Electron and Phonon Thermal Waves in Semiconductors: an Application to Photothermal Effects

G. González de la Cruz and Yu. G. Gurevich,
Departamento de Física,
Centro de Investigacion y de Estudios Avanzados del I.P.N.,
Apartado Postal 14–740, C.P. 07000,
México, D.F., México

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Abstract

The electron and phonon temperature distribution function are calculated in semiconductors. We solved the coupled one-dimensional heat-diffusion equations in the linear approximation in which the physical parameters on the sample are independent of the temperature. We also consider the heat flux at the surface of the semiconductor as a boundary condition for each electron and phonon systems instead of using a fixed temperature. From this, we obtain an expression for electron and phonon temperature respectively. The characterization of the thermal waves properties is discussed and some practical procedures for this purpose provide us information about the electron and phonon thermal parameters.

1 Introduction

Thermal wave physics is becoming a valuable tool in the study of material parameters as well as in the semiconductor industry for characterizing process in the manufacturing of electronic devices. These waves are created whenever there is a periodic heat generation in a medium. The most
common mechanism for producing thermal waves is the absorption of an intensity modulated light beam by a sample. The photothermal heating of a sample leads to thermal stress-induced changes in the physical properties of both the sample and the surrounding media. Based on this observation, several alternative detection techniques have been developed for monitoring the photothermally induced changes of given physical properties either of the sample or of its surrounding medium. Some of the different contact-type detection techniques, such as the conventional gas-microphone photoacoustic detection,\(^1\) photopyroelectric detection,\(^3\) or remote sensing techniques as photothermal reflection\(^4\) etc., have been reviewed in Ref. 5.

Being a photothermal technique, the detected signal is strongly dependent upon how the heat diffuses through the sample allows us to perform both thermal characterization of the sample (i.e., measurements of its thermal properties, such as thermal diffusivity and thermal conductivity), and carrier-transport properties.\(^6\) In the case of semiconductors the photoacoustic signal can provided us with additional information regarding the heat-transport properties and electron–phonon energy relaxation by the interacting electron and phonon systems, a fact which has been recognized since the earlier theory of heat conduction in semiconductors and hot electrons\(^6\)–\(^8\) Qualitatively, this may be understood as follows: in studies of the behavior of semiconductors heating by electromagnetic waves it is usual to assume that the phonon system remains in equilibrium, i.e., that the phonon temperature \(T_p\) is equal to the temperature \(T_0\) of the ambient medium.\(^8\) However, nonequilibrium carriers in the bulk of the sample can interact and transfer energy to the phonon system producing an essential increase in the average energy of phonons (energy nonequilibrium), which can be most conveniently described in terms of heating of the phonon gas (increase of its temperature \(T_p\)).\(^9\)

Let \(\nu_{pe}(q)\) be the characteristic phonon relaxation frequency owing to interaction with electrons. Gurevich at al.\(^9\) showed that the value of \(\nu_{pe}\) decreases rapidly for phonon wavevector \(q \geq 2\bar{p}\), tending ro zero, where \(\bar{p}\) is the average electron momentum, namely \(\bar{p} \sim \sqrt{2mT_e}\) for the nondegenerated electron gas, and \(\bar{p} \sim p_F\) (Fermi momentum) for the case of degeneracy. This mean that electrons are scattered by phonones having momentum values smaller than the average electron momentum \((q \leq 2\bar{p})\). Those phonones are knowen as long-wave (LW), in contrast to short-wave (SW) phonones, whose momentum satisfy \(q \geq 2\bar{p}\). The degree of nonequilibrium of the LW (and hence SW) phonones is determinated by the relationship of the phonon-
phonon collision frequency $\nu_{pp}$ and $\nu_{pe}$:

i) Strong phonon-phonon interaction

This case satisfies the following inequality $\nu_{pp} \gg \nu_{pe}$. This situation means that the phonon-phonon collisions are more frequent than phonon-electron collisions and more efficient in terms of energy relaxation than energy transfer from the phonon to the electron system. As a result, the Planck distribution function describes the phonon system with its own temperature $T_p$ different from $T_e$. Since the phonon-phonon collision frequency depends on the phonon temperature, the inequality $\nu_{pp} \gg \nu_{pe}$ holds for phonon temperature $T_p > 50^\circ K$ for n-type Ge and GaAs semiconductors with the charge density concentration $n \propto 10^{14} \text{ cm}^3$.

