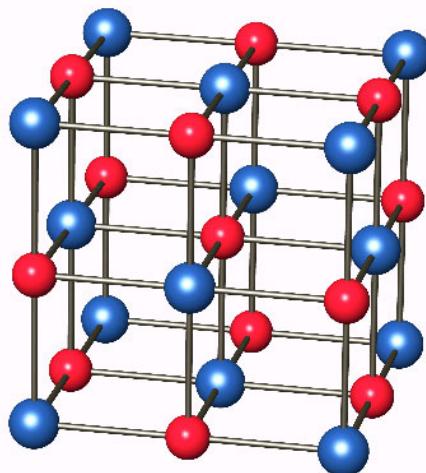
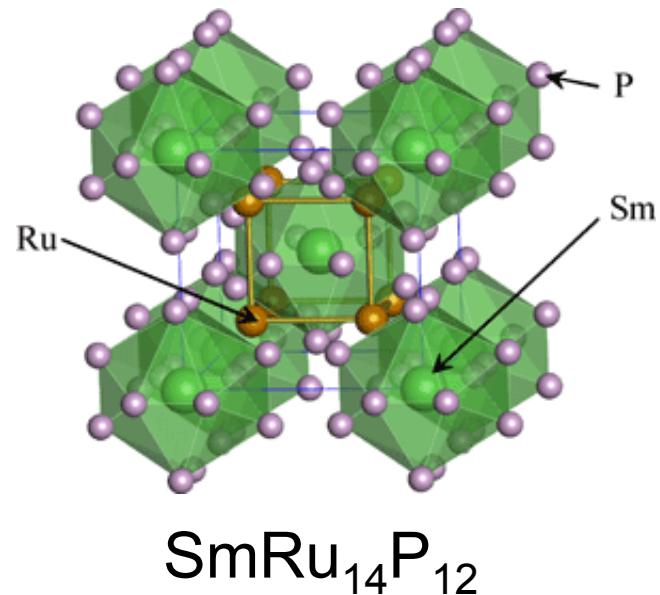


