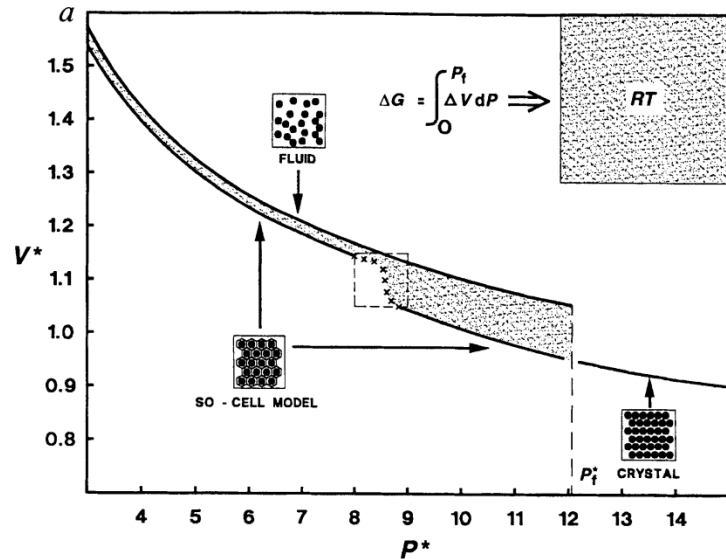
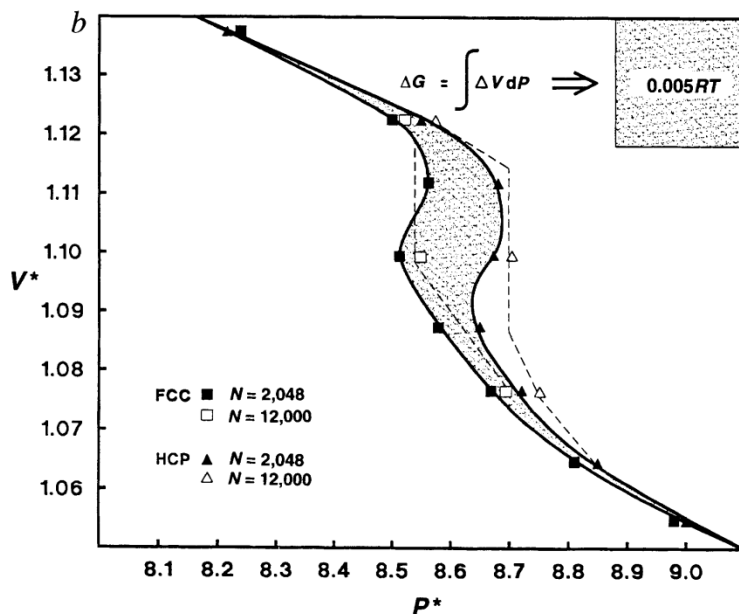


Class 2: fcc, hcp, diamond, zinc blende, wurtzite, SiC, semiconductors



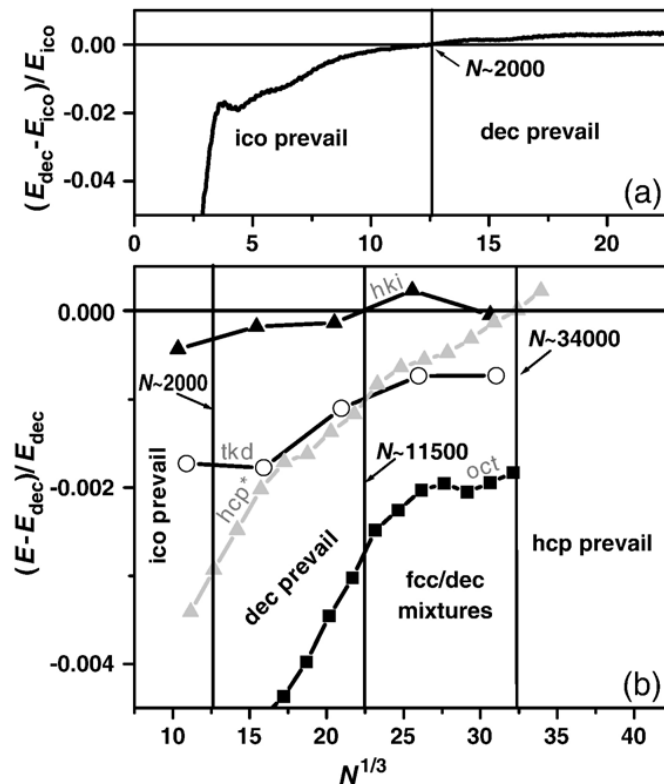
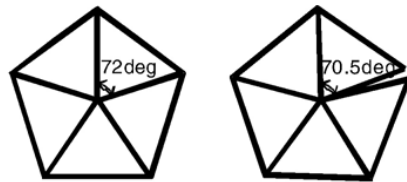
Hard spheres: fcc is slightly stabilized by entropy over hcp, by $0.005 R$ for all temperatures up to the melting point.

