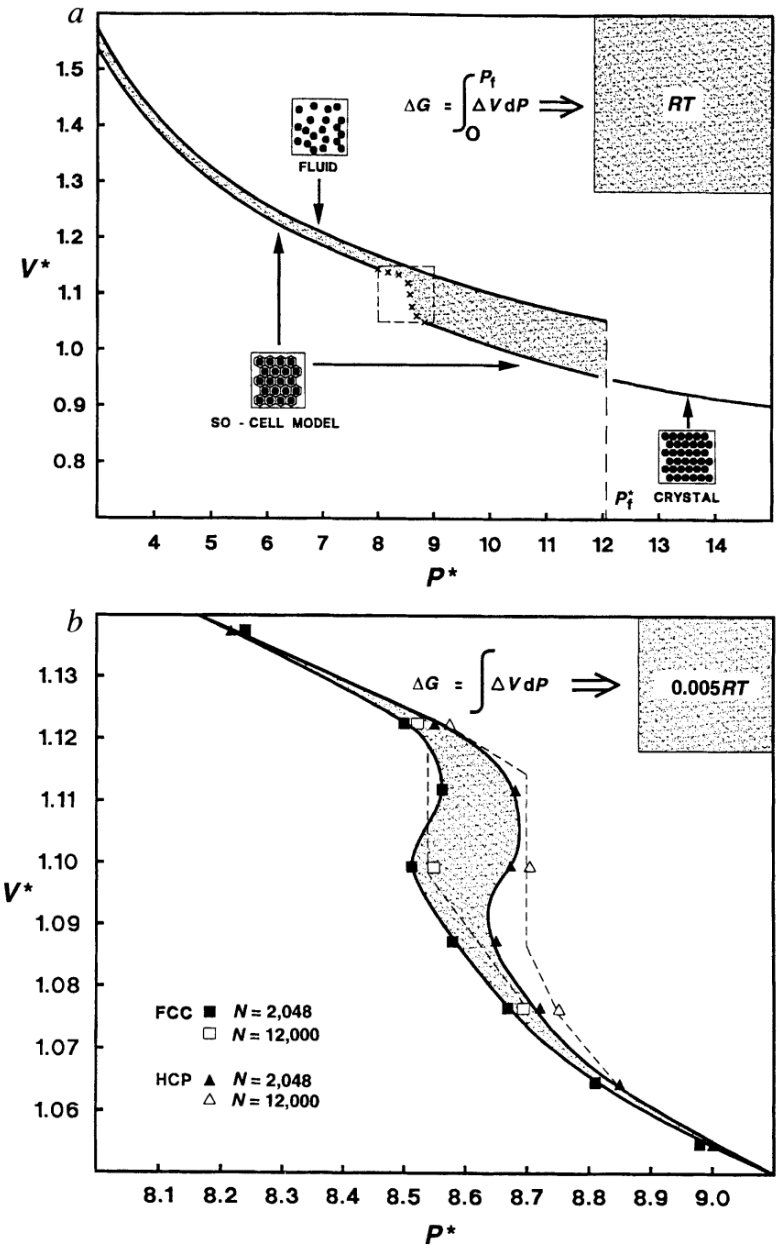
Close packings: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



