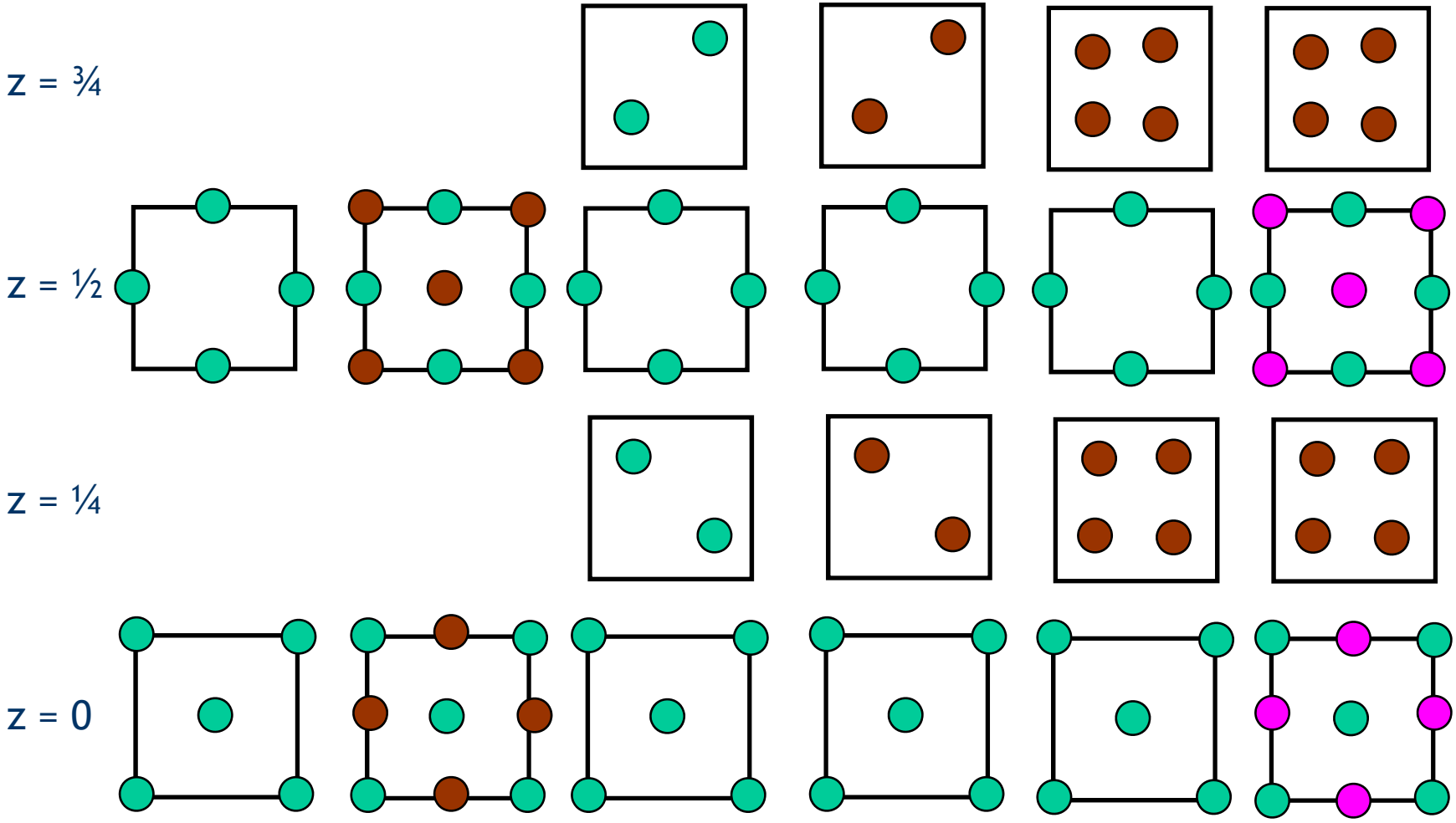
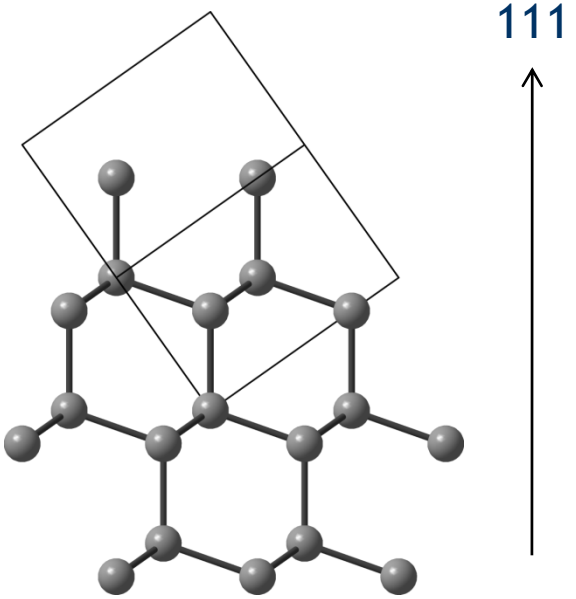
