Lessons from Nanoscience:
A Lecture Note Series

Vol. 3

THERMAL ENERGY AT THE NANOSCALE

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Lessons from Nanoscience: A Lecture Note Series

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(Purdue University, USA)

"Lessons from Nanoscience" aims to present new viewpoints that help understand, integrate, and apply recent developments in nanoscience while also using them to re-think old and familiar subjects. Some of these viewpoints may not yet be in final form, but we hope this series will provide a forum for them to evolve and develop into the textbooks of tomorrow that train and guide our students and young researchers as they turn nanoscience into nanotechnology. To help communicate across disciplines, the series aims to be accessible to anyone with a bachelor's degree in science or engineering.

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Vol. 1 Lessons from Nanoelectronics: A New Perspective on Transport
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Vol. 3 Thermal Energy at the Nanoscale
by Timothy S Fisher

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To my wonderful and amazing wife Amy

Preface

These notes provide a detailed treatment of the thermal energy storage and transport by conduction in natural and fabricated structures. Thermal energy by two main carriers–phonons and electrons–are explored from basic principles. For solid-state transport, a common Landauer framework is used for heat flow, and issues including the quantum of thermal conductance, ballistic interface resistance, and carrier scattering are elucidated. Bulk material properties, such as thermal conductivity, are derived from transport theories, and the effects of spatial confinement on these properties are established.

The foregoing topics themselves are not unique as elements in a book; many other outstanding texts cover these topics admirably and are cited in context herein. At the same time, the present content emphasizes a basic theoretical framework based on the Landauer formalism that is as self-consistent as possible, not only internally but also with respect to similar efforts in this book series on the subject of electrical transport. The other series titles, written by Profs. Supriyo Datta and Mark Lundstrom, have therefore provided much inspiration to the present work, as have my related conversations with these two amazing colleagues. The end result is (hopefully) an accessible exposition on the foundations of the subject that remains concise by avoiding lengthy digressions into the vast array of related contemporary research topics. At the same time, it is my hope that readers, after studying this work, will be ready to enter the field well-equipped to contribute to this wonderful body of research and community of researchers.

T. S. Fisher

Acknowledgments

This text has been thoroughly inspired by the large number of outstanding students whom I have been privileged to teach both in the classroom and laboratory during my career. The content of this text has been refined over the years through teaching students at Vanderbilt University, Purdue University, and the Jawaharlal Nehru Centre for Advanced Scientific Research (Bangalore, India), as well as those from around the world who participated in the first offering of an online course by the same name, first delivered through the nanoHUB-U initiative in Spring 2013. I convey particular gratitude to students Alfredo Tuesta, Anurag Kumar, Guoping Xiong, Jeff Engerer, Kim Saviers, Menglong Hao, and Stephen Hodson for assistance with proofreading and indexing. The nanoHUB-U team, and particularly Amanda Buckles, Joe Cychosz, Erich Huebner, and Mike McLennan, provided tremendous support in launching the class and allowing me to focus on content, most of which appears herein. I also express appreciation to members of Purdue's Mechanical Engineering Heat Transfer faculty, a group with whom I am humbly privileged to serve; and particularly in the context of this book, I express gratitude to Professors Jayathi Murthy (now at UT-Austin), Xiulin Ruan, and Xianfan Xu, each of whom has inspired substantial content herein. Other Purdue faculty colleagues whose influence has significantly shaped my interpretation of the subject matter include Supriyo Datta, Bob Lucht, Mark Lundstrom, Ron Reifenberger, Tim Sands, and Ali Shakouri. The content herein draws from many sponsored research projects in which I have participated over the years, and I convey my sincere appreciation to those sponsors. In terms of active research projects during the writing of the book, the most relevant is that from the US Office of Naval Research (Program Manager: Dr. Mark Spector) on interfacial heat transfer. I also thank the publisher, World Scientific, and particularly Song Yu for supporting this book series and assisting with the publication details.

Lastly, I offer my most sincere thanks and recognition to Sridhar Sadasivam and Ishan Srivastava, two doctoral graduate students in my group at Purdue. Sridhar has served impeccably as a sounding board for the explanations and content in the text, as well as providing great help in composing and organizing graded content for the companion online course offered through nanoHUB-U. Ishan has patiently tolerated my pedestrian capabilities in graphic arts and created most of the graphics contained herein. He has also developed a suite of simple, web-accessible simulation tools (using Wolfram's CDF driver) for use in the online course that draws from the content here. Aside from the foregoing specific contributions, our regular meetings to discuss ideas, explanations, theory, and content for these notes and the online course have been tremendously invigorating. In these days of much chaos for academic researchers, with the various and sundry demands of our profession, finding time to focus on what really matters with these two gifted colleagues has been delightful; I thank them for their engagement.

