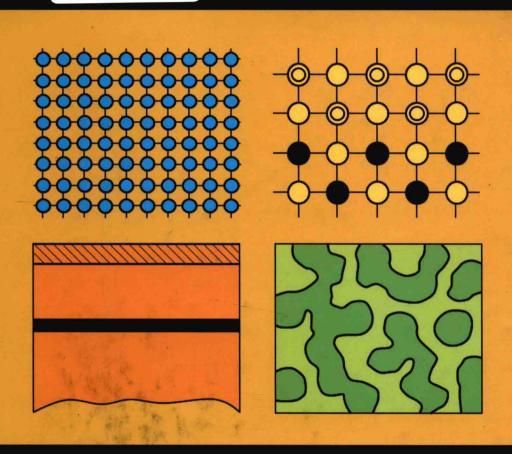
MATERIALS CONCEPTS FOR SOLAR CELLS

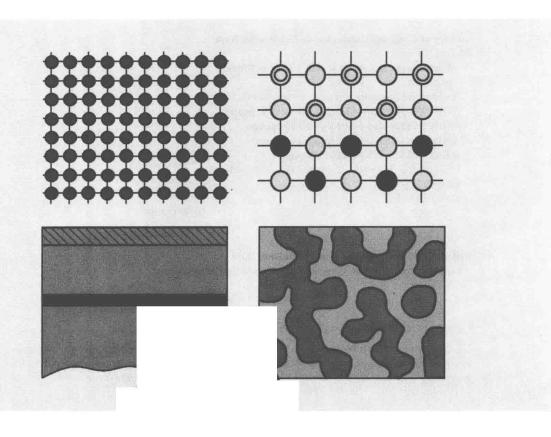


Thomas Dittrich

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MATERIALS CONCEPTS FOR SOLAR CELLS



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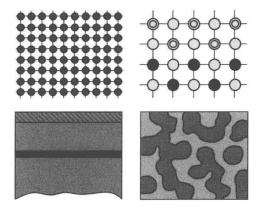
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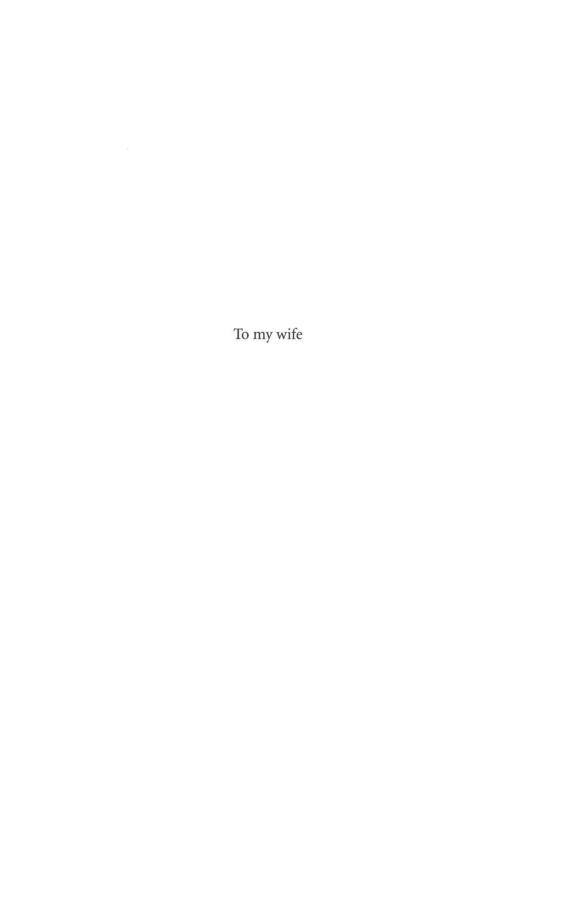
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MATERIALS CONCEPTS FOR SOLAR CELLS







Preface

This textbook results from lecture courses I have been giving to students who are interested in principles of solar energy conversion and in solar cell materials. Students listening to my courses usually study in the fields of engineering, materials science or natural science at universities around the world. I have had, and I continue to have, the great pleasure to teach not only in Europe but also in Asia, Africa and Latin America. A broad understanding of materials and combinations of materials for photovoltaic solar energy conversion helps to implement renewable energy worldwide. The textbook gives a comprehensive introduction to materials concepts for solar cells including basic principles and materials specific concepts.