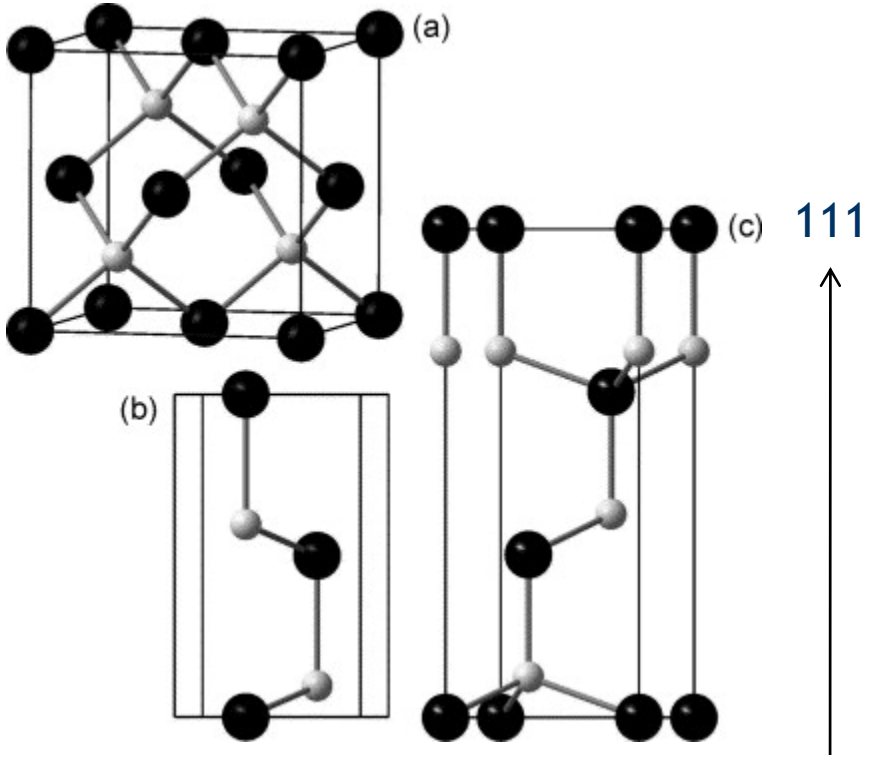
Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