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Nomenclature

α	thermal diffusivity (length^2/time)
β	inverse of thermal energy, $(k_BT)^{-1}$ (1/energy)
χ	carrier energy scaled by k_BT (-)
η_a	unit cells per volume of real space (1/volume)
η_e	volumetric electron density (1/volume)
$\hat{G}_Q$	quantum of thermal conductance (energy/time/temperature)
κ	thermal conductivity (power $\times$ length/('area' $\times$ temperature))
Λ	particle mean free path (length)
$\mathcal{D}$	plate bending stiffness (force $\times$ distance = energy)
$\mathcal{F}$	plate loading (force/area)
$\mathcal{L}$	boundary scattering length scale (length)
$\mathcal{T}$	carrier transmission function (-)
μ	mass density of a continuum string (mass/length)
ν	Poisson ratio (-)
Ω	number of possible states of a statistical ensemble (-)
ω	frequency (radians/time)
ω_D	Debye frequency (radians/time)
ω_E	Einstein frequency (radians/time)
ϕ	emitter work function (energy)
ρ	mass density (mass/volume)
σ	scattering cross section (area)
σ_e	electrical conductivity (current/(length $\times$ voltage))
τ	scattering time (time)
τ^{-1}	scattering rate (1/time)
τ_b^{-1}	boundary scattering rate (1/time)
θ_D	Debye temperature (temperature)
θ_E	Einstein temperature (temperature)

θ_F	Fermi temperature (temperature)
$\tilde{G}'_Q$	scaled spectral thermal conductance (-)
ε	boson energy (energy)
$\vec{a}_i$	real-space lattice translational vectors (length)
$\vec{b}_i$	reciprocal lattice translation vectors (lattice)
$\vec{G}$	reciprocal lattice vector (1/length)
$\vec{R}$	real-space lattice vector (length)
$\vec{v}_g$	group velocity (length/time)
a	lattice constant (length)
c	phase velocity (length/time)
c_0	speed of light in vacuum, 2.99792458×10^8 m/s
c_v	volumetric specific heat (energy/(volume × temperature))
$D(\omega)$	density of boson states, frequency basis (time/volume)
$D(\varepsilon)$	density of boson states, energy basis (volume energy)$^{-1}$
$D(E)$	density of fermion states, energy basis (volume energy)$^{-1}$
$D(K)$	density of boson states, **k**-space basis (length/volume)
D_α^β	dynamical matrix (force/(length × mass))
E	energy (energy)
E_b	bond energy (energy)
E_F	Fermi energy (energy)
E_Y	Young's modulus (force/area)
E_{vac}	vacuum energy level (energy)
F	boundary scattering fitting factor (-)
F	force on an atom due to bond stretching (force)
f_i^o	equilibrium carrier distribution function (-)
$f(t)$	forward-wave string displacement (length)
g	spring constant of an interatomic bond (force/length)
G'_Q	spectral thermal conductance (power/temperature, per unit frequency for phonons, or per unit energy for electrons)
$g(t)$	reflected-wave string displacement (length)
G_Q	thermal conductance (power/temperature)
h	plate thickness (length)
J	electrical current density (current/'area')
J_Q	heat flux (power/'area')
K	phonon wavevector (1/length)
k	electron wavevector (1/length)
K_D	Debye wavevector (1/length)
k_F	Fermi wavevector (1/length)

L_e	Lorenz number, dimensionless constant $\times \left(\frac{k_B}{q}\right)^2$
m	atomic mass (mass)
$M(\omega)$	number of phonon modes (-)
$M(E)$	number of electron modes (-)
m_e	electron mass, $9.10938188 \times 10^{-31}$ kg
$M_{dD}(\omega)$	phonon mode density, d = system dimension (1/'area')
$M_{dD}(E)$	electron mode density, d = system dimension (1/'area')
N	number of atoms (-)
N'	electron number (-)
N_A	Avogadro's number, 6.0221415×10^{23} (-)
n_i	defect density of impurity scatterers (1/volume)
N_{dD}	number of allowed phonon states, d = system dimension (-)
N_k	number of allowed electron states (-)
N_K	number of phonons with wave vector K (-)
P	acoustic wave power (energy/time)
P_ν	probability of a statistical state (-)
q	elementary electron charge, 1.602×10^{-19} C
r	distance coordinate (length)
R_b	thermal boundary (interface) resistance (temperature/power)
R_b''	area-normalized thermal boundary (interface) resistance (area$\times$temperature/power)
S	entropy (power/temperature)
t_{12}	interfacial energy transmittance from medium 1 to medium 2 (-)
U	internal energy (energy)
U	potential energy (energy)
u	atomic displacement away from equilibrium (length)
u	specific internal energy (energy/volume)
$u'(x)$	spectral energy density (energy/volume, per unit x, where x is a spectral quantity such as frequency or wavelength)
v_a	acoustic wave velocity (length/time)
v_F	Fermi velocity (length/time)
$y(x,t)$	total string displacement (length)
Z	acoustic impedance of a string under tension (mass/time)

Contents

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