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



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*.

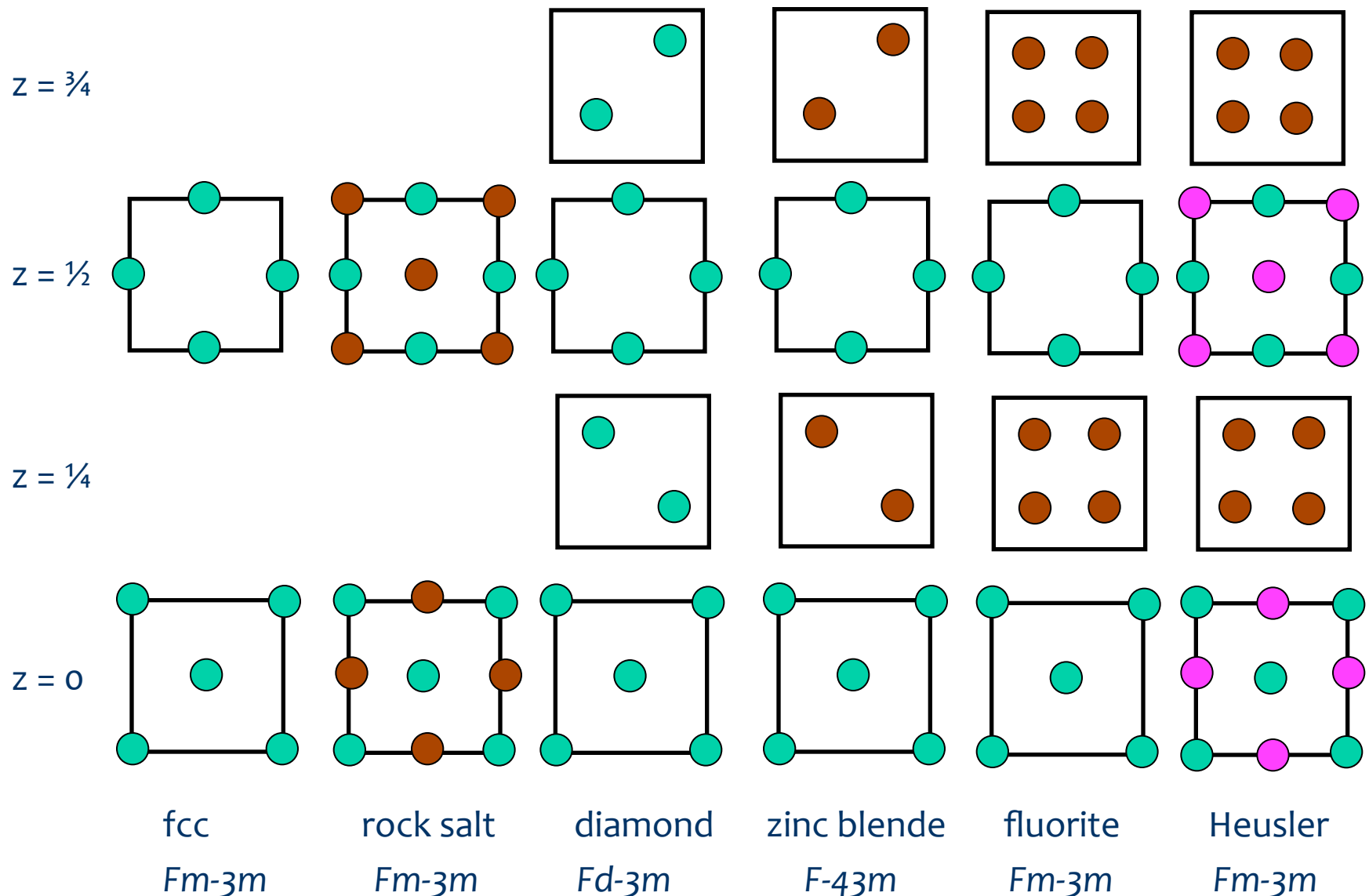


N. V. Krainyukova, The “crystal structure problem” in noble gas nanoclusters, *Thin Solid Films*, **515** (2006) 1658–1663.

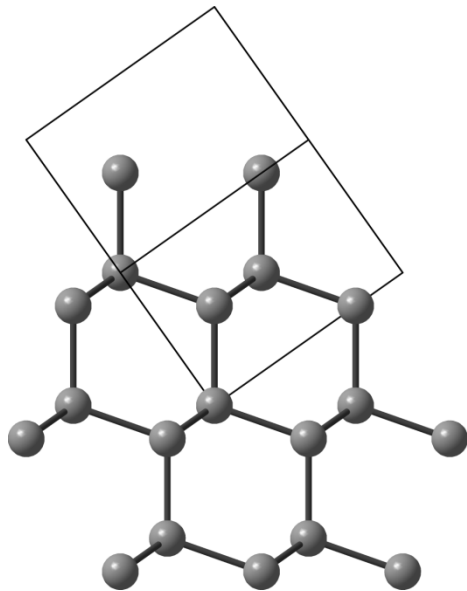
Calculations of the energetics of multiply twinned particles (MTPs) such as icosahedra and decahedra with fivefold symmetry as well as facecentered cubic (fcc) and hexagonal close-packed (hcp) particles in the size interval from 13 up to ~45,000 atoms were made applying Lennard-Jones potentials.