Diamond

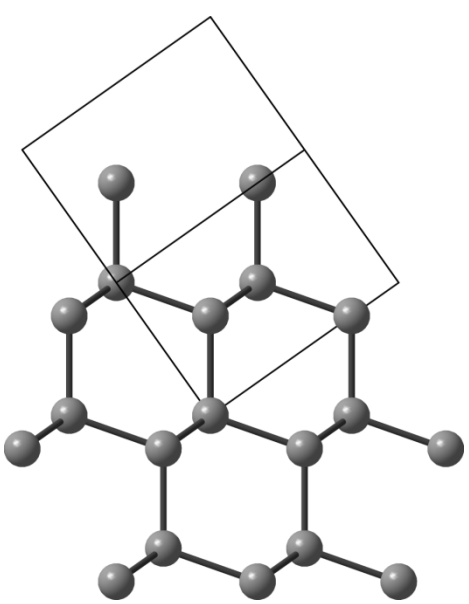


Wurtzite and zinc blende

P63mc and *R3m*/*F-43m*

2*H* and 3*R*

Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



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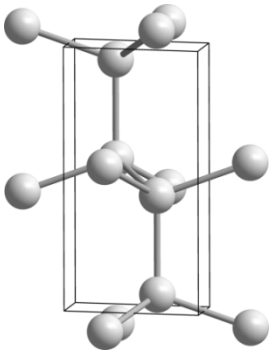
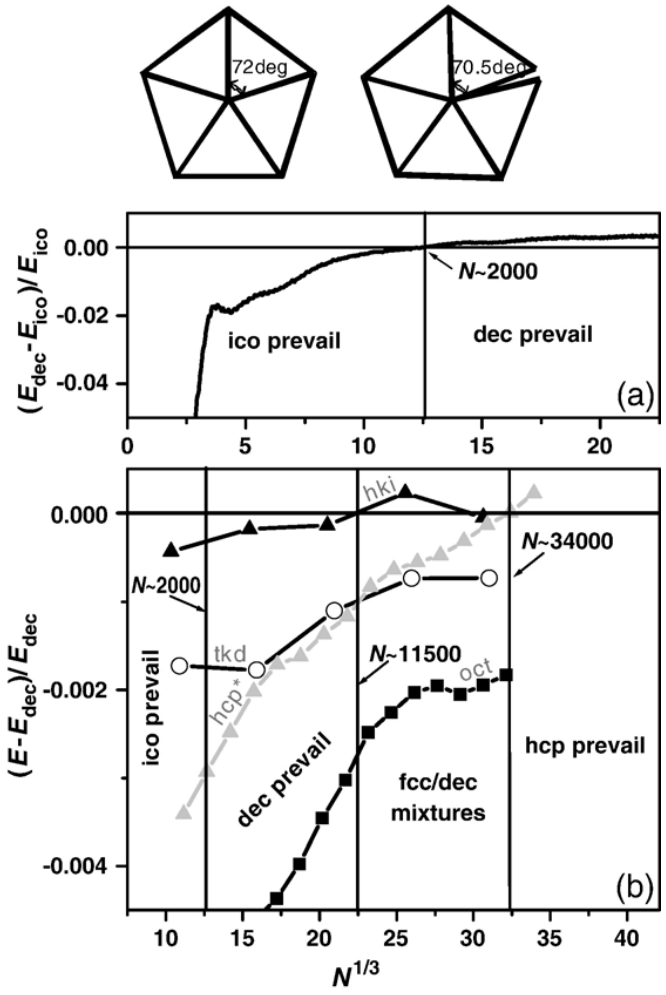


