

Overview

ATLAS understands a library of materials for reference to material properties and models of various regions in the semiconductor device. These materials are chosen to represent those most commonly used by semiconductor physicists today. Users of BLAZE or BLAZE3D will have access to all of these materials. S-PISCES or DEVICE3D users will have only access to Silicon and Polysilicon.

S-PISCES is designed to maintain backward compatibility with the standalone program SPISCES2 version 5.2. In the SPISCES2 syntax, certain materials could be used in the REGION statement just by using their name as logical parameters. This syntax is still supported.

Semiconductors, Insulators and Conductors

All materials in ATLAS are strictly defined into three classes as either semiconductor materials, insulator materials or conductors. Each class of material has particular properties to which all users should be aware.

Semiconductors

All equations specified by the user's choice of models are solved in semiconductor regions. All semiconductor regions must have a band structure defined in terms of bandgap, density of states, affinity etc. The parameters used for any simulation can be echoed to the run-time output using MODELS PRINT. For complex cases with mole fraction dependent models these quantities can be seen in Tonyplot by specifying OUTPUT BAND.PARAM and saving a solution file.

Any semiconductor region that is defined as an electrode is then considered to be a conductor region. This is typical for polysilicon gate electrodes.

Insulators

In insulator materials only the Poisson and lattice heat equations are solved. Therefore for isothermal simulations, the only parameter required for an insulator is dielectric permittivity defined using MATERIAL PERM=<n>.

Materials usually considered as insulators (eg. SiO₂) can be treated as semiconductors using BLAZE, however all semiconductor parameters are then required.

Conductors

All conductor materials must be defined as electrodes. Conversely all electrode regions are defined as conductor material regions. If a file containing regions of a material known to be a conductor are read in, these regions will automatically become un-named electrodes. As noted below if the file contains materials that are unknown, these region will become insulators.

During electrical simulation only the electrode boundary nodes are used. Nodes that are entirely within an electrode region are not solved. Any quantities seen inside a conductor region in TONYPLOT are spurious. Only optical ray tracing and absorption for LUMINOUS and lattice heating are solved inside of conductor/electrode regions.

Unknown Materials

If a mesh file is read containing materials not in Table B-1 these will automatically become insulator regions with a relative permittivity of 3.9. All user-defined materials from ATHENA, irrespective of the material name chosen by the user, will also become such insulator materials.

ATLAS Materials

ATLAS materials are listed in Table B-1 below.

Table B-1. The ATLAS Materials

Single Element Semiconductors

Silicon ¹	Poly ²	Germanium	Diamond
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Binary Compound Semiconductors

GaAs ³	GaP	CdSe	SnTe
SiGe	InP	CdTe	ScN
a-SiC	InSb	HgS	GaN
b-SiC	InAs	HgSe	AlN
AlP	ZnS	HgTe	InN
AlAs	ZnSe	PbS	BeTe
AlSb	ZnTe	PbSe	
GaSb	CdS	PbTe	

Ternary Compound Semiconductors

AlGaAs	GaSbP	InAlAs	GaAsP
InGaAs	GaSbAs	InAsP	HgCdTe
InGaP	InGaN	AlGaN	

Quaternary Compound Semiconductors

InGaAsP	AlGaAsP	AlGaAsSb	InAlGaN
InGaNAs	InGaNp	AlGaNAs	AlGaNp
AlInNAs	AlInNP	InAlGaAs	InAlGaP
InAlAsP			

Insulators

Vacuum	Oxide	Nitride	Si3N4
Air	SiO2	SiN	Sapphire
Ambient			

Conductors⁴

Polysilico 2	Palladium	TiW	TaSi
Aluminum	Cobalt	Copper	PaSi
Gold	Molybdenum	Tin	PtSi
Silver	Lead	Nickel	MoSi
AlSi	Iron	WSi	ZrSi
Tungsten	Tantalum	TiSi	AlSi
Titanium	AlSiTi	NiSi	Conductor
Platinum	AlSiCu	CoSi	Contact

Notes

1. The material models and parameters of Silicon are identical to those of **S-PISCES** version 5.2. Users should be aware that although these band parameters may be physically inaccurate compared to bulk silicon measurements, most other material parameters and models are empirically tuned using these band parameters.
2. Polysilicon is treated differently depending on how it is used. In cases where it is defined as an electrode, it is treated as a conductor. It can also be used as a semiconductor such as in a polysilicon emitter bipolars.
3. The composition of SiGe is the only binary compound that can be varied to simulate the effects of band gap variations.
4. Conductor names are only associated with electrodes. They are used for the specification of thermal conductivities and complex index of refraction and for display in `TonyPlot`.

