www.nextnano.com
stefan.birner@nextnano.com

How to treat Quaternaries in nextnano

Dr. Stefan Birner, Managing Director

next**nano** GmbH, Garching b. München, Germany

Material parameters needed

GaAs/AlGaAs heterostructures (no strain)

- **effective masses** (m_e, m_{hh}, m_{lh}, m_{so}, ...) or **k·p** parameters
- **band gap** E_{gap}, split-off energy
- **band offsets** (CBO, VBO)
- dielectric constant (Poisson equation)

Ternaries

a. Linear interpolation
b. Quadratic interpolation using a **constant** bowing parameter
c. Interpolation using a bowing parameter which depends on **alloy content** *x*

Ternaries

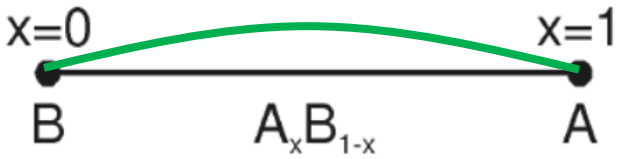
Ternary

- Binaries GaAs, AlAs

  ➔ Ternary $Al_xGa_{1-x}As$ = x AlAs + (1-x) GaAs – C x (1-x)

- **Bowing parameter** C – C(x) x (1-x)

might depend on alloy content x

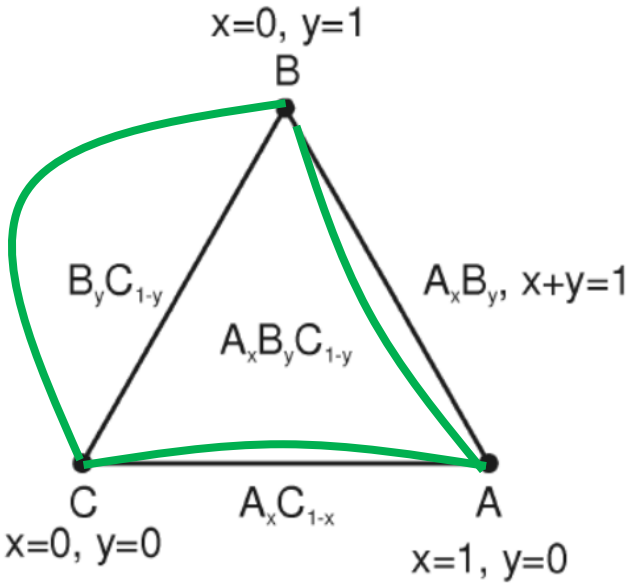


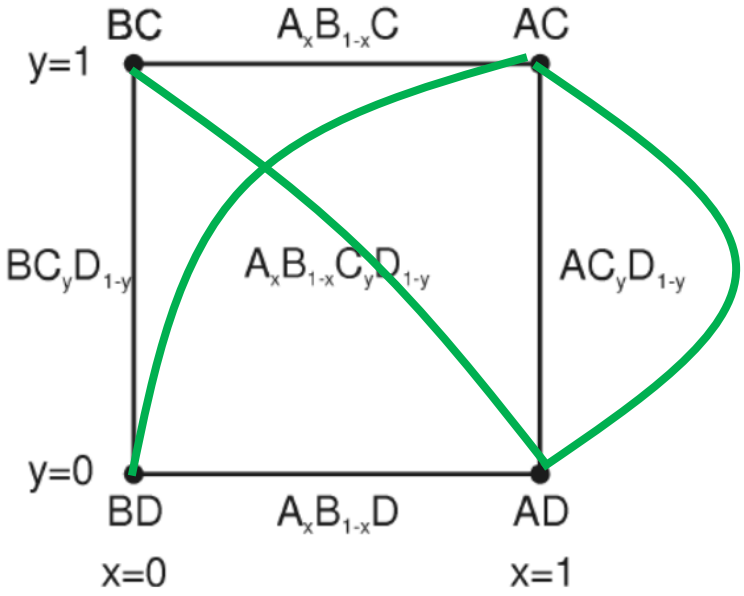
Quaternaries

- Quaternary: $Al_xGa_{1-x}As_yP_{1-y}$

III-III-III-V, III-V-V-V

III-III-V-V





Quaternaries

Alloys of the type $A_xB_yC_{1-x-y}$

$Al_xGa_{1-x}In_{1-x-y}As$

III-III-III-V

III-V-V-V

10 parameters!