Diamond

Lonsdaleite

Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors

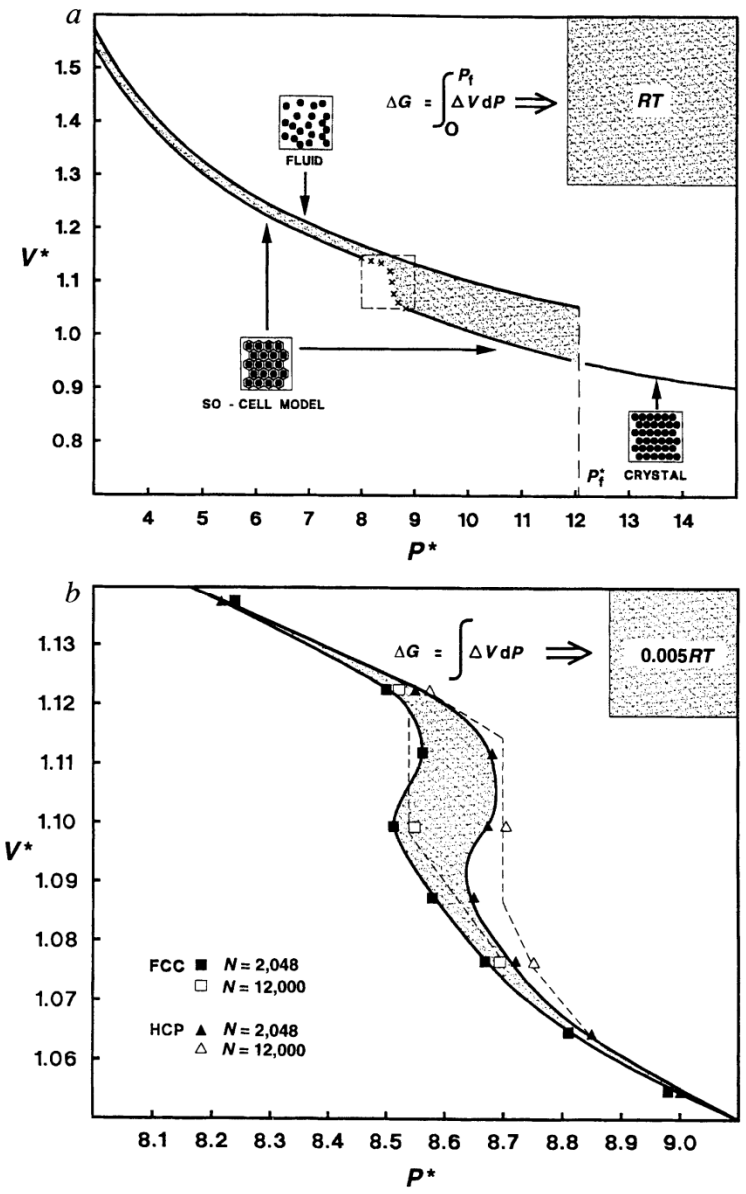
The *hcp-fcc* dilemma: Why is *fcc* more frequent than *hcp* ? [25% of elements are *fcc* and 20% are *hcp*.



N. V. Krainyukova, The crystal structure problem' in noble gas nanoclusters, *Thin Solid Films*, **515** (2006) 1658–1663.

Calculations of the energetics of multiply twinned particles (MTPs) such as icosahedra and decahedra with fivefold symmetry as well as facecentered cubic (fcc) and hexagonal close-packed (hcp) particles in the size interval from 13 up to ~45,000 atoms were made applying Lennard-Jones potentials.
For the cluster size N from minimal up to N~2000 atoms the binding energy is highest for icosahedra, in the size interval from 2000 up to ~11,500 atoms decahedra prevail, above N~11,500 atoms decahedra and optimized fcc clusters were found to alternate. The hcp structure was revealed to become favorable above N~34,000 atoms. Thus, hcp clusters can attain their preference with respect to MTPs (comprising fcc fragments) and optimized fcc clusters only for very large sizes

Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



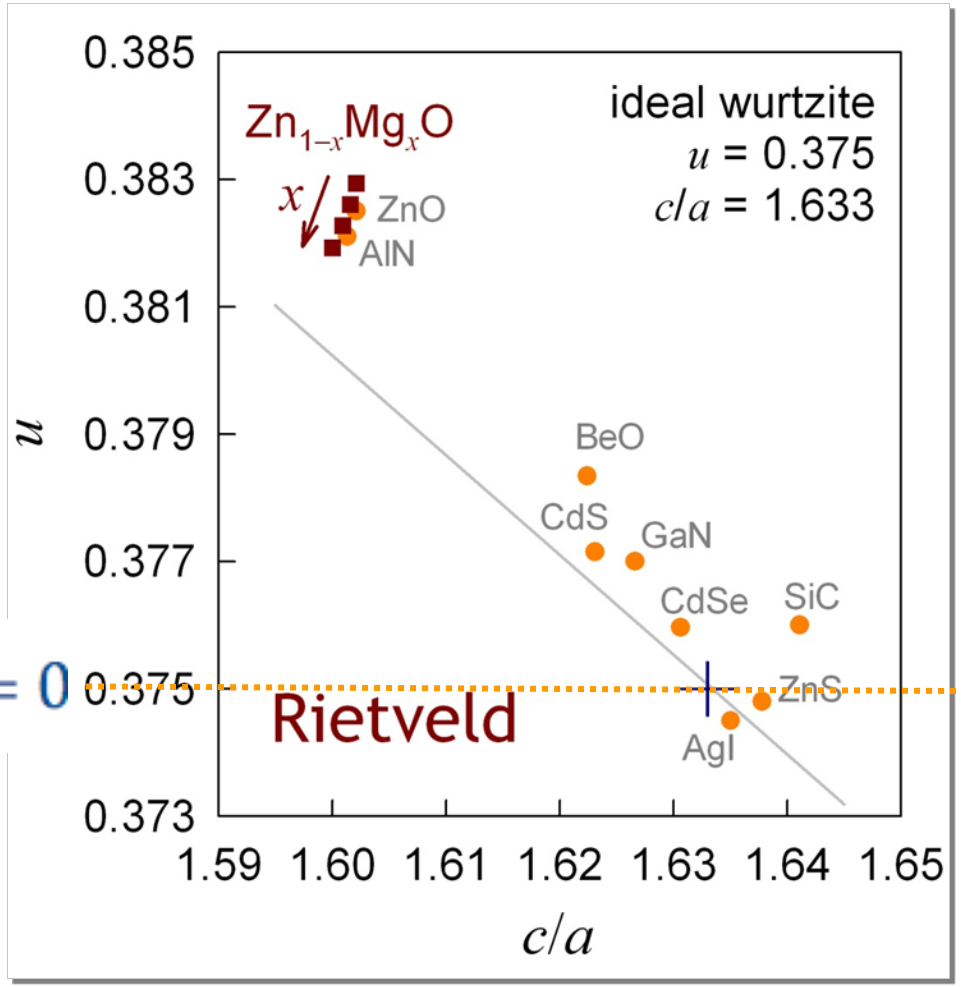
Hard spheres: *fcc* is slightly stabilized by entropy over *hcp*, by 0.005 R for al temperatures up to the melting point.

L. V. Woodcock, *Nature* **385** (1997) 141.

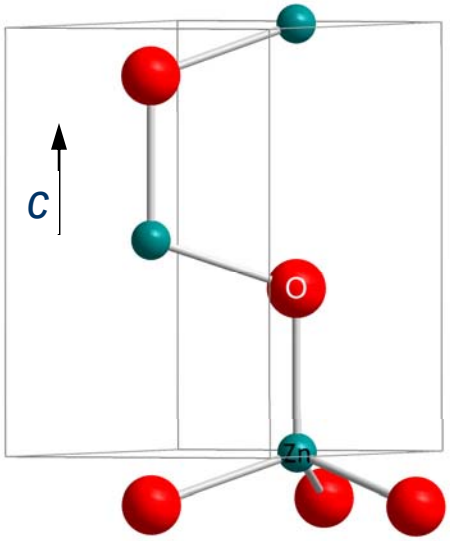
Wurtzite structures and static polarization

[Dr. Young-Il Kim]

$$u = \frac{3}{8}; P_s = 0$$



Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



Consider one ZnO_4 tetrahedron (polarization unit)

Zn $(\frac{1}{3}, \frac{2}{3}, 0)$

O_{axial} $(\frac{1}{3}, \frac{2}{3}, u)$

O_{basal} $(\frac{2}{3}, \frac{1}{3}, u - \frac{1}{2})$

$(\frac{2}{3}, -\frac{2}{3}, u - \frac{1}{2})$

$(-\frac{1}{3}, \frac{1}{3}, u - \frac{1}{2})$

dipole moment along $c-$direction

$$\mu(\text{Zn-O}_{axial}) = \tfrac{1}{4} \times (-2) \times u \times c$$

$$\mu(\text{Zn-O}_{basal}) = 3 \times \tfrac{1}{4} \times (-2) \times (u - \tfrac{1}{2}) \times c \qquad (\text{in } e \cdot \text{Å})$$