Rules for Specifying Compound Semiconductors

The rules for specifying the order of elements for compound semiconductors are derived from the rules used by the International Union of Pure and Applied Chemistry:

1. Cations appear before anions.
2. When more than one cation is present the order progresses from the element with the largest atomic number to the element with the smallest atomic number.
3. The order of anions should be the in order of the following list: B, Si, C, Sb, As, P, N, H, Te, Se, S, At, I, Br, Cl, O, and F.
4. The composition fraction x is applied to the cation listed first.
5. The composition y is applied to the anion listed first.

To accomodate popular conventions, there are several exceptions to these rules.

- **SiGe**: The composition fraction x applies to the Ge component. SiGe is then specified as $\text{Si}_{(1-x)}\text{Ge}_{(x)}$, an exception to rule #4.
- **AlGaAs** : This is specified as $\text{Al}_{(x)}\text{Ga}_{(1-x)}\text{As}$. This is an exception to rule #2.
- **InGaAsP**: The convention $\text{In}_{(1-x)}\text{Ga}_{(x)}\text{As}_{(y)}\text{P}_{(1-y)}$ as set forth by Adachi is used. This is an exception to rule #4.

Silicon and Polysilicon

The material parameters defaults for Polysilicon are identical to those for Silicon. The following paragraphs describe some of the material parameter defaults for Silicon and Polysilicon.

Note: Within the Physics section of this manual, a complete description is given of each model. The parameter defaults listed in Chapter Three are all Silicon material defaults.

Silicon and Polysilicon Band Parameters

Table B-2. Band parameters for Silicon and Poly						
Material	Eg300 eV	α	β	Nc300 per cc	Nv300 per cc	χ eV
Silicon	1.08	4.73×10^{-4}	636.0	2.8×10^{19}	1.04×10^{19}	4.17
Poly	1.08	4.73×10^{-4}	636.0	2.8×10^{19}	1.04×10^{19}	4.17

Silicon and Polysilicon Dielectric Properties

Table B-3. Static dielectric constants for Silicon and Poly	
Material	Dielectric Constant
Silicon	11.8
Poly	11.8

Silicon and Polysilicon Default Mobility Parameters

The default mobility parameters for Silicon and Poly are identical in all cases. The defaults used depend on the particular mobility models in question. A full description of each mobility model and their coefficients are given in Chapter 3.

Table B-4 contains the silicon and polysilicon default values for the low field constant mobility model.

Table B-4. Lattice Mobility Model Defaults for Silicon and Poly				
Material	MUN cm ² /Vs	MUP cm ² /Vs	TMUN	TMUP
Silicon	1000.0	500.0	1.5	1.5
Poly	1000.0	500.0	1.5	1.5

Table B-5 contains the silicon and polysilicon default values for the field dependent mobility model.

Table B-5. Parallel Field Dependent Mobility Model Parameters for Silicon and Poly		
Material	BETAN	BETAP
Silicon	2	1
Poly	2	1

Silicon and Polysilicon Bandgap Narrowing Parameters

The default values used in the bandgap narrowing model for Silicon and Polysilicon are defined in Table B-6.

Table B-6. Bandgap Narrowing Parameters for Silicon and Poly			
Statement	Parameter	Defaults	Units
MATERIAL	BGN.E	6.92×10^{-3}	V
MATERIAL	BGN.N	1.3×10^{17}	cm^{-3}
MATERIAL	BGN.C	0.5	—

Silicon and Polysilicon Recombination Parameters

The default parameters for Shockley-Read-Hall recombination are given in Table B-7.