ii) Strong phonon-electron interaction

Now, consider the situation represented by the inequality $\nu_{pe} \gg \nu_{pp}$. This is the case when phonon-phonon collisions alone cannot bring the phonon system to an internal equilibrium, and the description becomes more complicated. If $T_p$ is the characteristic phonon temperature, than the momentum $T_p/s$ ($s$ is the sound velocity) sets a limit to the phase space volume occupied by phonons (with $q > T_p s$ the number of phonons is exponentially low). The number of LW and SW phonons depend on the relation between $2\hbar$ and $T_p/s$. If $T_p/s \gg 2\hbar$ is true i.e., LW phonones occupy a much smaller phase volume than SW phonones, then the subsystem of SW phonones has enough time to redistribute the energy recived from LW phonones between its constituent quasiparticles. As a result, the distribution function of SW phonones becomes Plankian, with some temperature $T_{SW}^p$. Then the electron-LW phonon interaction relax their energy more efficiently than the phonon subsystem and the LW phonons emitted by electrons of temperature $T_e$ are characterized by the same temperature $T_e = T_p^{SW}$. In this situation we also have two different subsystems; one corresponds to th SW phonons with Temperature $T_p^{SW}$ and the other one corresponds to electrons and LW phonons with a characteristic temperature $T_e = T_p^{LW} \neq T_p^{SW}$. If $T_p/s \ll 2\hbar$ holds, then all phonons interact efficiently with electrons, and hence the phonon system cannot be subdivided into LW and SW phonons. In this case, the phonons emitted by electrons of temperature $T_e$ are characterized by the same temperature $T_e = T_p$ and all the phonons show $\nu_{pe} \gg \nu_{pp}$ for $T_p < 50^\circ K$.

At this point it's important to mention that thermal waves phenomenon is present in the same only for modulated frequency of the incident light $\omega$ (chopper frequency) of the same order as the frequency of the relaxation energy between the quasiparticle systems $\nu_e$. In the limit $\omega \gg \nu_e$ the system
cannot respond to this external perturbation; therefore the dynamic part of
the heat flux is negligible as compared with the static part and the transferred
heat is only static. For $\omega \ll \nu_e$, the variation of the electron and phonon
temperature oscillates with the same modulated frequency of the incident
light.\textsuperscript{10} For the case when $\nu_{pp} \gg \nu_{pe}$ then $\nu_e \sim \nu_{pe}$ otherwise ($\nu_{pp} \ll \nu_{pe}$)
$\nu_e \sim \nu_{pp}$.\textsuperscript{9} Typical values of $\nu_e$ are in the range of $10^8$–$10^{10}$ sec$^{-1}$.\textsuperscript{6}

Recently,\textsuperscript{10} there has been some interest in studying thermal characterization of layered systems using the photoacoustic effect. In particular, from
the theoretical point of view, thermal diffusion of one and two layer system
has been investigated using the heat-diffusion equation in the approxima-
tion when both the electron and phonon temperature distribution are equal.
This approximation is only valid in the limit of infinite electron-phonon en-
ergy interaction in which the size of the sample is greater than the cooling
length.\textsuperscript{7} The effective diffusivity and thermal conductivity of the two layer
were obtained assuming continuity of heat flux, instead of the temperature
distribution, at each interface and taking into account the physical solution
of the dynamical part of the temperature fluctuation in each layer.

In this work we further extend the earlier model for thin film semicon-
ductors by taking into account the so far neglected important features the
behavior of electrons and phonons under time varying excitation namely, the
electron and phonon temperature distribution function. In Part II the elec-
tron and phonon temperature distribution for semiconductors is calculated
by solving the coupled heat-diffusion equations, for both of quasiparticles
systems. In Section III a discussion of our results is presented, and a com-
parison to the predictions of the existing theories is also made. Finally, in
Section IV we present our conclusions.