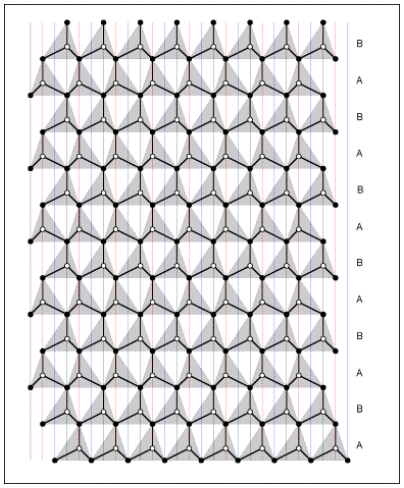
$$P_s = \frac{\mu_{sum}}{\text{unit volume}} = \frac{-2 \times (u - \frac{3}{8}) \times c}{\frac{\sqrt{3}}{4} a^2 c} = \frac{-2 \times (u - \frac{3}{8})}{\frac{\sqrt{3}}{4} a^2} \left(\frac{e}{\text{Å}^2} \right) \times \left(1.60 \times 10^3 \, \frac{\mu\text{C}}{\text{cm}^2} \cdot \frac{\text{Å}^2}{e} \right)$$

$(u - \frac{3}{8}) \cdot c$ can be obtained also from the separation between centers of $(-)$ and $(+)$ charges.

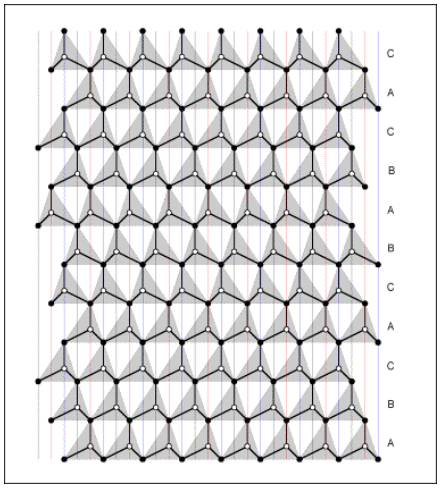
[Dr. Young-Il Kim]

Polytypism in SiC

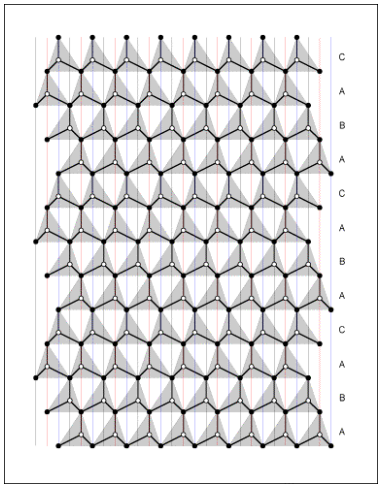
Professor Marek Skowronski
http://neon.mems.cmu.edu/skowronski/



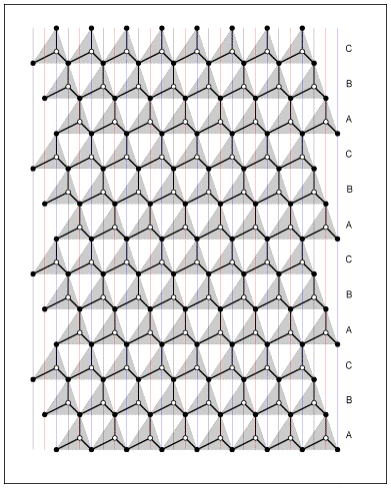
3*C*



4*H*



3*H*



2*H*

Specifying the total number of layers in the hexagonal unit cell followed by the letter *H* , *R* or *C* to indicate the lattice type. Thus a symbol *nH* represents a structure with *n* layers in the primitive hexagonal unit cell while *mR* denotes a structure whose primitive lattice is rhombohedral and contains *m* layers in its hexagonal unit cell.