Crystal lattice

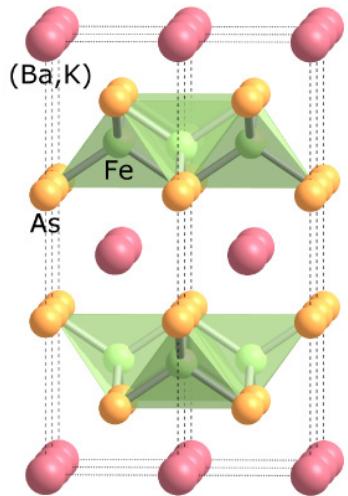
1



NaCl



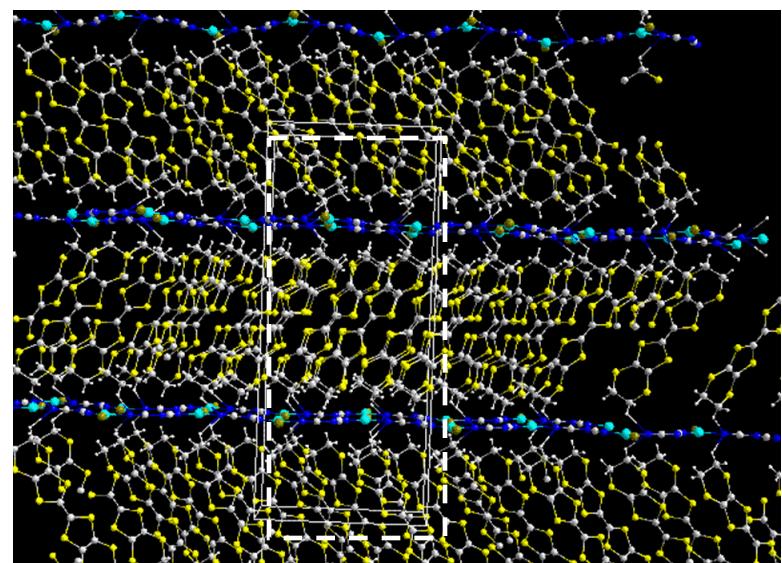
$\text{SmRu}_{14}\text{P}_{12}$



$(\text{Ba},\text{K})\text{FeAs}$

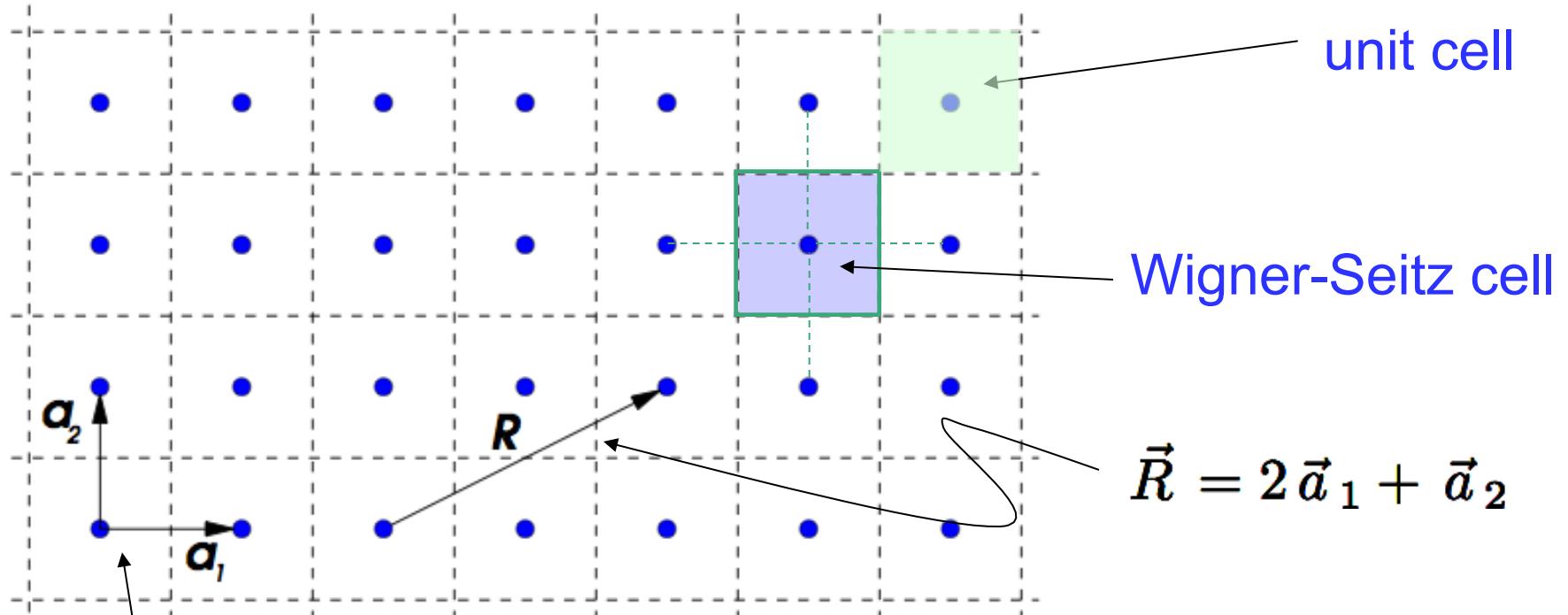
periodic array
of atoms

complex
sub-structures



$\text{K}-(\text{BEDT-TTF})_2\text{Cu}[\text{N}(\text{CN})_2]\text{Br}_x\text{Cl}_{1-x}$

Crystal lattice



primitive
lattice vectors
basis set

lattice vectors

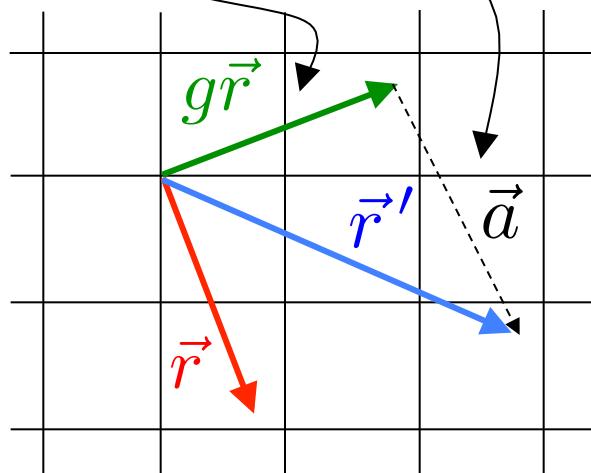
$$\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2$$