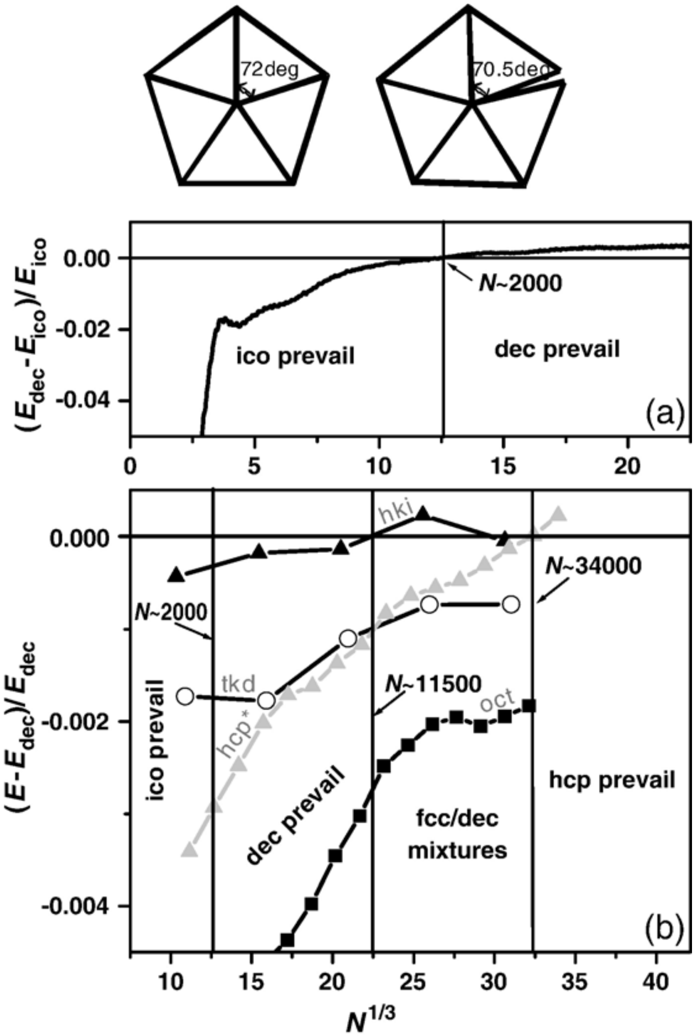
Hard spheres: *fcc* is slightly stabilized by entropy over *hcp*, by 0.005 R for all temperatures up to the melting point.

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*.

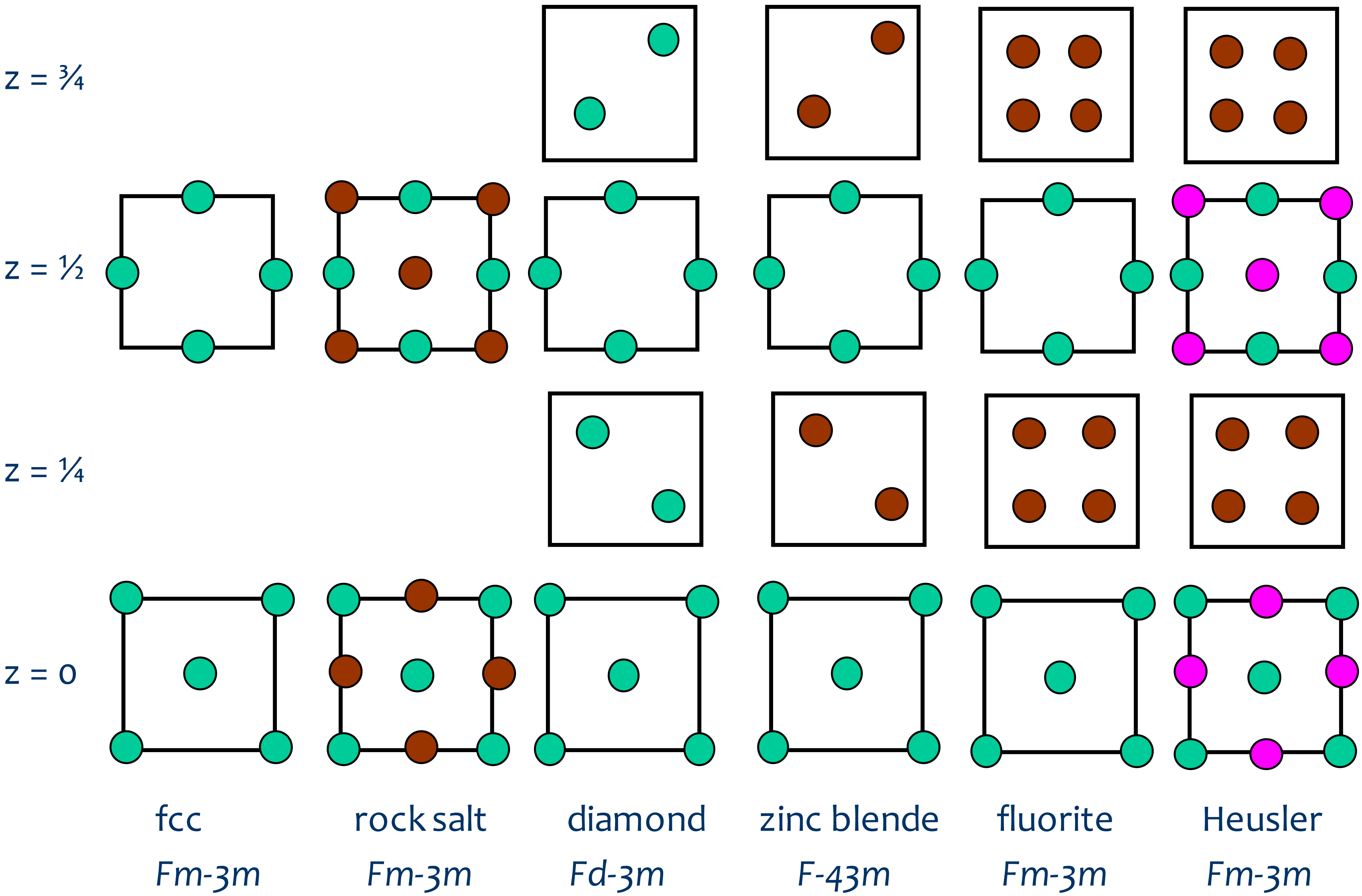
N. V. Krainyukova, The "crystal structure problem" in noble gas nanoclusters, *Thin Solid Films*, **515** (2006) 1658–1663.



