

Electron-phonon coupling of the iron pnictide superconductor $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$

Alexander Bartenev¹, Roman S. Kolodka¹, Ki-Tae Eom², Jong-Hoon Kang², Adrian Rua¹, Larry Theran³, Camilo Verbel¹, Eric E. Hellstrom⁴, Chang-Beom Eom², Armando Rua¹, Sergiy Lysenko¹

¹Department of Physics, University of Puerto Rico, Mayaguez, Puerto Rico 00681, USA

²Department of Materials Science and Engineering, University of Wisconsin-Madison, WI 53706, USA

³Department of Electrical and Computer Engineering, University of Puerto Rico, Mayaguez, Puerto Rico 00681, USA

⁴Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA
e-mail: alexander.bartenev@upr.edu

Abstract: Femtosecond photoexcitation of $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ superconductors reveals distinct dynamics of laser fluence-dependent ultrafast processes. The modified two-temperature model shows the complex interplay between thermalization time constants, electron-phonon coupling parameters, and level of optical excitation. © 2023 The Author(s)

$\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ is iron-based 122-type superconductor with suppressed antiferromagnetism and superconducting transition temperature T_c above 15 K [1]. Significant variations in T_c , structural transition temperature T_S , and electronic heat capacity in BaFe_2As_2 were observed with respect to electron doping, suggesting a multiband superconductivity [1,2]. The electron-phonon (*e-ph*) coupling in superconductors requires rigorous study what can be performed by using the phenomenological two- or three-temperature models [3, 4]. The Allen's theory [5] allows deriving the *e-ph* coupling constant λ [3, 4], and T_c can be calculated using the McMillan formula. However, the calculated T_c values show a notable divergence from experimental ones, revealing the unconventional nature of BaFe_2As_2 superconductor. Despite these efforts, the role of *e-ph* coupling in superconductivity and its sensitivity to lattice temperature, external pressure, and electromagnetic excitation, still remains poorly understood.

In this work, we study the *e-ph* coupling for $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ in its superconducting state at 8 K, exploring the evolution of the second moment of Eliashberg function $\lambda\langle\omega^2\rangle$ versus the laser excitation fluence. Time-resolved reflectivity data were analyzed in terms of the modified two-temperature model (TTM) that includes the non-instantaneous electron thermalization time [6].

Thin films were grown by pulsed laser deposition on $(\text{La,Sr})(\text{Al,Ta})\text{O}_3$ [LSAT] single crystal employing the SrTiO_3 [STO] epitaxial buffer layer. To achieve TiO_2 terminated surface, STO template was etched by buffered hydrofluoric acid. By using the x-ray diffraction and resistance measurement data, an 80-nm-thick $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ film was selected for optical studies. The pump-probe reflectivity measurements were performed with Ti:Sapphire femtosecond laser, operating at 1 kHz repetition rate and producing 35 fs laser pulses with $\lambda=800$ nm central wavelength. The pump laser fluence ranging from 1 mJ/cm^2 to 5.1 mJ/cm^2 was computer-controlled by a half-wave plate affixed to a motorized rotary stage in the front of the Glan polarizer. The probe pulse was overlapped with the pump pulse, and its intensity was significantly attenuated to prevent nonlinear interaction with the sample. The sample was mounted inside the optical cryostat operating at 8 K.

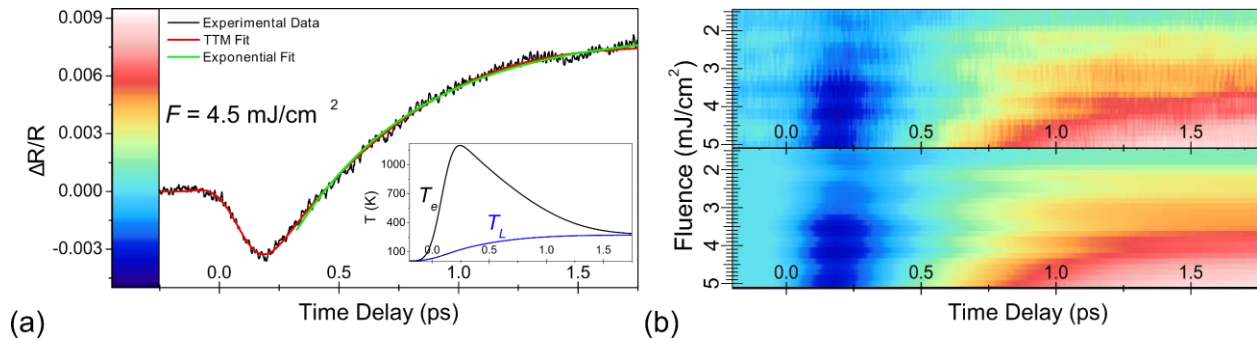


Fig. 1. Transient reflectivity of $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ (a) at pump fluence $F=4.5 \text{ mJ}/\text{cm}^2$, along with TTM and single exponent fit curves. The inset illustrates the temperatures of the electron and lattice subsystems versus delay time t ; (b) Comparison of the $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ transient reflectivity versus laser fluence within 2 ps scale [upper panel], and its TTM-modelled counterpart [lower panel].