The success in the development and application of solar cells is closely related to countless improvements of materials and to the development of new materials for solar cells. Quality criteria of solar cell materials are consequences of basic principles of solar cells. Materials and technological concepts follow from the ways in which different photovoltaic absorbers can be realized. Materials concepts of solar cells are based (i) on the growth of large crystals (wafer-based technology), (ii) on the growth of sophisticated layer systems on substrate crystals (epitaxy-based technology), (iii) on the deposition of absorber layers on foreign substrates (thin-film photovoltaics) and (iv) on the combination of very different materials on a nanometer scale (nano-composite solar cells). Interfaces between materials for charge separation, electric contacts to external leads and passivation are considered for all kinds of solar cells.

I would like to express my appreciation to all of my students, but especially those from the Free University Berlin for their interest and questions, to my former teacher Fred Koch for inspiration, to Günther Seliger for the opportunity to teach at GPE (Global Production Engineering for Solar Technology) at the Technical University Berlin, to friends at the Kasetsart University in Bangkok and other universities around the world for supporting my teaching projects, to Martha Lux-Steiner at the Helmholtz Centre Berlin for giving me the opportunity to teach alongside my scientific work, to Bernhard Reinhold for discussing aspects of this textbook, to Brian Edlefsen Lasch for his critical reading of the manuscript, and to Catharina Weijman from Imperial College Press for excellent collaboration.

Thomas Dittrich Berlin, 2013

Symbols and Abbrevations

Those Beginning with Latin Letters

A, A acceptor, ionized acceptor

A surface area

A ampere, unit of the current

a distance between two grid fingers

A/cm² unit of the current density
A_{cr} area of a cross section

a₀ Bohr radius of the hydrogen atom (0.051 nm)

a₀ interatomic distance A_{cell} area of the solar cell

a_{elhl,b} radius of an exciton with the lowest energy in bulk

semiconductor

a_{lc} lattice constant

A_{fc} area of the front contact ALD atomic layer deposition

AM air mass AM0 air mass zero

AM1.5d air mass 1.5 for direct irradiation

AM1.5G air mass 1.5 for global irradiation ($P_{sun}(AM1.5G) \equiv$

1000 W/cm²)

As unit of the charge (ampere-second or Coulomb)

a-Si:H hydrogenated amorphous silicon

a-SiC:H hydrogenated amorphous silicon carbide

AU astronomical unit

B width

B radiative recombination rate constant

B_{ideal} radiative recombination rate constant of an ideal

absorber

C heat capacitance

C_A Auger recombination rate constant

C_{A,e} Auger recombination rate constant of electrons C_{A,h} Auger recombination rate constant of holes

c velocity of light (2.99 · 10⁸ m/s)

C_{i0} initial concentration of impurity atoms

C_{is} concentration of impurity atoms in the growing crystal

C_m concentration of impurity atoms in the melt

c-Si crystalline silicon
CSS close space sublimation

 Cu_{In}^{2-} copper replacing an In atom at a lattice side of a

chalcopyrite

CuInS₂ copper indium disulfide

Cu(In,Ga)Se₂ copper indium gallium diselenide

CVD chemical vapor deposition

D diffusion coefficient
D, D⁺ donor, ionized donor

d thickness

d_{abs} thickness of the absorber

D_e density of states for free electrons in the conduction band

dE interval of energy

 d_{em} thickness of the emitter layer $d(h\nu)$ interval of photon energies

D_h density of states for free holes in the valence band

D_i diffusion constant of an impurity

 d_k thickness of kuvette d_{local} local thickness

 D_n diffusion coefficient of free electrons D_p diffusion coefficient of free holes

dbs dangling bonds

DOS_{st,a} density of donor-like surface states
DOS_{st,d} density of acceptor-like surface states

dR resistance of a very thin slice D_{th} thermal diffusion constant

dx interval of distances
DSSC dye-sensitized solar cell

E energy (in units of eV)

e, e free electron

E_A energy of an acceptor E_A activation energy

 $\begin{array}{ll} E_{Ai} & \text{activation energy of a diffusing impurity} \\ E_{A}^{SRH,pn} & \text{activation energy for Shockley-Read-Hall} \end{array}$

recombination in a pn-junction

E_{ab} energy of an anti-bonding state

 $E_{abs}(r_{\mathrm{QD}})$ absorption edge of a semiconductor quantum dot

E_b energy of a bonding state

E_C energy of the conduction band edge, conduction band

edge

 $E_{C(n)}$ conduction band edge in an n-type doped region $E_{C(p)}$ conduction band edge in a p-type doped region $E_{C,abs}$ conduction band edge of the photovoltaic absorber $E_{C,pass}$ conduction band edge of the passivation layer

