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* denotes a volume which contains a Classified Index starting from Volume 36

H. Overhof P. Thomas

Electronic Transport in
**Hydrogenated
Amorphous
Semiconductors**

With 65 Figures



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Preface

Systematic research on amorphous semiconductors started more than thirty years ago. At that time the motivation for research was mainly academic interest in a field which was still new to researchers because of the absence of periodicity and the presence of disorder: Deviations of the electronic properties of amorphous semiconductors from those of crystalline semiconductors were observed, and theoretical concepts and models were developed which rested on well-known principles that had been used with success in the field of crystalline semiconductors. On the other hand, new theoretical methods were also introduced which explicitly took care of the disorder.

A dramatic rise in experimental activities started when it was realized that under suitable preparation conditions amorphous semiconductors, in particular hydrogenated amorphous silicon, could be used as a cheap basis material for large-scale electronic thin-film devices. Some new and surprising features of electronic properties, especially transport properties, were found. The theoretical models and methods, however, still remained at a somewhat immature state, which in view of the high complexity of the real amorphous semiconducting materials and the lack of a well-defined microscopic symmetry is not surprising. In the last few years, however, a coherent theoretical picture has begun to emerge which allows the interpretation of equilibrium transport properties of amorphous semiconductors to be placed on a more general footing.

This book is devoted to a detailed presentation of the model, the basic theoretical concepts and the interpretation of equilibrium transport data of tetrahedrally coordinated amorphous semiconductors. Most of the material covered by this book has been published in the last few years and is scattered over the literature. We found it therefore useful to give a coherent presentation of our approach, which also includes the discussion of other theoretical work in this field. The book is organized in such a way as to allow the occasional reader not interested in theoretical details to follow the main ideas, while theoreticians are invited to concentrate on the theoretical chapters and sections.

The authors are indebted to Professor Sir Nevill Mott for numerous discussions concerning the prefactor problem of the activated conductivity, and to Professor W. Götze for helpful discussions about his mode-coupling theory of Anderson localization. We thank our colleagues in Marburg, Professor J. Stuke, Professor W. Fuhs and Dr. H. Mell, as well as Dr. W. Beyer from Jülich, and their coworkers, for their continuous and fruitful cooperation in all problems related to experiments. We have benefitted from many fruitful discussions with Professors

H. Fritzsche, E.N. Economou, W.E. Spear and P.G. LeComber. From discussions with Dr. K. Kempter and his colleagues at Siemens AG we learnt many details related to the applications of amorphous semiconductors. Last but not least we thank our numerous students for their valuable and creative contributions to the present subject over the past decade, and Mrs. Anastasia Leventi for her gentle linguistic assistance.

Paderborn and Marburg,
October 1988

H. Overhof
P. Thomas

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List of Symbols*

a	lattice constant of the site lattice	63
A, A^*	heat of transport term of the thermoelectric power	27
A_{iq}	electron-phonon coupling constant	64
a_{loc}	decay length of a localized basis state	29
B_{MNR}	intercept of the Meyer–Neldel rule	128
B	magnetic (induction) field	
b_q, b_q^\dagger	phonon annihilation (creation) operator	64
c_i, c_i^\dagger	electron annihilation (creation) operator	16
d	dimensionality of the system	
d_i, d_i^\dagger	annihilation (creation) operator for displaced oscillators	123
e	elementary charge	
E	energy	
E_C, E'_C	mobility edge in the conduction band	17
E_F	Fermi energy	
E_F^q	quasi-Fermi energy	51
E_g^{opt}	optical band gap	11
E_H^*	activation energy of the Hall effect	50
E_m	mobility edge	27
E_{MNR}	characteristic energy of the Meyer–Neldel rule	41
E_Q, E_Q^*	activation energy of the Q function	46
E_S, E_S^*	activation energy of the thermoelectric power	28
E_t, E_t^*	dominant transport energy	76
E_T	slope of the tail density of states distribution	75
E_V	mobility edge of the valence band	24
E_σ, E_σ^*	activation energy of the conductivity	26
F, F_0	electric field	
f_0^e, f_0^h	Boltzmann distribution function for electrons (holes)	24
$f_F(E, E_F, T)$	Fermi distribution function	24
$g(E)$	density of states distribution	13
$g(L)$	dimensionless conductance of a sample of linear size L	19
$g_C(E)$	conduction band density of states distribution	13
$g_V(E)$	valence band density of states distribution	13
H, H'	Hamiltonian	

* Symbols that are of local importance only are not listed here.