$$
\begin{aligned}
f^{(3)}(x,y) = {} & x f_{\mathrm{A}} + y f_{\mathrm{B}} + (1-x-y) f_{\mathrm{C}} + xy \left[x f_{\mathrm{AB}}^{\mathrm{A}} + y f_{\mathrm{AB}}^{\mathrm{B}} \right] \\
& + x(1-x-y) \left[x f_{\mathrm{AC}}^{\mathrm{A}} + (1-x-y) f_{\mathrm{AC}}^{\mathrm{C}} \right] \\
& + y(1-x-y) \left[y f_{\mathrm{BC}}^{\mathrm{B}} + (1-x-y) f_{\mathrm{BC}}^{\mathrm{C}} \right] \\
& + xy(1-x-y) f_{\mathrm{ABC}}
\end{aligned}
$$

Quaternaries

Alloys of the type $A_xB_{1-x}C_yD_{1-y}$

$Al_xGa_{1-x}As_yP_{1-y}$

III-III-V-V

13 parameters!

$$
\begin{aligned}
f^{(2.4)}(x,y) = {} & xy f_{AC} + (1-x)\, y f_{BC} + x\,(1-y)\, f_{AD} + (1-x)\,(1-y)\, f_{BD} \\
& + x\,(1-x)\, y \left[x f^{A}_{AB,C} + (1-x)\, f^{B}_{AB,C}\right] + x\,(1-x)\,(1-y)\left[x f^{A}_{AB,D} + (1-x)\, f^{B}_{AB,D}\right] \\
& + xy\,(1-y)\left[y f^{C}_{CD,A} + (1-y)\, f^{D}_{CD,A}\right] + (1-x)\, y\,(1-y)\left[y f^{C}_{CD,B} + (1-y)\, f^{D}_{CD,B}\right] \\
& + x\,(1-x)\, y\,(1-y)\, f_{ABCD}
\end{aligned}
\tag{E.15}
$$

Material parameters needed

GaAs/InGaAs heterostructures (strain!)

- … +
- lattice constant
- elastic constants (2-3 parameters)
- piezoelectric constant
- deformation potentials (3-8 parameters)

nextnano++ software

- http://www.nextnano.com/nextnanoplus/software_documentation/input_file/structure.htm

```
quaternary_constant{
   name        = "Al(x)Ga(y)In(1-x-y)As" # quaternary material name for this region with constant alloy profile
   alloy_x     = 0.2                     # x content of the alloy (minimum value is 0.0, maximum value is 1.0)
   alloy_y     = 0.5                     # y content of the alloy (minimum value is 0.0, maximum value is 1.0)
}
```

For quaternaries of type $A_xB_yC_{1-x-y}H$, the following relation must hold: `x + y <= 1`

The interpolation of $A_xB_yC_{1-x-y}H$ is done according to eq. (E.10) in PhD thesis of T. Zibold apart from changes in sign of bowing parameters.

The interpolation of $A_xB_{1-x}C_yD_{1-y}$ is done according to eq. (E.15) in PhD thesis of T. Zibold apart from changes in sign of bowing parameters.

- http://www.nextnano.com/nextnanoplus/software_documentation/database/zincblende.htm

Example:

```
######### indium aluminum arsenide antimonide (InAlAsSb) ##############
quaternary4_zb {
 name      = "In(x)Al(1-x)As(y)Sb(1-y)"
 valence   = III_V
 binary1   = InAs                #
 binary2   = AlAs                #
 binary3   = AlSb                #
 binary4   = InSb                #
 ternary12 = "In(x)Al(1-x)As"    # Note: In(x)Al(1-x)As and In(1-x)Al(x)As are equivalent
 ternary23 = "AlAs(x)Sb(1-x)"    #       as can be seen in the above equation.
 ternary34 = "Al(x)In(1-x)Sb"    #       So one has to use the name that is already defined in the database.
 ternary14 = "InAs(x)Sb(1-x)"
}
```

More information

- PhD thesis T. Zibold (Appendix E)

PHD THESES RELATED TO THE NEXTNANO++ SOFTWARE

Walter Schottky Institute, Technische Universität München, Germany

- Optoelectronic and spin-related properties of semiconductor nanostructures in magnetic fields
  T. Andlauer
  Selected Topics of Semiconductor Physics and Technology (G. Abstreiter, M.-C. Amann, M. Stutzmann, and P. Vogl, eds.), Vol. **105**, Verein zur Förderung des Walter Schottky Instituts der Technischen Universität München e.V., München, 171 pp. (2009)
- Semiconductor based quantum information devices: Theory and simulations
  T. Zibold
  Selected Topics of Semiconductor Physics and Technology (G. Abstreiter, M.-C. Amann, M. Stutzmann, and P. Vogl, eds.), Vol. **87**, Verein zur Förderung des Walter Schottky Instituts der Technischen Universität München e.V., München (2007)

- http://www.nextnano.com/information/publications.php

- nextnano³ software
  http://www.nextnano.com/nextnano3/input_parser/database/docu/quaternaries.htm
  http://www.nextnano.com/nextnano3/tutorial/1Dtutorial_AlGaInP_onGaAs.htm