E_{Cs} conduction band edge at the surface of a photovoltaic

absorber

E_D energy of a donor

E_{e1h1} lowest energy of an exciton

E_{e1h1,b} lowest energy of an exciton in a bulk semiconductor

E_F Fermi-energy

E_{F0} Fermi-energy in thermal equilibrium

E_{Fm} Fermi-energy of a metal

E_{Fn} Fermi-energy of free electrons

 $E_{Fn(n)}$ Fermi-energy of free electrons in an n-type doped region $E_{Fn(p)}$ Fermi-energy of free electrons in a p-type doped region $E_{F(n)}^0$ Fermi-energy in thermal equilibrium in an n-type

doped region

E_{Fp} Fermi-energy of free holes

 $\begin{array}{ll} E_{Fp(n)} & \text{Fermi-energy of free holes in an n-type doped region} \\ E_{Fp(p)} & \text{Fermi-energy of free holes in a p-type doped region} \\ E_{F(p)}^0 & \text{Fermi-energy in thermal equilibrium in a p-type doped} \end{array}$

region

E_{Fn}-E_{Fp} Fermi-level splitting

E_{Fs} Fermi-energy at the surface of a photovoltaic absorber

Eg energy of the forbidden band gap

E_{g0} energy of the forbidden band gap at the temperature of

0 K

E_{HL} energy of the HOMO–LUMO gap of an organic

semiconductor

E^{absorption} energy of the HOMO–LUMO gap for the absorption of

an organic semiconductor

E_{HL} transport energy of the HOMO–LUMO gap for the transport in

an organic semiconductor

E_{HOMO} lowest energy of an unoccupied state in the HOMO

band of an organic semiconductor

E_i intrinsic Fermi-level

 $E_{\rm ion}^{\rm D,A}$ ionization energies of donor and acceptor states $E_{\rm ion}^{\rm H}$ ionization energy of the hydrogen atom (13.56 eV)

 $E_{kin,e}$ kinetic energy of a free electron $E_{kin,h}$ kinetic energy of a free hole

E_{LUMO} lowest energy of an occupied state in the LUMO band of

an organic semiconductor

E_{og} energy of the optical band gap

E_{ph} photon energy

E_{redox} potential of a redox reaction

 $E_{S/S+}$ energy of the ground state and of the ionized state of a

dye molecule

E_S* energy of the excited state of a dye molecule

E_t energy characterizing exponential absorption tails
E_t energy of a trap state in the forbidden band gap
E_V energy of the valence band edge, valence band edge

valence band edge in an n-type doped region $E_{V(n)}$ valence band edge in a p-type doped region $E_{V(p)}$ valence band edge of the photovoltaic absorber E_{V,abs} valence band edge of the passivation layer E_{V,pass}

valence band edge at the surface of a photovoltaic E_{Vs}

absorber

energy of the vacuum Evac

eV electron Volt, unit of energy

f occupation probability of an electron

FF fill factor

fluorine-doped tin oxide FTO

FZ float zone

G generation rate of free charge carriers

 G_0 thermal generation rate of an ideal absorber

emission rate of free electrons Ge

geometry factor for the diode saturation current density G_{fn}

of electron diffusion

 G_{fp} geometry factor for the diode saturation current density

of hole diffusion

 G_h emission rate of free holes

photo-generation rate of an ideal absorber G_{sun}

GaAs gallium arsenide GaP gallium phosphide

Ge germanium

Н height

h Planck constant $(6.626 \cdot 10^{-34} \text{ Js})$ ħ Planck constant in terms of $h/(2\pi)$

h, h+ free hole

 H_n thickness of the n-type doped region thickness of the p-type doped region $H_{\mathfrak{p}}$