For the cluster size N from minimal up to $N \sim 2000$ atoms the binding energy is highest for icosahedra, in the size interval from 2000 up to ~11,500 atoms decahedra prevail, above $N \sim 11,500$ atoms decahedra and optimized fcc clusters were found to alternate. The hcp structure was revealed to become favorable above $N \sim 34,000$ atoms. Thus, hcp clusters can attain their preference with respect to MTPs (comprising fcc fragments) and optimized fcc clusters only for very large sizes

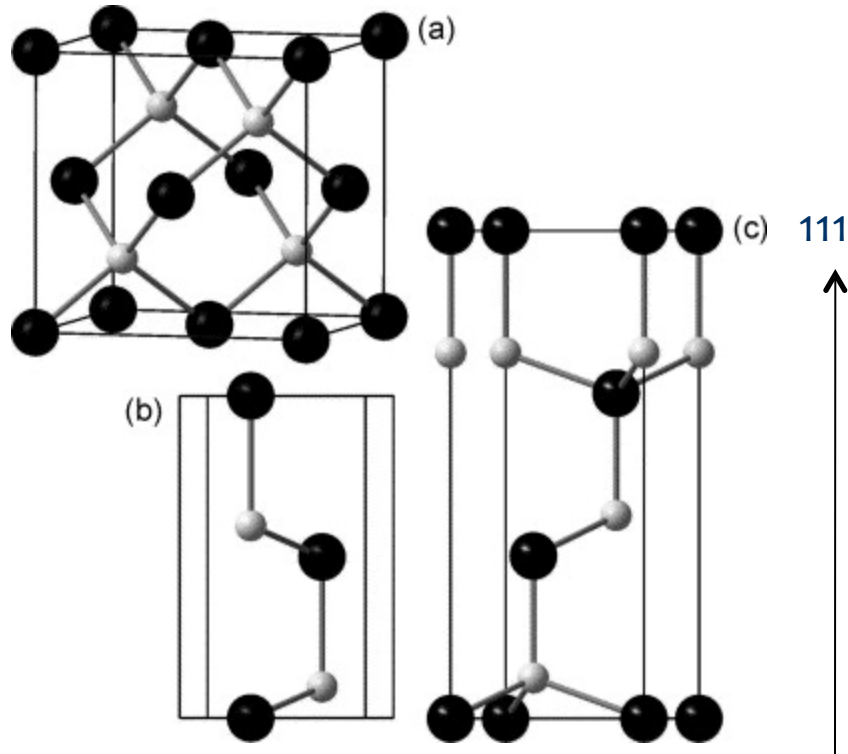
Class 2: fcc, hcp, diamond, zinc blende, wurtzite, SiC, semiconductors



