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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
$\boldsymbol{B}$	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
$\boldsymbol{F}$, $\boldsymbol{F}_0$	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
$\boldsymbol{j}$	electric current density	
J , J_{ij}	transfer matrix element	16
k	Boltzmann's constant	
$\boldsymbol{k}$	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
$\boldsymbol{q}$	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
$\boldsymbol{R}_i$	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_T	transit time in time-of-flight experiment	56
U_i , U_{eff}	Hubbard's correlation energy	123
V	voltage, potential	
$\boldsymbol{v}$	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
$\boldsymbol{w}$	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
Γ_{ij} , Γ_{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
Λ	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
$\varrho(E)$	density of electronic states per site 74
σ	conductivity
$\sigma(E)$	differential conductivity 36
σ_{ext} , σ_{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
$\Psi_{\boldsymbol{k}}$	electronic wave function 17
Ω	volume of the system
$\omega_{\boldsymbol{q}}$	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