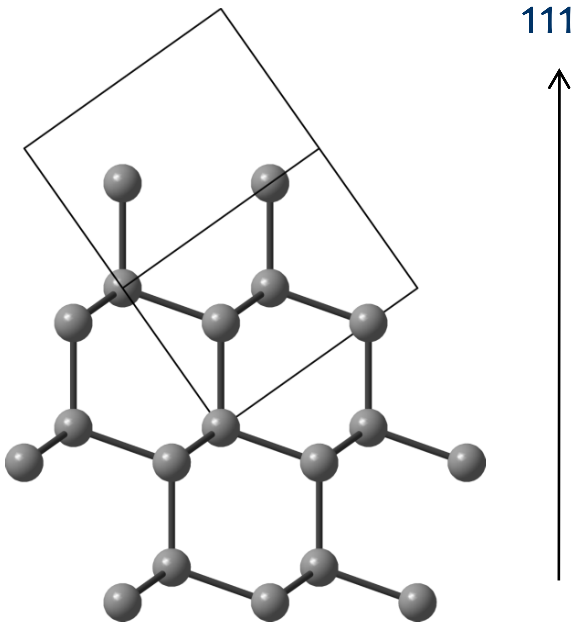
Calculations of the energetics of multiply twinned particles (MTPs) such as icosahedra and decahedra with fivefold symmetry as well as facecentered cubic (fcc) and hexagonal close-packed (hcp) particles in the size interval from 13 up to ~45,000 atoms were made applying Lennard-Jones potentials.

For the cluster size N from minimal up to N~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

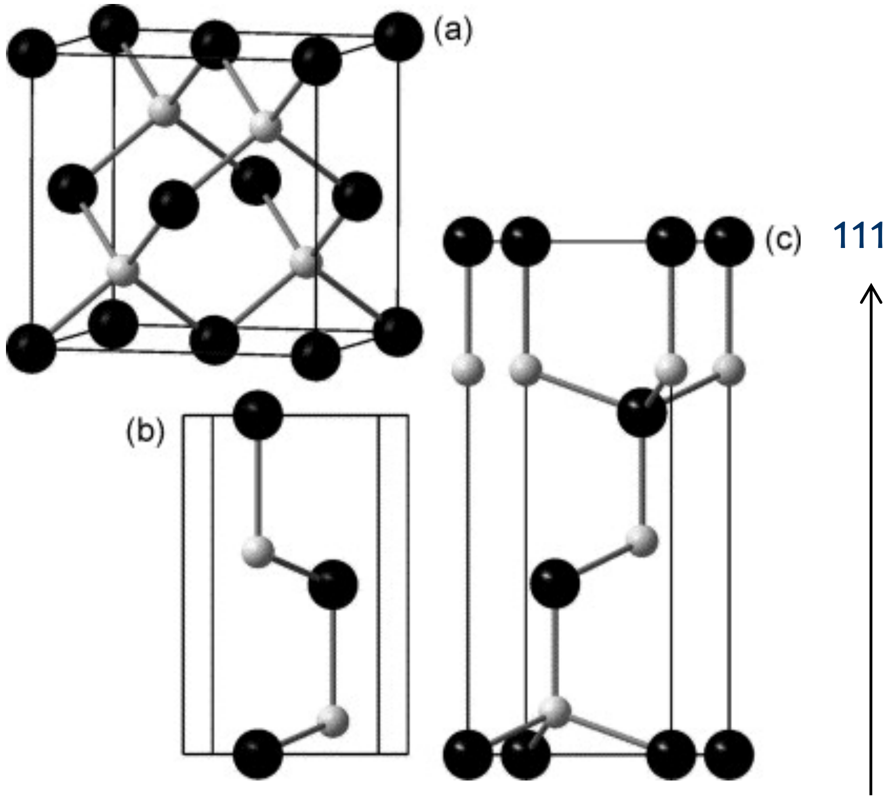
Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors



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



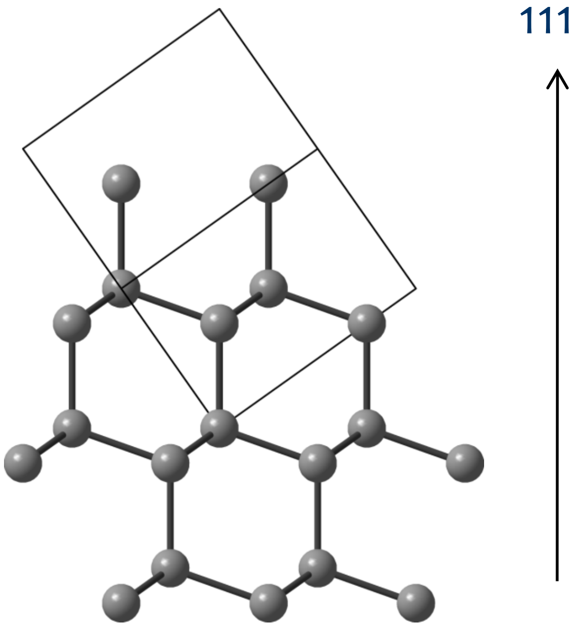
Diamond



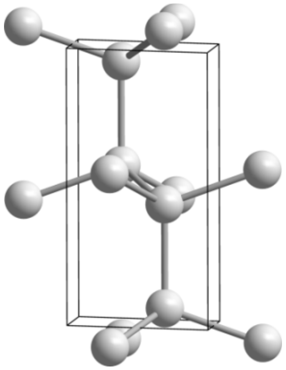
Wurtzite and zinc blende

*P*6₃*mc* and *R*3*m*/*F*-43*m*
2*H* and 3*R*

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



Diamond



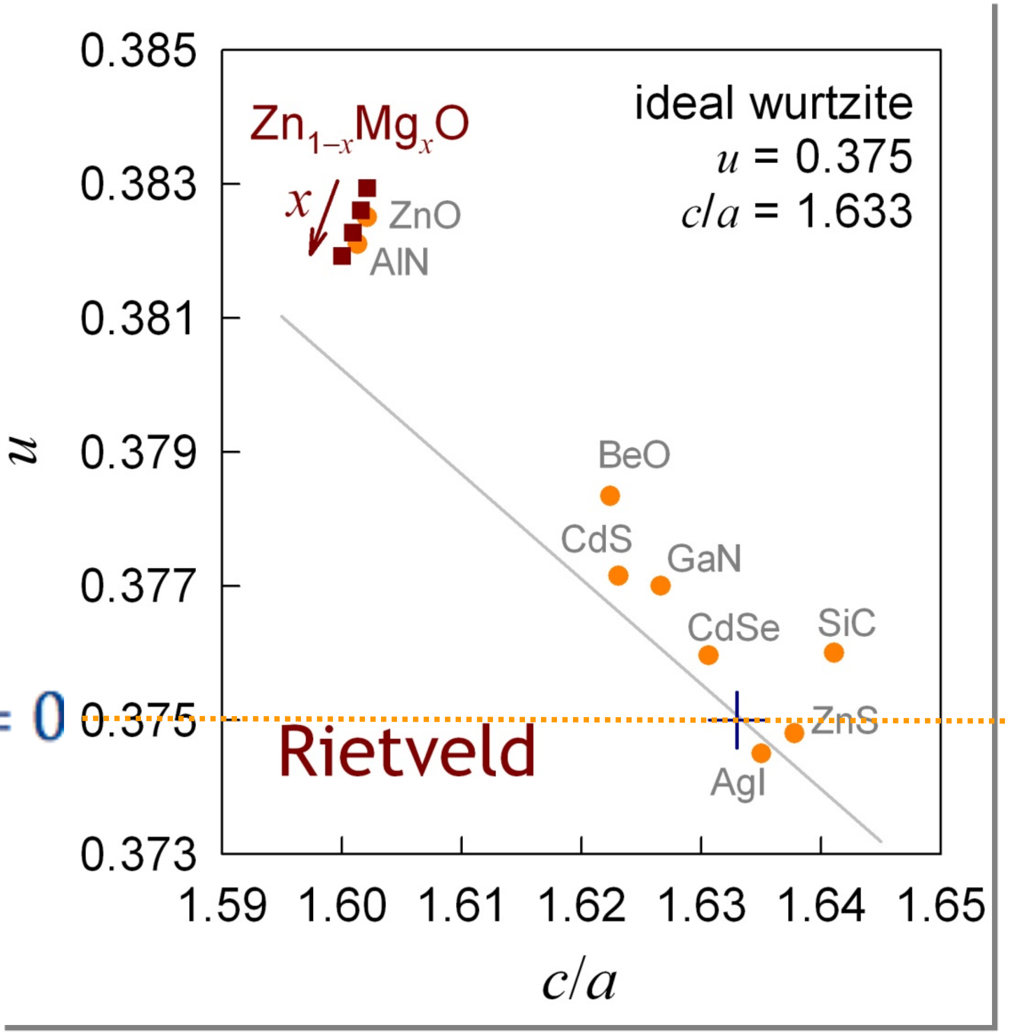
Lonsdaleite

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

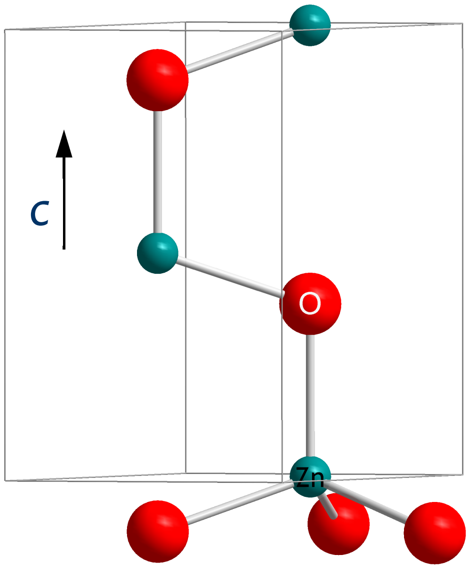
Wurtzite structures and static polarization

[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 $(\tfrac{1}{3}, \tfrac{2}{3}, 0)$

O$_{\text{axial}}$ $(\tfrac{1}{3}, \tfrac{2}{3}, u)$

O$_{\text{basal}}$ $(\tfrac{2}{3}, \tfrac{1}{3}, u-\tfrac{1}{2})$