2 Formulation

It is well known the heat transport in solids is carried out by various quasi-
particles (electrons, holes, phonons, magnons, plasmons, etc.). Frequently
the interactions between these quasiparticles are such that each of these sub-
systems can have its own temperature and the physical conditions at the
boundary of the sample. We restrict our analysis to the case of monopolar
semiconductors under the conditions of strong phonon-phonon interaction
as discussed previously.\textsuperscript{11} Therefore steady state heat conduction can be de-
scribed by the following system of equations

\[ \text{div } Q_e = -P_{ep}(T_e - T_p), \quad \text{div } Q_p = P_{pe}(T_e - T_p). \]
(1)

The term \( P_{ep}(T_e - T_p) \) describes the transfer of heat between electrons and phonons. Here \( P_{ep} \) is a parameter proportional to the energy frequency between electron and phonon systems (\( P_{ep} = P_{pe} = P \approx n\nu_e \)) and the heat flux of electron \( Q_e \) and phonon \( Q_p \) subsystems are described by the usual relationships:

\[ Q_e = -\kappa_e \text{ grad } T_e, \quad Q_p = -\kappa_p \text{ grad } T_p, \]
(2)

where \( \kappa_e, \kappa_p \) is the electron (phonon) thermal conductivity. So far, Eqs. (1) include only the static contribution of the heat transport, i.e. the heat flux is independent of time. However, in the photothermal experiments, the incident radiation is modulated in time by the chooper, and in this case it is necessary to consider the dynamic contribution to the heat transport in the electron and phonon systems. Let us assume the one dimensional model for the heat flux. Assuming that the sample is optically opaque to the incident light (i.e., all the incident light is absorbed at the surface), the electron and phonon temperature distribution function are the solutions of

\[ \frac{\partial^2 T_e(z,t)}{\partial z^2} - k_{e,p}^2 [T_e(z,t) - T_p(z,t)] = \frac{1}{\alpha_e} \frac{\partial T_e(z,t)}{\partial t}, \]
(3)

\[ \frac{\partial^2 T_p(z,t)}{\partial z^2} + k_{e,p}^2 [T_e(z,t) - T_p(z,t)] = \frac{1}{\alpha_p} \frac{\partial T_p(z,t)}{\partial t}, \]

where \( k_{e,p}^2 = \frac{P}{\kappa_{e,p}} \) and the diffusivity for each system is given as \( \alpha_{e,p} = \kappa_{e,p}/(\rho c)_{e,p} \) and \( \rho_e, c_e \) (\( \rho_p, c_p \)) is the electron (phonon) density and specific heat respectively.

The temperature fluctuation \( T_{e,p}(z,t) \) should be supplemented by boundary conditions at the surface of the semiconductor \((z = 0)\). In the photothermal experiment, the most common mechanism to produce thermal waves is the absorption by the sample of an intensity modulated light beam with frequency modulation \( \omega \leq \nu_e \). It is clear that when the intensity of the radiation is fixed, the light-into-heat conversion at the surface of the sample can be written in general as

\[ Q_{e,p}(z,t)|_{z=0} = Q_{e,p} + \Delta Q_{e,p} e^{i\omega t} \]
(4)
where $Q_{e,p}$ is proportional to the intensity of high frequency light and the other term represents the modulation of this light.

The general solution of the coupled heat-diffusion equation for the electron and phonon system can be written as

$$T_{e,p} = A + Bz \pm \frac{k_{e,p}^2}{k^2} Ce^{-kz} + \theta_{e,p}(z)e^{i\omega t}$$

where $k^2 = k_e^2 + k_p^2$ represents the inverse of cooling length\(^7\) and $\theta_{e,p}(z)$ satisfies a similar set of Eqs. (3) but instead of the term $(1/\alpha_{e,p})\partial T_{e,p}/\partial t$ we substitute $(i\omega/\alpha_{e,p})T_{e,p}$, and the solution is given by

$$\theta_e(z) = Fe^{-\sigma z}$$

$$\theta_p(z) = Ge^{-\sigma z}.$$ 

Here $F$ and $G$ are related each other by the following relationship

$$G = -\frac{\sigma^2 - \sigma_e^2}{k_e^2} F$$

and the values of $\sigma$ are given by

$$\sigma_{1,2}^2 = \frac{1}{2} (\sigma_e^2 + \sigma_p^2) \pm \frac{1}{2} \left[ (\sigma_e^2 - \sigma_p^2)^2 + 4k_e^2k_p^2 \right]^{1/2}$$

Eq. (8) represents the condition for non-trivial solutions of the coupled electron-phonon differential equations and $\sigma_{e,p}^2$ are given by

$$\sigma_{e,p}^2 = \frac{i\omega}{\alpha_{e,p}} + k_{e,p}^2.$$ 

It is worth mentioning that the increasing exponential term $\exp kz$ and $\exp \sigma_{1,2}z$ which are solution of the static and the dynamical part of heat-diffusion equations respectively have not been considered because they do not represent a physical solution (heat flux cannot be reflected).