H_e, H_{ep}, H_p	electronic, electron-phonon, and phonon contribution to H	63, 64
\hbar	Planck's constant	
I	current	
I_0^*, I_{00}	prefactor of the current	53
I_D	drift current of the time-of-flight experiment	56
I_{FB}	flat band current of the field effect experiment	131
I_{SD}	Source-drain current of the field effect experiment	54
j	electric current density	
J, J_{ij}	transfer matrix element	16
k	Boltzmann's constant	
k	quantum number for electronic states	17
k_F	Fermi wave number	18
l	electrode distance	51
l_{free}	mean free path	18
L_i	inelastic scattering length	22
L_{ij}	Onsager's transport coefficients	23
l_{max}	maximum fluctuation length of the long-ranged potential	110
l_{min}	minimum mean free path	18
m	mass of the electron	
n	electron density	51
N_C, N_V	effective density of extended conduction (valence) states	26
n_i	particle number operator	16
$p(V)$	distribution function of random potentials	115
$P(\varepsilon_i)$	distribution function of site energies	63
p_c	critical bond concentration in percolation theory	31
q	charge of a particle ($\pm e$)	25
q	quantum number for phonons	16
Q	combination of conductivity and thermoelectric power	28
Q_0, Q_0^*	intercept of the Q function	46
r	parameter for the electron-phonon coupling strength	74
R_c	critical radius in the percolation analysis for hopping	31
R_i	position of site i	16
R_{ij}	distance between sites i and j	30
s	frequency exponent of the ac conductivity	59
S	thermoelectric power, Seebeck coefficient	27
T	temperature	
T_{ac}	characteristic temperature of the ac conductivity data	60
T_{SLC}	characteristic temperature in the superlinear current	119
T_{TOF}	characteristic temperature of the TOF data	58
T_0	slope parameter of variable range hopping formula	33
t	time	
t_r	transit time in time-of-flight experiment	56
U_i, U_{eff}	Hubbard's correlation energy	123
V	voltage, potential	
v	velocity	
V_D	applied voltage of the TOF experiment	56

V_G	gate voltage of field effect	54
V_j	external potential	65
V_{SD}	Source-Drain voltage of field effect	54
w	heat current density	23
W	width of the distribution of disorder energies	17
y	coupling constant in the localization theory	68
z	complex frequency	
α_1, α_2	dispersion parameters of the TOF data	56
β	$1/kT$	
$\beta(g)$	scaling function	19
γ_F^*	temperature coefficient of the Fermi energy	127
$\Gamma_{ij}, \Gamma_{ij}^0$	hopping rate	30
γ_t^*	temperature coefficient of the transport energy	76
δ	rms potential fluctuation	111
ΔE_{opt}	slope of the Urbach tail	13
ΔE_σ^*	change of the apparent activation energy of the conductivity	78
ϵ''	imaginary part of the dielectric constant	13
ϵ_i	site energy	16
ϵ_s, ϵ_d	static dielectric constant of the semiconductor (dielectric)	
ϵ_0	vacuum dielectric constant	
η	rms width of the distribution of site energies	63
θ	dimensionless temperature	74
λ	critical exponent	20
A	phonon propagator	74
μ, μ_0	mobility	25
μ_H, μ_{H0}	Hall mobility	49, 116
ξ	correlation length	21
ξ_{loc}	localization length of an Anderson localized state	19
Π	Peltier coefficient	27
$\rho(E)$	density of electronic states per site	74
σ	conductivity	
$\sigma(E)$	differential conductivity	36
$\sigma_{ext}, \sigma_{hopp}$	extended states (hopping) contribution to σ	38
σ_M	minimum metallic conductivity	18
σ_h, σ_t	hopping (tunneling) contribution to σ	104
σ_0, σ_0^*	prefactor of the conductivity	26
τ_{deph}	dephasing time	96
τ_j, τ_n	current (density) relaxation time	66
χ, χ_{ij}	generalized susceptibility	65
Ψ_k	electronic wave function	17
Ω	volume of the system	
ω_q	phonon frequency	64
ω_0	frequency of order phonon frequency	59

List of Acronyms

CFO	Cohen-Fritzsche-Ovshinsky Model	4
CRN	Continuous Random Network	12
ESR	Electron Spin Resonance	14
fcc	face centered cubic	10
gd	glow discharge	5
MIS	Metal Insulator Semiconductor device	54
MNR	Meyer-Neldel Rule	42
NMR	Nuclear Magnetic Resonance	15
TOF	Time-of-Flight	55
RDF	Radial Distribution Function	12
SAW	Surface Acoustical Wave	146
SCLC	Space Charge Limited Current	51
SIMS	Secondary Ion Mass Spectroscopy	15
SLC	Super Linear Current	118
SWE	Staebler-Wronski Effect	42
TROK	Tietje-Rose-Orenstein-Kastner model	57
VLSI	Very Large Scale Integrated devices	1