Table B-7. SRH Lifetime Parameter Defaults for Silicon and Poly				
Material	TAUN0 (s)	TAUP0 (s)	NSRHN (cm^{-3})	NSRHP (cm^{-3})
Silicon	1.0×10^{-7}	1.0×10^{-7}	5.0×10^{16}	5.0×10^{16}
Poly	1.0×10^{-7}	1.0×10^{-7}	5.0×10^{16}	5.0×10^{16}

The default parameters for Auger recombination are given in Table B-8;

Table B-8. Auger Coefficient Defaults for Silicon and Poly		
Material	AUGN	AUGP
Silicon	8.3×10^{-32}	1.8×10^{-31}
Poly	8.3×10^{-32}	1.8×10^{-31}

Silicon and Polysilicon Impact Ionization Coefficients

The default values for the SELB impact ionization coefficients are given in Table B-9.

Parameter	Value
EGRAN	4.0×10^5
BETAN	1.0
BETAP	1.0
AN1	7.03×10^5
AN2	7.03×10^5
BN1	1.231×10^6
BN2	1.231×10^6
AP1	6.71×10^5
AP2	1.582×10^6
BP1	1.693×10^6
BP2	2.036×10^6

Silicon and Polysilicon Thermal Parameters

The default values used for thermal conductivity and capacity are given in Table B-10.

Material	TCA	TCB	TCC	HCA	HCB	HCC	HCD
Silicon	0.03	1.56×10^{-3}	1.65×10^{-6}	1.97	3.6×10^{-4}	0.0	-3.7×10^4
Poly	0.03	1.56×10^{-3}	1.65×10^{-6}	1.97	3.6×10^{-4}	0.0	-3.7×10^4

Silicon And Polysilicon Effective Richardson Coefficients

Table B-11. Effective Richardson Coefficients for Silicon and Poly		
Material	ARICHN (A/cm²/K²)	ARICHP (A/cm²/K²)
Silicon	110.0	30.0
Poly	110.0	30.0

The Al_(x)Ga_(1-x)As Material System

AlGaAs Recombination Parameters.

The default recombination parameters for AlGaAs are given in Table B-12.

Table B-12. Default Recombination Parameters for AlGaAs		
Parameter	Value	Equation
TAUN0	1.0×10^{-9}	3-213
TAUP0	1.0×10^{-8}	3-213
COPT	1.5×10^{-10}	3-226
AUGN	5.0×10^{-30}	3-227
AUGP	1.0×10^{-31}	3-227

GaAs and AlGaAs Impact Ionization Coefficients.

The default values for the SELB impact ionization coefficients used for GaAs are given in Table B-13. AlGaAs uses the same values as GaAs.

Table B-13. Impact Ionization Coefficients for GaAs	
Parameter	Value
EGRAN	0.0
BETAN	1.82
BETAP	1.75
EGRAN	0.0
AN1	1.889×10^5
AN2	1.889×10^5
BN1	5.75×10^5
BN2	5.75×10^5
AP1	2.215×10^5
AP2	2.215×10^5
BP1	6.57×10^5
BP2	6.57×10^5

AlGaAs Thermal Parameters.

The default thermal parameters used for AlGaAs are given in Table B-14.

Table B-14. Default Thermal Parameters for GaAs	
Parameter	Value
TCA	2.27
HCA	1.738

GaAs Effective Richardson Coefficients.

The default values for the effective Richardson coefficients for GaAs are $6.2875 \text{ A/cm}^2/\text{K}^2$ for electrons and $105.2 \text{ A/cm}^2/\text{K}^2$ for holes.

The $\text{In}_{(1-x)}\text{Ga}_{(x)}\text{As}_{(y)}\text{P}_{(1-y)}$ System

InGaAsP Thermal Parameters.

The default material thermal models for InGaAsP assumes lattice-matching to InP. The material density is then given by;

$$\rho = 4.791 + 0.575y.\text{composition} + 0.138y.\text{composition}$$

The specific heat for InGaAsP is given by;

$$C_p = 0.322 + 0.026y.\text{composition} - 0.008y.\text{composition}$$

The thermal resistivities of InGaAsP are linearly interpolated from Table B-15.

Table B-15. Thermal Resistivities for InGaAsP Lattice-Matched to InP	
Composition Fraction y	Thermal Resistivity (deg/cm/w)
0.0	1.47
0.1	7.05
0.2	11.84
0.3	15.83
0.4	19.02
0.5	21.40
0.6	22.96
0.7	23.71
0.8	23.63
0.9	22.71
1.0	20.95

The default thermal properties of the binary compounds in the InGaAsP system are given in Table B-16.