Using the boundary conditions at the surface of the sample given by Eq. (4) the electron and phonon temperatures are given by

$$T_e = A + Bz + \frac{k_{e}^2}{k^2} Ce^{-kz} + e^{i\omega t} [F_1e^{-\sigma_1z} + F_2e^{-\sigma_2z}],$$
\[ T_p = A + Bz + \frac{k_e^2}{k^2} e^{-kz} + e^{i\omega t} \left[ G_1 e^{-\sigma_1 z} + G_2 e^{-\sigma_2 z} \right], \]  

where the constants \( B, C, F_{1,2}, G_{1,2} \) can be written as

\[ \begin{align*}
B &= -\frac{1}{k^2} \left( \frac{Q_e k_p^2 + Q_p k_e^2}{\kappa_e} \right) \\
C &= \frac{1}{k} \left( \frac{Q_e}{\kappa_e} - \frac{Q_p}{\kappa_p} \right) \\
F_1 &= \frac{1}{\sigma_1 (\sigma_2^2 - \sigma_1^2)} \left[ \frac{\Delta Q_p k_e^2 \kappa_p^2}{\kappa_e} + \frac{\Delta Q_e (\sigma_2^2 - \sigma_e^2)}{\kappa_e} \right] \\
F_2 &= -\frac{1}{\sigma_2 (\sigma_2^2 - \sigma_1^2)} \left[ \frac{\Delta Q_p k_e^2 \kappa_p^2}{\kappa_e} + \frac{\Delta Q_e (\sigma_1^2 - \sigma_e^2)}{\kappa_e} \right] \\
G_{1,2} &= -\frac{\sigma_{1,2}^2 - \sigma_e^2}{k_e^2} F_{1,2}
\end{align*} \]

Here \( A \) is a constant which cannot be determined from these boundary conditions and it is not important in obtaining the physical results.

Once we know the electron and phonon temperature distributions in the sample, we can calculate the response of the surrounding medium due to the photothermal heating of the sample using one of the several alternative detection techniques mentioned before.

3 Special Cases

We now turn to a discussion on the results obtained so far and compare them with previous theories on thermal waves. We shall first consider a nondegenerate semiconductors. In this case, the typical ratio of the heat conductivity of electrons to phonon satisfies \( \kappa_e/\kappa_p \sim 10^{-3} \) then \( k_e \gg k_p \). Under these circumstances, after simplifying the expression for \( T_e, T_p \) and \( \sigma_{1,2} \) can be written as

\[ T_e(z,t) = A + Bz + Ce^{-kz} + e^{i\omega t} \left( F_1 e^{-\sigma_1 z} + F_2 e^{-\sigma_2 z} \right) \]  

\[ (12a) \]
\[
T_{p}(z,t) = A + Bz - \frac{k_{p}^{2}}{k_{e}^{2}}Ce^{-kz} + G_{2}e^{i\omega t - \sigma z}
\]  

(12b)

where \( G_{1} \approx 0, \sigma_{1} = \sigma_{e} \) and \( G_{2} = \left[ 1 - \frac{i\omega}{k_{e}^{2}} \left( \frac{1}{\alpha_{p}} - \frac{1}{\alpha_{e}} \right) \right] F_{2} \), \( \sigma_{2} = i\omega/\alpha_{p} \). It is important to note that the contribution of the electron diffusivity disappears in the phase of the dynamical part of the phonon temperature.

Because the main source of the photothermal signal arises from the periodic heat flow from the semiconductor, the periodic diffusion process produces a periodic temperature variation in the semiconductor given by the sinusoidal (AC) component of Eqs. (12).

Information about electron and phonon parameters can be obtained from photothermal experiments depending upon the decay length \( s_{1,2} = \Re \sigma_{1,2} \) of the AC component of the electron and phonon temperature at \( z = d \) (where \( d \) is the thickness of the sample).