HF hydrofluoric acid

HIT hetero-junction with intrinsic thin layer highest occupied molecular orbital HOMO

v	v	1	37
А	А	1	v

I	current, current density
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I₀ diode saturation current, diode saturation current

density

I₀₀ pre-factor of the diode saturation current density

I_{0,SRH} diode saturation current density related to

Shockley-Read-Hall recombination

I_D current across a diode

I_{mp} current, current density in the maximum power point

I_{ph} photo current, photo current density

Is ionization energy of a semiconductor (in units of eV)
Isc short-circuit current (in units of A), short circuit current

density (in units of A/cm²)

I_{SC} short-circuit current density in the diode equation I_{SC} short-circuit current density following from the I–V

characteristics

I^{abs} short-circuit current density under consideration of

transmission losses

I^{max} maximum short-circuit current density

I_{SRH} diode current related to Shockley–Read–Hall

recombination

 $I_{tunn,e}$ tunneling current density for electrons $I_{tunn,h}$ tunneling current density for holes

ILGAR® ion layer gas reaction

In²⁺ indium replacing a copper atom at a lattice side of a

chalcopyrite

InP indium phosphide ITO indium tin oxide

I–V current–voltage (characteristics)

J_S solar constant (1356 W/m²)

k wave vector

k heat conductivity

 k_0 segregation coefficient in equilibrium k_B Boltzmann constant $(1.38 \cdot 10^{-23} \text{ J/K})$

k_e momentum of a free electron k_h momentum of a free hole k_s segregation coefficient KCN potassium cyanide

kWh kilowatt hour, unit of the electrical energy

L length

 $\begin{array}{ll} L & & \text{diffusion length} \\ L_{\text{drift}} & & \text{drift length} \end{array}$

L_f length of a grid finger

 $\begin{array}{ll} L_n & \text{diffusion length of electrons} \\ L_p & \text{diffusion length of holes} \\ L_{th} & \text{thermal diffusion length} \\ LPE & \text{liquid phase epitaxy} \end{array}$

LUMO lowest unoccupied molecular orbital

 m_e electron mass in free space $(9.1 \cdot 10^{-31} \text{ kg})$

m_e* effective mass of free electrons in the conduction band

of a semiconductor

m_b* effective mass of free holes in the valence band of a

semiconductor

MBE molecular beam epitaxy mc-Si multi-crystalline silicon

MOCVD metal organic chemical vapor deposition MOVPE metal organic vapor phase deposition

MOSFET metal oxide semiconductor field-effect transistor

N number

N density of particles (units of cm^{-3})

N_C effective density of states in the conduction band

N_{db} density of dangling bonds

 N_e number of photo-generated electrons N_{i0} initial number of impurity atoms

 N_{im} number of impurity atoms N_{ph} number of incident photons N_{st} density of surface defects

N_{st,a} density of acceptor-like surface defects N_{st,d} density of donor-like surface defects

N_t density of defects in the forbidden band gap

7	7	٦	,	ч	71	1
2	١.	2	١	А	r J	u

N_V	effective density of states in the valence band
n	ideality factor in the diode equation
n	density of free electrons (unit in cm^{-3})
n_i	intrinsic density of free charge carriers
$n^{+}(n^{++})$	density of free electrons in a highly (very highly) n-type
	doped semiconductor
n_0	density of free electrons in thermal equilibrium
n_n	density of free electrons in an n-type doped region
n_n^0	density of free electrons in an n-type doped region in
	thermal equilibrium
n_p	density of free electron in a p-type doped region
n_p^0	density of free electron in a p-type doped region in
P	thermal equilibrium
n_s	density of free electrons at the surface of a photovoltaic
	absorber
n_t	density of occupied traps
n _{air}	refractive index of air
n_{AR}	refractive index of an antireflection coating layer
n_S	refractive index of a photovoltaic absorber
n_{TCO}	refractive index of a TCO layer
nwSC	nanowire solar cell
OVC	ordered vacancy compound
OSC	organic solar cell
P	electric power (in units of W)
Pe	sun's power received on earth
P _i	phosphorus atom at an interstitial lattice side
P _{inst}	installed power (in units of W _p)
	light intensity (in units of W/cm ²)
$P_{ ext{light}}$ $P_{ ext{loss}}$	electric power losses due to resistive heating
P _{mp}	electric power in the maximum power point
P _{Si}	phosphorus atom at a lattice side in a silicon crystal
P _{Si}	ionized phosphorus atom at a lattice side in a silicon
Si	crystal
P_{sun}	areal density of the power of the sun received on earth
Juli	(in units of W/m^2)