$(\tfrac{2}{3}, -\tfrac{2}{3}, u-\tfrac{1}{2})$
$(-\tfrac{1}{3}, \tfrac{1}{3}, u-\tfrac{1}{2})$

dipole moment along c – direction

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

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

$$P_s = \frac{\mu_{\text{sum}}}{\text{unit volume}} = \frac{-2\times\left(u-\frac{3}{8}\right)\times c}{\frac{\sqrt{3}}{4}a^2 c} = \frac{-2\times\left(u-\frac{3}{8}\right)}{\frac{\sqrt{3}}{4}a^2}\left(\frac{e}{\text{Å}^2}\right)\times\left(1.60\times10^3\,\frac{\mu\text{C}}{\text{cm}^2}\cdot\frac{\text{Å}^2}{e}\right)$$

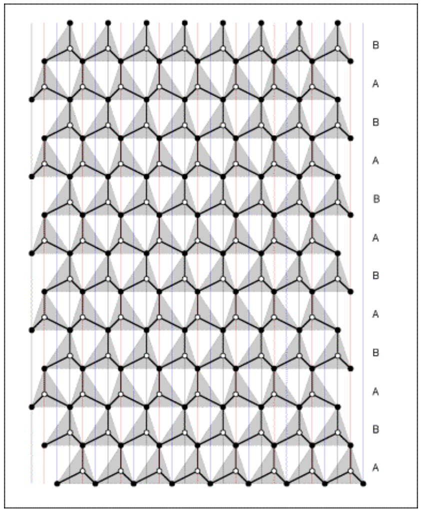
$(u-\tfrac{3}{8})\cdot c$ can be obtained also from the separation between centers of (–) and (+) charges.