Table B-16. Default Thermal Properties of InP InAs GaP and GaAs		
Material	Thermal Capacity (J/cm3)	Thermal Resistivity (deg/cm/W)
InP	1.543	1.47
InAs	1.994	3.70
GaP	1.292	1.30
GaAs	1.738	2.27

The default thermal properties for the ternary compounds in the InGaAsP system: $\text{In}_{(1-x)}\text{Ga}_{(x)}\text{As}$, $\text{In}_{(1-x)}\text{Ga}_{(x)}\text{P}$, $\text{InAs}_{(y)}\text{P}_{(1-y)}$, and $\text{GaAs}_{(y)}\text{P}_{(1-y)}$ are given, as a function of composition fraction, by linear interpolations from these binary compounds.

Silicon Carbide (SiC)

SiC Impact Ionisation Parameters

The default values for the SELB impact ionization coefficients used for SiC are given in Table B-17.

Parameter	Value
EGRAN	0.0
BETAN	1.0
BETAP	1.0
AN1	1.66×10^6
AN2	1.66×10^6
BN1	1.273×10^7
BN2	1.273×10^7
AP1	5.18×10^6
AP2	5.18×10^6
BP1	1.4×10^7
BP2	1.4×10^7

SiC Thermal Parameters.

The default thermal parameters used for both 6H and 4H-SiC are shown in Table B-18.

Parameter	Value	
	4H-SiC	6H-SiC
TCA	0.204	0.385
HCA	0	0

Miscellaneous Semiconductors

The remainder of the semiconductors available have defined default parameter values to various degrees of completeness. The following sections describe those parameter defaults as they exist. Since many of the material parameters are not available at this time, it is recommended that care be taken in using these materials. It is important to make sure that the proper values are used

Note: The syntax `MODEL PRINT` can be used to echo the parameters used to the run-time output.

Miscellaneous Semiconductor Band Parameters

Material	E _g (0)eV	E _g (300)eV	α	β	m _c	m _v	χ eV
Silicon							
Poly-silicon							
Ge	0.7437		4.77×10^{-4}	235.0	0.2225	0.2915	4.0
Diamond		5.45	4.77×10^{-4}	0.0	(a)	(b)	7.2
6H-SiC	2.9	2.9	0.0	0.0	0.454	0.33	
4H-SiC	2.2	2.2	0.0	0.0	0.41	0.165	
AlP	2.43	2.43	0.0	0.0			
AlAs	2.16	2.16	0.0	0.0			
AlSb	1.6		2.69×10^{-4}	2.788	(c)	0.4	
GaSb	0.81		3.329×10^{-4}	-27.6622	(c)	0.24	3.65
InSb	0.235		2.817×10^{-4}	90.0003	0.014	0.4	4.06
ZnS	3.8	3.8	0.0	0.0	0.4		4.59
ZnSe	2.58	2.58	0.0	0.0	0.1	0.6	
ZnTe	2.28		0.0	0.0	0.1	0.6	4.09
Cds	2.53	2.53	0.0	0.0	0.21	0.8	3.5
CdSe	1.74	1.74	0.0	0.0	0.13	0.45	4.5
CdTe	1.5	1.5	0.0	0.0	0.14	0.37	
HgS	2.5	2.5	0.0	0.0			4.28
HgSe							
HgTe							

Material	Eg(0)eV	Eg(300)eV	α	β	m_c	m_v	χ eV
PbS	0.37	0.37	0.0	0.0	0.25	0.25	
PbSe	0.26	0.26	0.0	0.0	0.33	0.34	
PbTe	0.29	0.29	0.0	0.0	0.17	0.20	4.6
SnTe	0.18	0.18	0.0	0.0			
ScN	2.15	2.15	0.0	0.0			
GaN	3.45	3.45	0.0	0.0	0.172	0.259	
AlN	6.28	6.28	0.0	0.0	0.314	0.417	
InN	1.89	1.89	0.0	0.0	0.11	0.17	
BeTe	2.57	2.57	0.0	0.0			

