3541 (at $T = 175 \text{K}$, experiment [28]) and additionally taking a thermal energy increment by $5 \times \frac{3}{2}T$ (i.e., the equipartition theorem with five atoms in a formula unit).

3.2. Lattice-spin cooperative phenomena

In the potential energy manifolds for SDW and NM$_{T>T_c}$ obtained in figure 3(a), a schematic description of the photoinduced dynamics starting from NM$_{T>T_c}$ is provided in figure 3(b). Optical pumping creates the photoexcited charge density and the consequential electron–phonon and spin–phonon couplings cast the potential energy curve $\sim \frac{1}{2}z^2$ to the optically
induced curve $\sim -\frac{1}{2}z^2 + z(N' + \Delta'_s) + \mathcal{E}'$, where $z$ is a configurational coordinate. $N'$ and $\Delta'_s$ are terms related to electron–phonon and spin–phonon couplings, respectively, and $\mathcal{E}'$ includes additional excitation energies. This makes a shifted oscillation over a new equilibrium position, i.e., smaller $z_{As}$, which causes the energy $\mathcal{E}'_{s}$ of the lattice part as shown in the sketch of figure 3(b). The shifted oscillation and its strong coupling to the electron spin can drive the electronic part to be cooled down effectively below $T_s$ by opening the SDW gap. Note that $\mathcal{E} - \mathcal{E}'_{s}$ is lower than the minimum of NM$_{T>T_s}$. This will be the physical picture of the optically regenerated SDW at $T$ > $T_s$. Let us also note that the optically induced potential curve (red solid line) of figure 3(b) is essentially the same as the TDGL free energy including $\mathcal{F}'_{s}(\tau) = \frac{1}{2}\omega_0\xi^2 - \omega_0\bar{g}\xi\Delta_s - \omega_0\bar{g}\xi N(\tau)$, where a negative sign to $\xi$ is due to a difference in definition of $\xi$ and $z$. 

**Figure 3.** (a) Total energy of the SDW state (blue solid line) as a function of the fractional coordinate of As ion, $z_{As}$. Extrapolation for the total energy of NM$_{T>T_s}$ (we actually assume $T = 175$ K; see the text) is given in black solid line. (b) Sketch of photoinduced dynamics from the initial potential energy (i.e., NM$_{T>T_s}$; black solid line) to the optically induced potential energy (red solid line). $\mathcal{E}$ is the energy after the optical excitation. $\mathcal{E}'$ is the excitation energy of the lattice part and $\mathcal{E} - \mathcal{E}'$ is the remaining energy of the electronic part. $z$ is a configurational coordinate. $N'$ and $\Delta'_s$ are terms relevant with lattice couplings. The system shifts toward a new equilibrium position by the optical pumping. SDW$_{T=0}$ (blue solid line) corresponds to SDW in (a). In the figure, the shift is intentionally exaggerated.
Figure 4(a) gives us an insight of spin–phonon coupling in terms of the first-principles calculation for the SDW state. One may have

\[
\xi \frac{\partial \mathcal{E}_{e-p}}{\partial n} \left( \frac{\partial n_i}{\partial z_{\text{As}}} - \frac{\partial n_i}{\partial z_{\text{As}}} \right) \approx \bar{g} \left( n_\uparrow - n_\downarrow \right),
\]

where \( \mathcal{E}_{e-p} \) is the electron–phonon coupling energy. If one takes \( n_\uparrow - n_\downarrow \sim O(1) \) and \( \frac{\partial n_i}{\partial z_{\text{As}}} - \frac{\partial n_i}{\partial z_{\text{As}}} \sim O(10) \) from figure 4(a) and further assumes \( \xi \frac{\partial \mathcal{E}_{e-p}}{\partial n} \sim O(10^{-2}) \) eV Å, one may have \( \bar{g} \sim O(10^{-3}) \) eV Å. As manifested in figure 4(a), \( n_\uparrow \) or \( n_\downarrow \) in equation (6) implies the total number of spin up or spin down electrons. However, even in the present dynamics starting from the NM state, equation (6) is still useful by putting \( n_i = n_i^0 + n_i^{\text{ex}} \) and \( n_i = n_i^{\text{ex}} \), where \( n_i^{\text{ex}} \), means electrons remaining nonmagnetic, i.e., \( n_i^{\text{ex}} = n_i^0 \), and \( n_i^{\text{ex}} \) photoexcited electrons. In this sense, \( \bar{g} \sim O(10^{-3}) \) eV Å just obtained from equation (6) and figure 4(a) would be consistent with \( \bar{g} = 0.11 \) eV Å taken in figures 1 and 2. A shifted oscillation to smaller \( z_{\text{As}} \) gives an increase of the effective spin–phonon coupling strength \( \bar{g} \) according to equation (6) and
Further intuitive understanding may be available from the stationary limit of dynamics after termination of the optical pumping and relaxation of the photoexcited charges ($N \to 0$) by taking $\partial F / \partial \Delta_s = 0$ and $\partial F / \partial \xi = 0$ from equation (3). We find an effective cooling of the system like $T \to T - \tilde{g}^2 / \alpha$ (for a fixed $T_s$), or an effective increase of $T_s$ like $T_s \to T_s + \tilde{g}^2 / \alpha$ (for a fixed $T$) with regard to a new equilibrium position $\tilde{\xi} = 0 \to \tilde{\xi} = \tilde{g} \Delta_s / \omega_0$. It is interesting to explicitly estimate the effective cooling induced by the coherent phonon. From figure 2, the $A_{1g}$ mode displacement (i.e., As displacement) would be about $10^{-3}$Å and $\Delta_s$ about $10^{-5}$, which lead to $\tilde{g} \sim O\left(10^{-1}\right)$ eVÅ. We can then find that an effective cooling of the system would be $\tilde{g}^2 / \alpha \sim O\left(10^{-1}\right)$ K. The effective cooling of the system (or effective increase of $T_s$) could be regarded to induce the SDW gap. It was in fact reported that $T_s$ of Ba$_{1-x}$Sr$_x$Fe$_2$As$_2$ increases as $x (0 \leq x \leq 1)$ increases [30], where $z_{As}$ decreases with an increase of $x$.

In order to investigate how the As displacement affects the electronic structure of BaFe$_2$As$_2$, the partial density of states (PDOS) is presented for the SDW state in figure 4(b). It is noticeable that the systematic band narrowing occurs as $z_{As}$ increases. It is also noted from figure 4(a) that the local magnetic moment of the Fe atom increases from 1.32 $\to$ 1.94 $\to$ 2.34 $\mu_B$ as $z_{As}$ increases from S1 to S3, which is clearly demonstrated in the inset. This is physically intuitive in that the As ion going away from the Fe layer may induce the strong exchange correlation between Fe ions, which typically leads to the band narrowing and an increase of the magnetic moment.

4. Summary

In summary, in a model incorporating TDGL of the ultrafast cooperative interplay among charge, spin, and lattice, we investigated the subpicosecond transient dynamics of BaFe$_2$As$_2$. We found that the coherent phonon (i.e., a shifted macroscopic oscillation) generated by the optical excitation couples to the SDW order parameter, which drives reconstruction of the SDW order at $T > T_s$. Employing the first-principles electronic structure calculation, a change in the potential energy between NM and SDW was calculated with respect to the fractional coordinate of As ion. This substantiates that SDW can be reached by a macroscopic shift of As ion in NM through an excitation of the coherent lattice oscillation. This finding explains the recent experimental observation.

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