[Dr. Young-Il Kim]

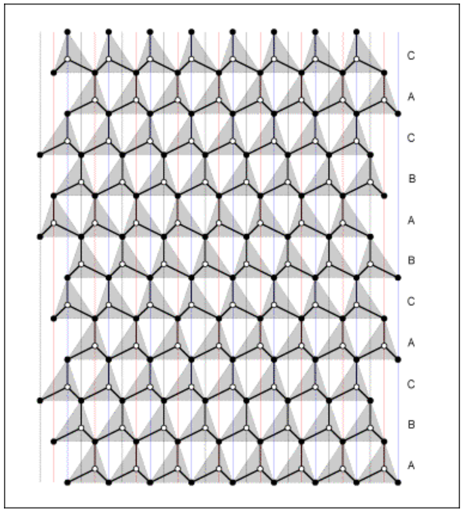
Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors

Polytypism in SiC

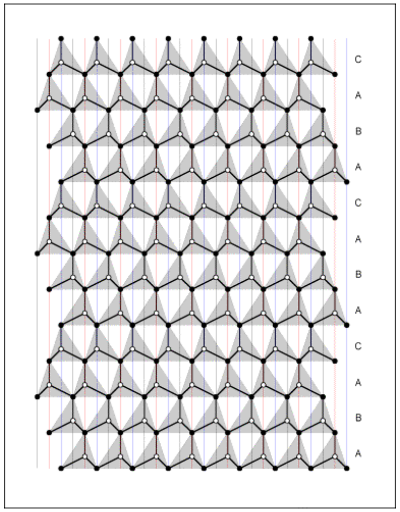
Professor Marek Skowronski
http://neon.mems.cmu.edu/skowronski/



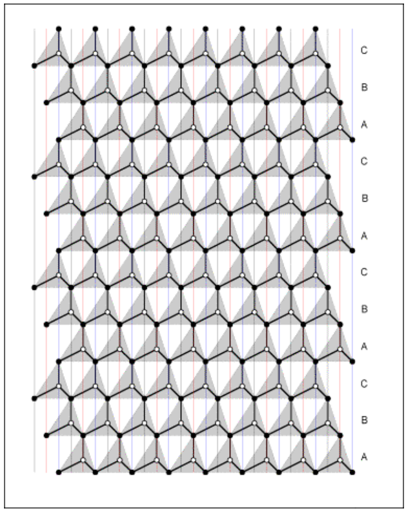
3*C*



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.