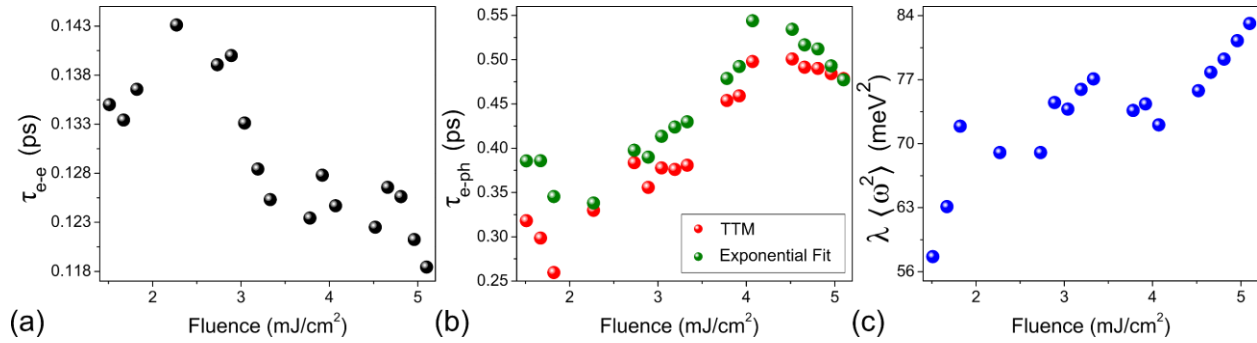


Fig. 2. The $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ constants obtained from experimental data fitting: (a) the electron thermalization time τ_{e-e} , (b) the electron-phonon relaxation time τ_{e-ph} , and (c) the second moment of the Eliashberg function $\lambda \langle \omega^2 \rangle$.

The nonlinear signal $\Delta R(t)/R(0)$ of $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ shows an initial drop in the transient reflectivity $\Delta R(t)$ within the first 200 fs [Fig.1(a)], followed by a gradual rise above the equilibrium value $R(0)$. The experimental data of laser fluence-dependent signal is shown in [Fig.1(b), upper panel]. The TTM was applied to model the electron-electron ($e-e$) and electron-phonon thermalization dynamics $\Delta R(t)/R(0)=a\Delta T_e(t)+b\Delta T_L(t)$ [Fig.1(b), lower panel], where a and b are fitting parameters. The electronic T_e and lattice T_L temperatures [see inset in Fig.1(a)] were computed in TTM using the Runge-Kutta method with additional fitting algorithms for $e-ph$ coupling G constant and thermalization time τ_{e-e} , with the heat capacities from [2]. This allows estimating the second moment of the Eliashberg function associated with the strength of the $e-ph$ interaction as [5]:

$$\lambda \langle \omega^2 \rangle = \frac{\pi k_B G}{3 \hbar \gamma} \quad (1)$$

where γ is the electronic specific heat, k_B is the Boltzmann constant, and \hbar is the reduced Planck constant.

The initial drop of the transient reflectivity signal is associated with $e-e$ thermalization, showing that the τ_{e-e} time exceeds the excitation pump pulse. With a modified laser source term in the TTM [6], the time τ_{e-e} was estimated to be within a 120-145 fs range, showing a slight decrease with increasing pump fluence [Fig.2(a)].

Figure 2(b) shows $e-ph$ relaxation time τ_{e-ph} obtained using two different approaches: from TTM and from single exponential fit. Both approaches indicate a rise of the τ_{e-ph} with pump fluence, converging more closely at higher fluences. The Eliashberg function's second moment values, calculated here, match those in [3] for similar fluences, and are slightly higher than values for overdoped and undoped samples [4]. The rapid rise of electronic temperature with subsequent $e-ph$ energy transfer results in strong uniaxial stress that can affect $\lambda \langle \omega^2 \rangle$.

In summary, the ultrafast nonequilibrium optical dynamics of $\text{Ba}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ were measured and evaluated using TTM to compute characteristic time constants for $e-e$ and $e-ph$ processes. While the electron thermalization time shows a slight decrease with the pump fluence, the $e-ph$ thermalization time and second moment of the Eliashberg function both show an increase associated with photoinduced stress in the film.

The work was supported at UPRM by the NSF Award# DMR-1905691. The work at University of Wisconsin-Madison (Thin film synthesis and characterization) was supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), under Award# DE-FG02-06ER46327.

References

- [1] N. Ni and S. L. Bud'ko, "Tuning the ground state of BaFe_2As_2 : Phase diagrams and empirical trends," MRS Bulletin **36**, 620–625 (2011).
- [2] F. Hardy, T. Wolf, R. A. Fisher, R. Eder, P. Schweiss, P. Adelmann, H. v. Löhneysen, and C. Meingast, Calorimetric evidence of multiband superconductivity in $\text{Ba}(\text{Fe}_{0.925}\text{Co}_{0.075})_2\text{As}_2$ single crystals, Phys. Rev. B **81**, 060501 (2010).
- [3] B. Mansart, D. Boschetto, A. Savoia, F. Rullier-Albenque, F. Bouquet, E. Papalazarou, A. Forget, D. Colson, A. Rousse, and M. Marsi, "Ultrafast transient response and electron-phonon coupling in the iron-pnictide superconductor $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$," Phys. Rev. B **82**, 024513 (2010).
- [4] L. Rettig, R. Cortès, H. S. Jeevan, P. Gegenwart, T. Wolf, J. Fink, and U. Bovensiepen, "Electron-phonon coupling in 122 Fe pnictides analyzed by femtosecond time-resolved photoemission," New J. Phys. **15**, 083023 (2013).
- [5] P. B. Allen, "Theory of thermal relaxation of electrons in metals," Phys. Rev. Lett. **59**, 1460–1463 (1987).
- [6] S. B. Naldo, A. V. Bernotas, and B. F. Donovan, "Understanding the sensitivity of the two-temperature model for electron-phonon coupling measurements," J. Appl. Phys. **128**, 085102 (2020).