Notes

(a). $N_{c300} = 5.0 \times 10^{18}$

(b). $N_{v300} = 1.8 \times 10^{19}$

(c). $m_c(X) = 0.39$

$m_c(G) = 0.09$

$N_c = N_c(X) + N_c(G)$

(d). $m_c(G) = 0.047$

$m_c(L) = 0.36$

$N_c = N_c(G) + N_c(L)$

Miscellaneous Semiconductor Dielectric Properties

Material	Dielectric Constant
Ge	16.0
Diamond	5.5
6H-SiC(a)	9.66
4H-SiC(b)	9.72
AlP	9.8
AlAs	12.0
AlSb	11.0

Table B-20. Static Dielectric Constants for Miscellaneous Semiconductors	
Material	Dielectric Constant
GaSb	15.7
InSb	18.0
ZnS	8.3
ZnSe	8.1
CdS	8.9
CdSe	10.6
CdTe	10.9
HgS	
HgSe	25.0
HgTe	20.
PbS	170.0
PbSe	250.0
PbTe	412.0
SnTe	
ScN	
GaN	9.5
AlN	9.14
InN	19.6
BeTe	

Miscellaneous Semiconductor Mobility Properties

Table B-21. Mobility Parameters for Miscellaneous Semiconductors				
Material	MUNO (cm²/Vs)	MUPO (cm²/Vs)	VSATN(cm/s)	VSAT(cmcm/s)
Ge	3900.0(a)	1900.0(b)		
Diamond	500.0	300.0	2.0×10^7	
SiC(a)	330.0	300.0	2.0×10^7	
SiC(b)	1000.0	50.0	2.0×10^7	
AlP	80.0			

Table B-21. Mobility Parameters for Miscellaneous Semiconductors				
Material	MUNO (cm ² /Vs)	MUPO (cm ² /Vs)	VSATN(cm/s)	VSAT(cmcm/s)
AlAs	1000.0	100.0		
AlSb	200.0	550.0		
GaSb	4000.0	1400.0		
InSb	7800.0	750.0		
ZnS	165.0	5.0		
ZnSe	100.0	16		
CdS	340.0	50.0		
CdSe	800.0			
CdTe	1050.0	100.0		
HgS				
HgSe	5500.0			
HgTe	22000.0	100.0		
PbS	600.0	700.0		
PbSe	1020.0	930.0		
PbTe	6000.0	4000.0		
SnTe				
ScN				
GaN	400.0	8.0	2.0×10^7	
AlN		14.0		
InN	3000.0			
BeTe				

Notes

- (a) Uses Equation B-4 with TMUN=1.66.
 (b) Uses Equation B-4 with TMUP = 2.33.

Insulators

The default material parameters for insulator materials are given in the following sections. As noted in the “Semiconductors, Insulators and Conductors” section the only parameter required for electrical simulation in insulator materials is the dielectric constant. Thermal and optical properties are required in GIGA and LUMINOUS respectively.

Insulator Dielectric Constants

Material	Dielectric Constant
Vacuum	1.0
Air	1.0
Ambient	1.0
Oxide	3.9
SiO ₂	3.9
Nitride	7.5
SiN	7.5
Si ₃ N ₄	7.55
Sapphire	12.0

Insulator Thermal Properties

Material	Thermal Capacity (J/cm ³)	Thermal Conductivity(deg/cm/W)	Reference
Vacuum	0.0	0.0	
Air	1.0	0.026	7
Ambient	1.0	0.026	7
Oxide	3.066	0.014	4
SiO ₂	3.066	0.014	4
Nitride	0.585	0.185	4

Material	Thermal Capacity (J/cm ³)	Thermal Conductivity(deg/cm/W)	Reference
SiN	0.585	0.185	4
Si3N4	0.585	0.185	4
Sap- phire			

Optical Properties

The default values for complex index of refraction in LUMINOUS are interpolated from tables from the "Handbook of Optical Constants," first and second editions. Rather than print the tables here, the ranges of optical wavelengths for each material are listed in Table B-24.