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

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

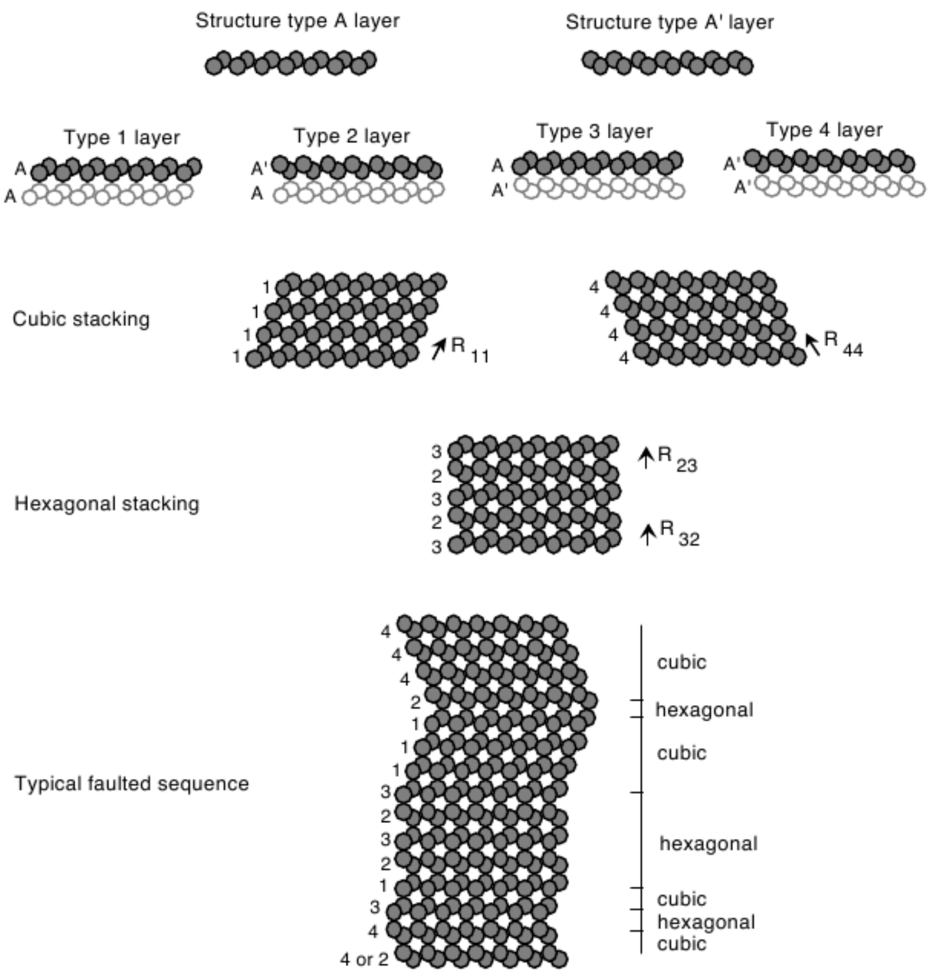
DIFFaX v 1.812

by

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

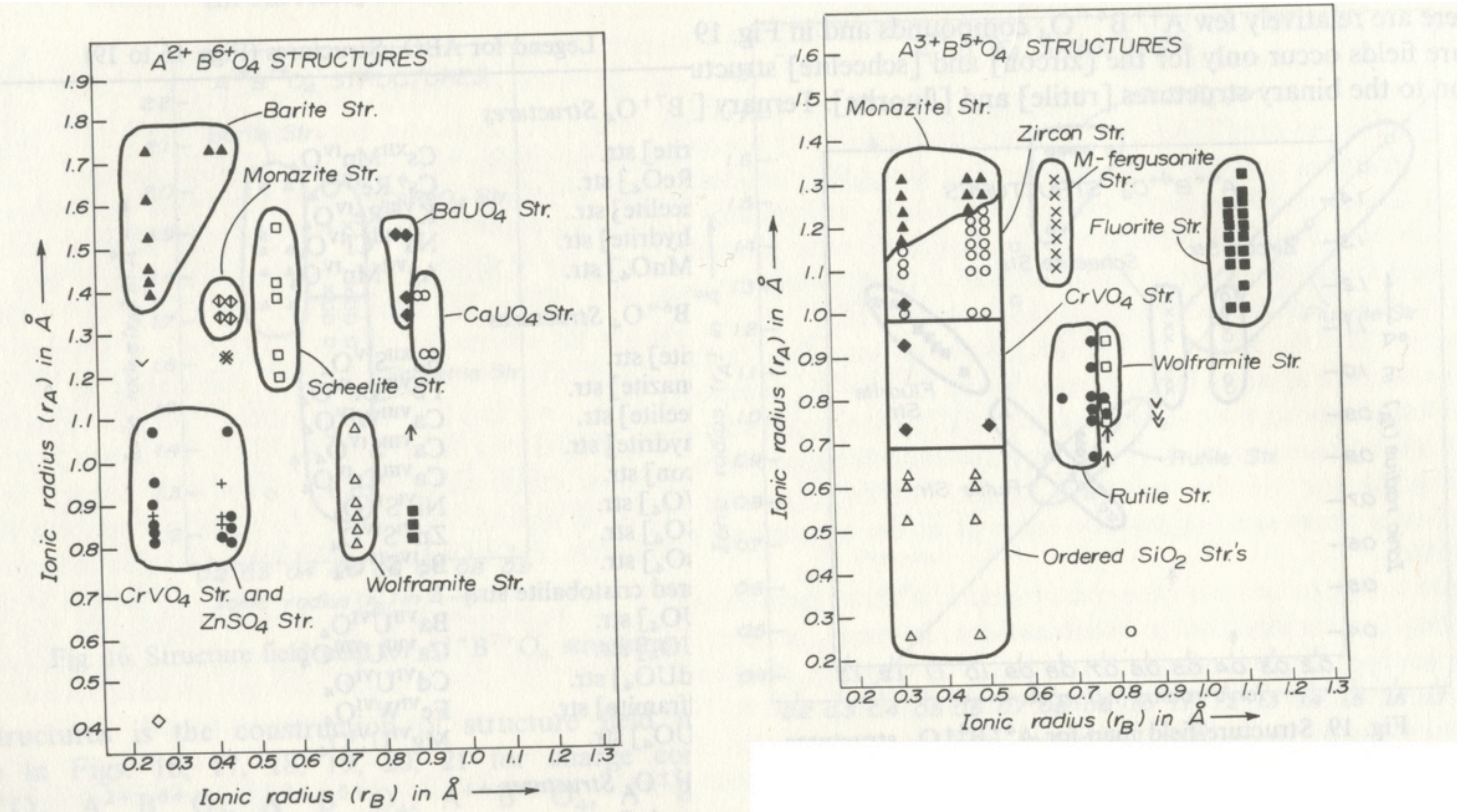
3rd July 2005

4 layers are required to describe fault clustering in diamond



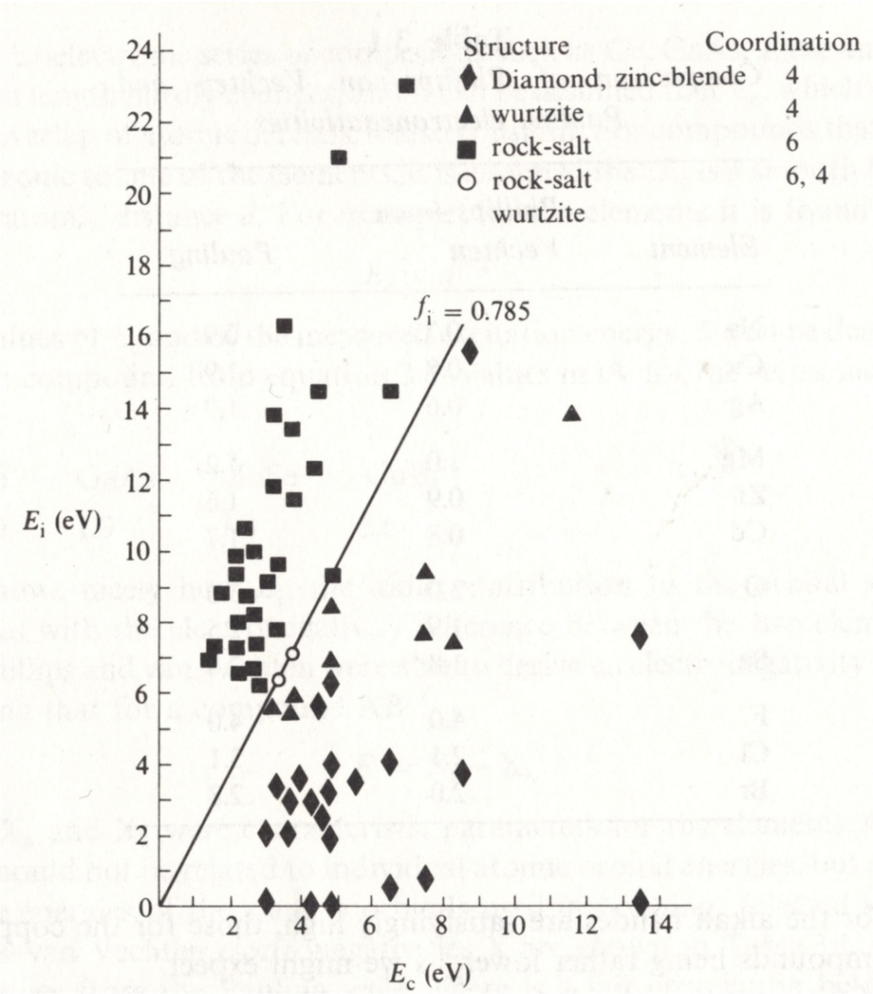
Class 2: *fcc*, *hcp*, diamond, zinc blende, wurtzite, SiC, semiconductors

Structure sorting: The major ternary structuraal families, Muller and Roy.



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

Semiconductors: Structure sorting (Phillips-van Vechten)



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

Chalcopyrite: $CuFeS_2$ and Kesterite, Cu_2ZnSnS_4