Ramsdell notation.

Stacking notation

Ramsdell notation	ABC sequence	Zhdanov number	h-c notation
2H	AB	(11)	h
3C	ABC		c
4H	ABCB	(22)	hc
$6H_1$	ABCACB	(33)	hcc
$6H_2$	ABCBAB	(2211)	hchchh
9R	ABACACBCB	(12)	hhc

http://www.iucr.org/iucr-top/comm/cteach/pamphlets/5/node0.html

Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors

DIFFaX: Diffraction from faulted structures:

DIFFaX v 1.80
DIFFaX v 1.80
DIFFaX v 1.80
DIFFaX v 1.80
DIFFaX v 1.80
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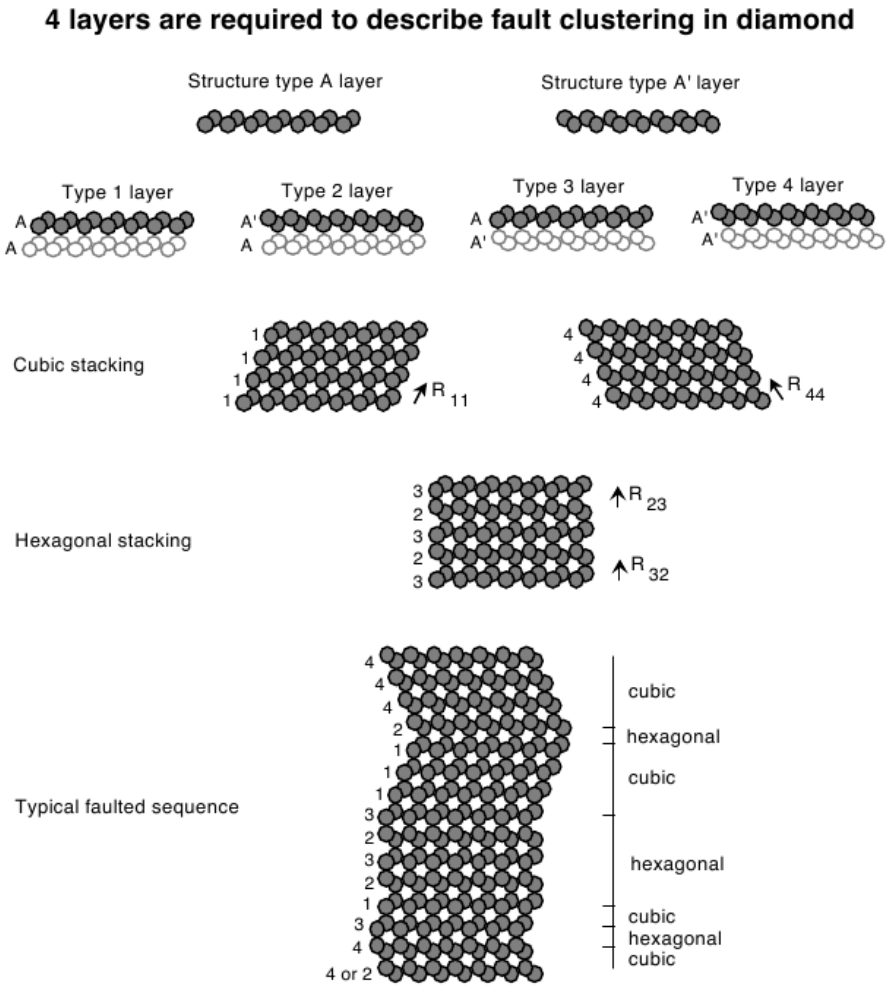
DIFFaX v 1.80
DIFFaX v 1.80

DIFFaX v 1.812

by

M. M. J. Treacy, M. W. Deem & J. M. Newsam

3rd July 2005



Semiconductors: Structure sorting (Phillips-van Vechten)