As can be seen in Fig. 1a, if \(|F_{1}| \gg |G_{2}| \geq |F_{2}|\) and \( s_{1} \ll s_{2} \) the time dependent component of the phonon temperature in the semiconductor attenuates rapidly to zero with increasing distance from the surface of the solid as compared with component of the electron temperature, and the electron thermal wave carries all the information about electron and phonon parameters through the coefficient \( F_{1} \). However if besides that \( \frac{\Delta Q_{e}}{\kappa_{e}} \ll \frac{\Delta Q_{p}}{\kappa_{p}} \), electron thermal wave provide us only information about thermal parameters of the electron system. Now if \( \frac{\Delta Q_{p}}{\kappa_{p}} \gg \frac{\Delta Q_{e}}{\kappa_{e}} \) information about the phonon system is only obtained from the photothermal experiments.

On the other hand if \(|F_{1}| \gg |G_{2}| \geq |F_{2}|\) and \( s_{1} \gg s_{2} \), in this case the time dependent component of the electron temperature is fully damped out as shown in Fig. 1b. Information about the electron or phonon parameters depend on the relation between \( d \) and \( s_{1}^{-1} \) and how the incident energy is distributed in the electron and phonon systems:

(1) \( d < s_{1}^{-1} \) and \( \frac{\Delta Q_{e}}{\kappa_{e}} \gg \frac{\Delta Q_{p}}{\kappa_{p}} \), Eqs. (11c) and (12a) tell us that thermal wave associated with the electron system only give information about the electron thermal parameters.

(2) \( d > s_{1}^{-1} \) and \( \frac{\Delta Q_{e}}{\kappa_{e}} \ll \frac{\Delta Q_{p}}{\kappa_{p}} \), in this case only a phonon thermal wave can be detected at \( z = d \) and the photothermal experiments give the thermal phonon parameters of the sample.

Similar behavior of photothermal waves in the semiconductors can be obtained if \(|G_{2}| \gg |F_{2}|, |F_{1}|\) and \( s_{2} \ll s_{1} \) and information about phonon thermal parameters is obtained from the photothermal experiments if in ad-
dition the inequality $\frac{\Delta Q_p}{\kappa_p} \gg \frac{\Delta Q_e}{\kappa_e}$ holds. If $|G_2| \gg |F_2|, |F_1|$ and $s_2 \gg s_1$, hence the photothermal experiments only detect the thermal parameters of the phonon system when $d \ll s_2^{-1}$ and $\frac{\Delta Q_p}{\kappa_p} \gg \frac{\Delta Q_e}{\kappa_e}$ or thermal parameters of the electron system if $d \gg s_2^{-1}$ and $\frac{\Delta Q_p}{\kappa_p} \gg \frac{\Delta Q_e}{\kappa_e}$ as shown in Figs. 2a and 2b.

In the case $k_{e,p} \to 0$ (electron-phonon interaction vanishes), it follows from Eqs. (11) that the electron and phonon temperatures reduce to

$$T_{e,p} = A_0 - \frac{Q_{e,p} z}{\kappa_{e,p}} + \frac{\Delta Q_{e,p}}{2\kappa_{e,p}} \left( \frac{2\alpha_{e,p}}{\omega} \right)^{1/2} (1 - i)e^{i\omega t - \sigma_{e,p} z}$$

where the constant $A$ has been chosen such that it exactly cancels out the divergent term from the Eq. (11b), i.e. for $P \to 0$ we have non-interacting systems of quasiparticles and heat transport is carried out by the electrons and phonon independently through the semiconductor.

We now consider the situation represented by the strong coupling between electrons and phonons i.e. $P \to \infty$. In this case the electron-phonon energy interaction is very efficient in terms of energy relaxation than energy transfer in the electron or phonon system. Here the solutions of Eq. (8) are given by

$$\sigma_1^2 = \frac{k^2 + i\omega}{k^2} \left( \frac{k_e^2}{\alpha_e} + \frac{k_p^2}{\alpha_p} \right)$$

$$\sigma_2^2 = \frac{i\omega}{k^2} \left( \frac{k_p^2}{\alpha_e} + \frac{k_e^2}{\alpha_p} \right)$$