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



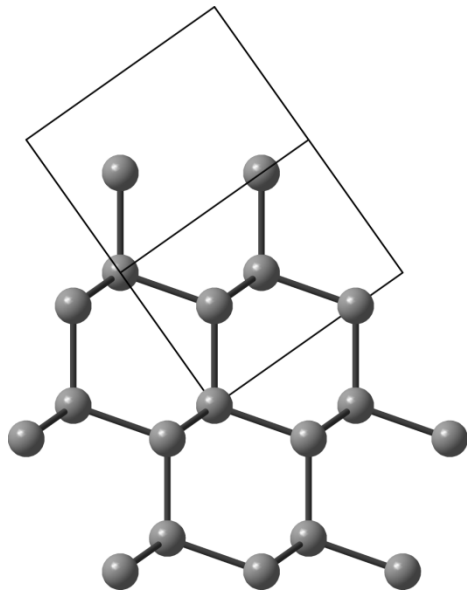
Diamond



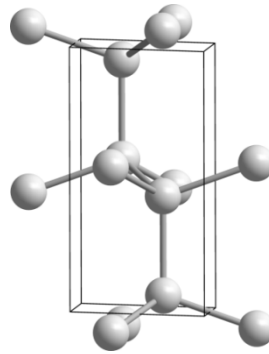
Wurtzite and zinc blende

P6₃mc and *R3m/F-43m*
2H and *3R*

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



Diamond

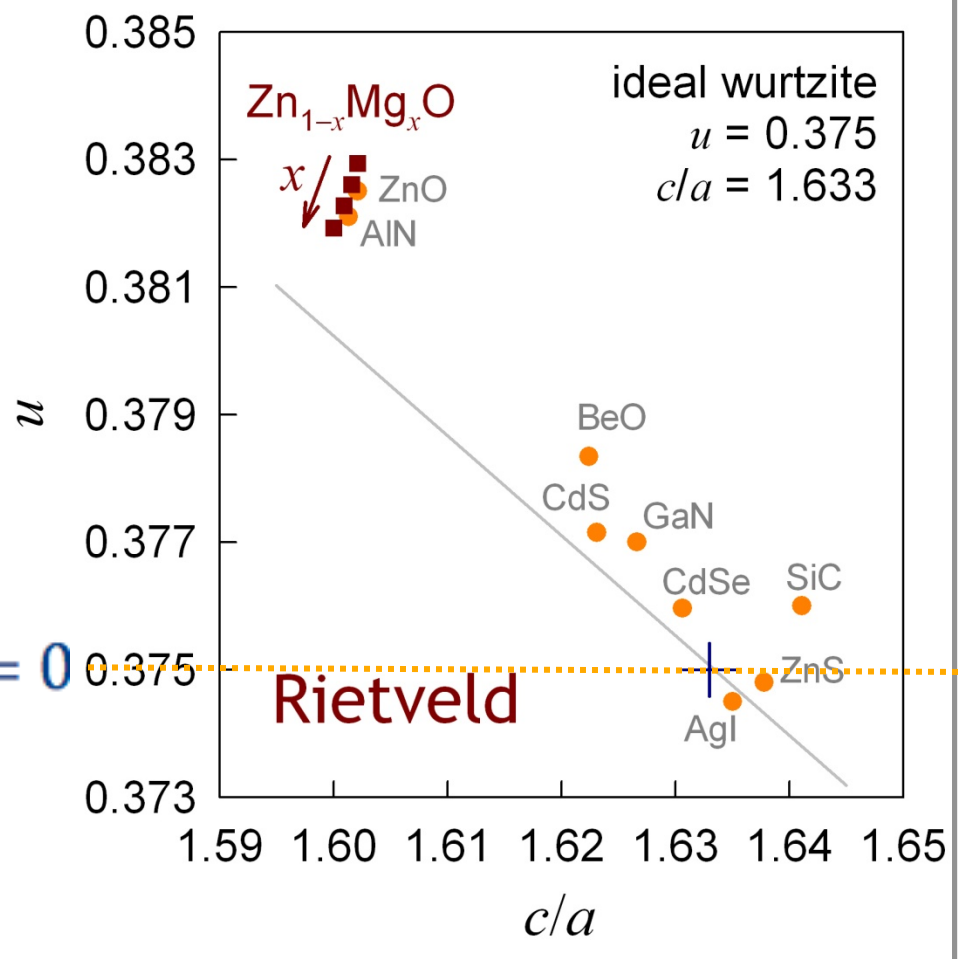


Lonsdaleite

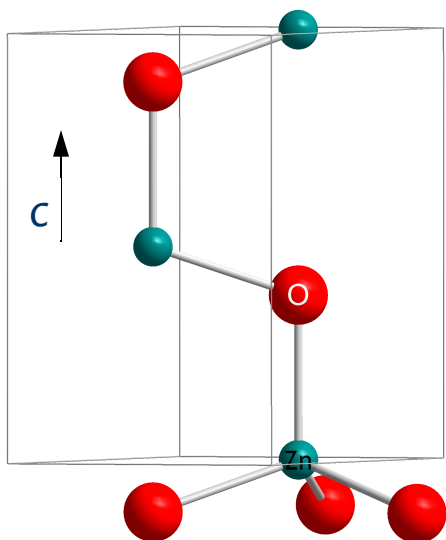
Wurtzite structures and static polarization

[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)

$$\text{Zn} \quad \left(\frac{1}{3}, \frac{2}{3}, 0\right)$$

$$\text{O}_{\text{axial}} \quad \left(\frac{1}{3}, \frac{2}{3}, u\right)$$