Table B-24. Wavelength Ranges for Default Complex Index of Refraction			
Material	Temperature(K)	Composition Fraction	Wavelengths (microns)
Silicon	300	NA	0.0103-2.0
AlAs	300	NA	0.2213 - 50.0
GaAs	300	NA	0.0 - 0.9814
InSb	300	NA	0.2296 - 6.5
InP	300	NA	0.1689 - 0.975
Poly	300	NA	0.1181 - 18.33
SiO2	300	NA	0.1145 - 1.7614

Note: The parameter INDEX.CHECK can be added to the SOLVE statement to list the values of real and imaginary index being used in each solution.

User Defined Materials

The current version of ATLAS does not directly support user defined materials. A simple workaround can be done using the already existing user specifications. This workaround is based on the use of an already existing material name and modifying the material parameters as appropriate.

In ATLAS material names are defined to give the user a reasonable set of default material parameters. Any of these defaults can be overridden using the `MATERIAL`, `IMPACT`, `MODEL`, and `MOBILITY` statements. The key to defining new materials is choosing a material name that is defined in ATLAS, then modifying the material parameters of that material to match the user material. Here it is best to choose a material that has default parameter values that might best match the user material, while being sure to choose a material that is not already in the user device. Next the user must associate this material name with the device regions where the new material is present. This is done by either specifying the chosen material name on the appropriate `REGION` statements (when the device is defined in the ATLAS syntax) or choosing the material name from the materials menu when defining the region in `DEVEDIT`.

Next, the user should modify the material statements using `MATERIAL`, `IMPACT`, `MOBILITY`, and `MODEL` statements. When doing this the `MATERIAL` parameter of the given statement should be assigned to the chosen material name.

For materials with variations in composition fraction, the user should choose a defined material with X and/or Y composition fractions (i.e., a ternary or quaternary material). The user may also find it convenient to use C interpreter functions to define the material parameters as a function of composition. The C interpreter functions that are useful for this approach are: `F.MUNSAT`, `F.MUPSAT`, `F.BANDCOMP`, `F.VSATN`, `F.VSATP`, `F.RECOMB`, `F.INDEX`, `F.BGN`, `F.CONMUN`, `F.CONMUP`, `F.COPT`, `F.TAUN`, `F.TAUP`, `F.GAUN`, and `F.GAUP`.

In defining new materials there exists a minimum set of parameters that should be defined. This set includes bandgap (`EG300`), electron and hole density of states (`NC300` and `NV300`), dielectric permittivity (`PERMITIVITY`), and electron and hole mobilities (`MUN` and `MUP`). For bipolar devices certain recombination parameters should also be defined such as: lifetimes (`TAUN` and `TAUP`), radiative recombination rates (`COPT`), and Auger coefficients (`AUGN` and `AUGP`). For devices with variations in material composition certain band-edge alignment parameters should also be defined: either electron affinity (`AFFINITY`) or edge alignment (`ALIGN`). If impact ionization is considered the impact ionization coefficients should also be defined.

As an example, consider the case where the user is simulating a device with an `AlInGaP` region. Consulting table B-1, we see that this material system is not defined in ATLAS. We then choose a material that is defined in ATLAS which has default material parameters that best approximate the material parameters of the new material. In this case, we choose `InGaAsP` since, at least for example purposes, we feel that this material is closest to the `AlInGaP`. Next, we must specify `InGaAsP` as the material of the region(s) that is/are composed of `AlInGaP`. This can be done either on the `REGION` statement if the structure is defined in ATLAS syntax or from the material menu when the region is defined in `DEVEDIT`.

Supposing that we are satisfied with the default values of the parameters from the "minimum set" discussed above, and that we are principally concerned with the recombination and heat flow parameters defaults, the following section of the input deck illustrates how these parameter defaults may be modified:

```
# new material AlInGaP
MATERIAL MATERIAL=InGaAsP
# SRH
MATERIAL MATERIAL=InGaAsP TAUN0=1.1e-9 TAUP0=2.3e-8
# Auger
MATERIAL MATERIAL=InGaAsP AUGN=5.8e-30 AUGP=1.1e-31
# Optical
material material=InGaAsP COPT=1.7e-30
```

```
# Thermoconductivity  
MATERIAL MATERIAL=InGaAsP TC.A=2.49  
# Heat capacity  
MATERIAL MATERIAL=InGaAsP HC.A=1.9
```