and $G_2 \approx F_2$, $B = -\frac{1}{\kappa_e + \kappa_p} (Q_e + Q_p)$ therefore, in this limit both temperatures are the same

$$T = T_e = T_p = A + B z + F_2 e^{i\omega t - \sigma_{e,p} z}$$

Here the amplitude and decay length of temperature fluctuation in the sample depend in a nontrivial way on the diffusivity, heat conductivity of electron and phonon system and energy frequency of electron-phonon interaction. Equation (15) can be obtained from Eqs. (3) in the limit when $P \to \infty$. In this situation the electron and phonon temperature are the same, the product $P(T_e - T_p)$ approaches to unknown finite value and the set of differential equations for $P(T_e - T_p)$ and $T_e = T_p = T$ reduce to one,

$$\frac{\partial^2 T}{\partial z^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t}$$
with

\[
\frac{1}{\alpha} = \frac{1}{k^2} \left( \frac{k_p^2}{\alpha_e} + \frac{k_e^2}{\alpha_p} \right)
\]

(17)

where the solution is similar to Eq. (15) with the appropriate boundary condition at the surface of the semiconductor given by

\[
Q(z, t) \bigg|_{z=0} = Q_e(z, t) + Q_p(z, t) \bigg|_{z=0} = Q_e + Q_p + (\Delta Q_e + \Delta Q_p) e^{i\omega t}
\]

(18)

At this point, the authors believe that it is important to remark the difference between thermal waves and electromagnetic waves (for example). In the absence of rigorous theoretical guidance from first principles, several workers find it necessary to introduce arbitrary algebraic factor into their calculations in order to get desirable fit to the data. As a consequence the controversial analogy between thermal waves and electromagnetic waves arises.

It is our contention that the main differences are the following:

i) As pointed out by Mandelis,\textsuperscript{12} electromagnetic waves satisfy a hyperbolic differential equation while in the case for thermal waves satisfy a parabolic differential equation. In other words heat conduction in solid is a diffusive process, quite different to electromagnetic wave propagation.

ii) It is well known from standard electromagnetic books that the tangential component of the electric field at the interface between two different media must to be continuous. In addition there are a reflected and transmitted electromagnetic waves through the interface. However for the thermal waves there is not such similarity i.e., the electron or phonon temperature distributions in solid is not continuous in general at the interface of two layer system (see Ref. 10) only heat flux (energy conservation) is continuous at the boundary between two thermal different media.

iii) It is also well known that a damped electromagnetic wave in a medium is of the form \(e^{i(\omega t - kx) - \lambda x}\) where in general the decaying length satisfies the following inequality \(\lambda^{-1} \geq k^{-1}\) where \(k\) is the wave vector associated with the electric field. As mentioned before, information about electron and phonon thermal parameters can be obtained from photothermal experiments. In particular when the electron-phonon interaction is strong such that \(k_e^2 \gg \omega/\alpha_e\), in this limit the decay length \((\Re \sigma_1)^{-1}\) is smaller than the wave length \((\Im \sigma_1)^{-1}\) of the thermal wave associated with the electron system. This behavior is impossible to get from the propagation of electromagnetic waves. This three
points show that the analogy between thermal and electromagnetic waves is not correct.

4 Conclusions

A theoretical analysis of thermal waves in thin films semiconductors has been studied. Using the appropriate boundary conditions, we obtain the electron and phonon temperature distribution taking into account the physical solution for the static and dynamical parts of the heat-diffusion equation. For typical parameters of the heat conductivity of electrons and phonon in semiconductors \((k_e \gg k_p)\), it is possible to obtain information about the physical parameters describing the diffusivity and electron-phonon interaction in photoacoustic experiments. It is shown, Eq. (12), that the photothermal signal is ultimately governed by the electron or phonon system depending on the relationship of the amplitude and the decay lengths of the temperature fluctuation in each system and the sample size. We also showed that it is possible that decaying parameter of the thermal wave be smaller than the wavelength. However, it is well known that from Maxwell equations this situation is forbidden for electromagnetic waves.

We have also derived exact solutions for electron and phonon temperature in semiconductors in the limit of weak and strong electron-phonon interactions. The above findings tell us that thermal waves in semiconductors can propagate independent each other or propagate as a thermal wave in the sample with an effective diffusivity including the contribution of the thermal parameters of the electron and phonon system.

Acknowledgments

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