$$\text{O}_{\text{basal}} \quad \left(\frac{2}{3}, \frac{1}{3}, u - \frac{1}{2}\right)$$

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

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

dipole moment along c – direction

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

$$\mu(\text{Zn} - \text{O}_{\text{basal}}) = 3 \times \frac{1}{4} \times (-2) \times \left(u - \frac{1}{2}\right) \times c \quad (\text{in } e \cdot \text{\AA})$$

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

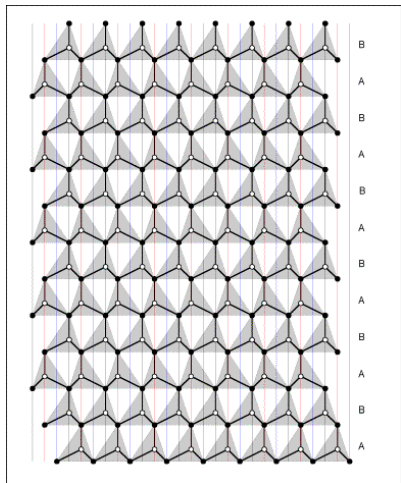
$\left(u - \frac{3}{8}\right) \cdot c$ can be obtained also from the separation between centers of $(-)$ and $(+)$ charges.

[Dr. Young-Il Kim]

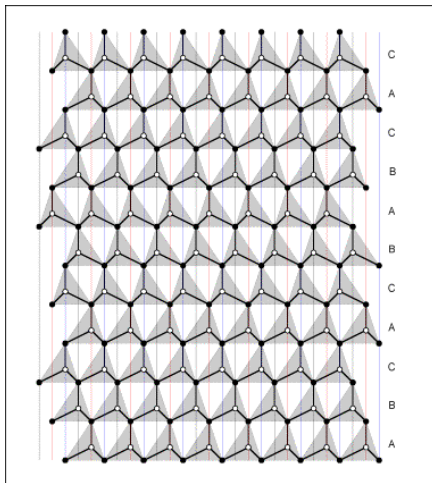
Professor Marek Skowronski

<http://neon.mems.cmu.edu/skowronski/>

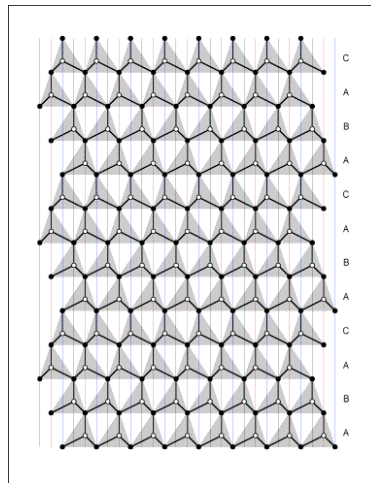
Polytypism in SiC



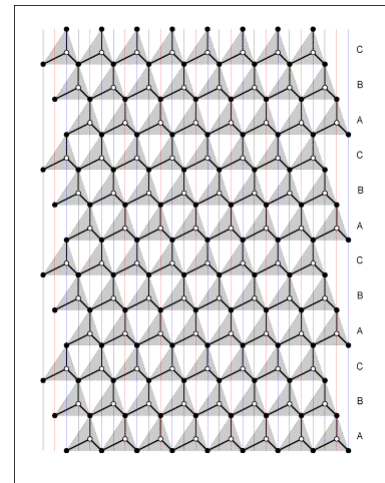
3C



4H



3H

 $2H$

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/nodeo.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

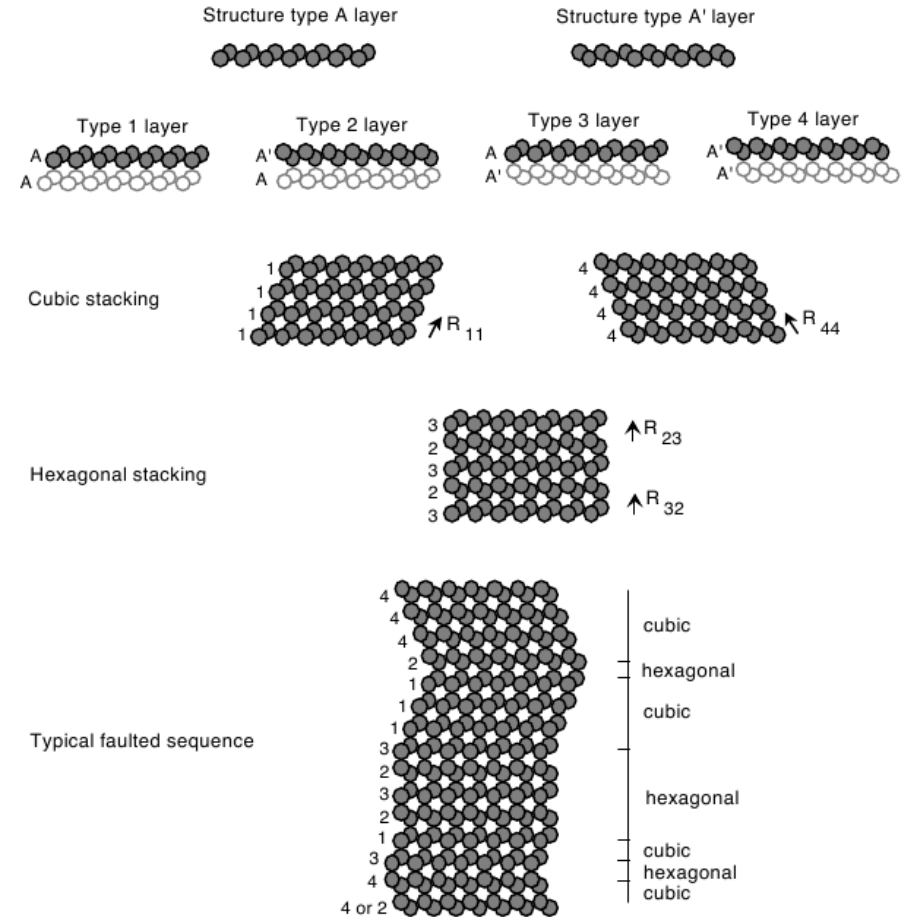
DIFFaX v 1.812

by

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

3rd July 2005

4 layers are required to describe fault clustering in diamond



Semiconductors: Structure sorting (Phillips-van Vechten)