Crystal lattice - Space Group

general symmetry operations in a crystal lattice

$$\vec{r}' = g\vec{r} + \vec{a} = \{g|\vec{a}\}\vec{r}$$

$\{g|\vec{a}\}$ space group element



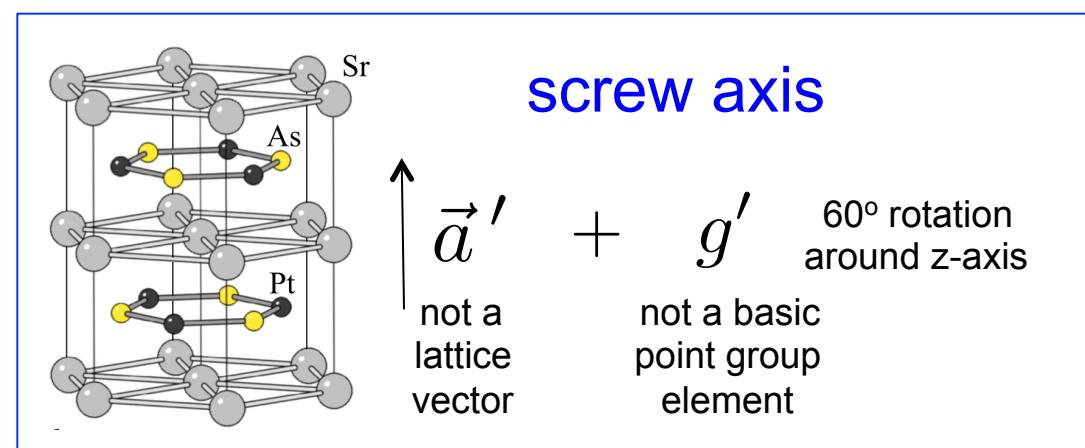
$g \in \mathcal{P}$ point group element
 \vec{a} lattice vector

basic elements

$\{E|\vec{a}\}$ basic translations

$\{g|\vec{0}\}$ rotations, reflections, inversions

$\{g'|\vec{a}'\}$ screw axis, glide plane



Crystal lattice - Space Group

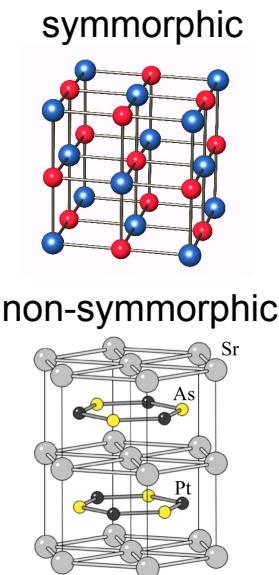
space group \mathcal{R} is a group

- multiplication $\{g|\vec{a}\}\{g'|\vec{a}'\} = \{gg'|g\vec{a}' + \vec{a}\}$ associative
- unit element $\{E|\vec{0}\}$ $\{E|\vec{0}\}\{g|\vec{a}\} = \{Eg|E\vec{a} + \vec{0}\} = \{g|\vec{a}\}$
- inverse $\{g|\vec{a}\}^{-1} = \{g^{-1}| - g^{-1}\vec{a}\}$
 $\{g|\vec{a}\}^{-1}\{g|\vec{a}\} = \{g^{-1}| - g^{-1}\vec{a}\}\{g|\vec{a}\} = \{g^{-1}g|g^{-1}\vec{a} - g^{-1}\vec{a}\} = \{E|\vec{0}\}$

space groups with
screw axes and
glide planes



non-symmorphic



230 space groups =
73 symmorphic + 157 non-symmorphic

crystal system (# point groups, # space groups)	point groups Schönflies symbols	space group numbers international tables
triclinic (2,2)	$C_1, C_{\bar{1}}$	1-2
monoclinic (3,13)	C_2, C_s, C_{2h}	3-15
orthorhombic (3,59)	D_2, C_{2v}, D_{2h}	16-74
tetragonal (7,68)	$C_4, S_4, C_{4h}, D_4, C_{4v}, D_{2d}, D_{4h}$	75-142
trigonal (5,25)	$C_3, S_6, D_3, C_{3v}, D_{3d}$	143-167
hexagonal (7,27)	$C_6, C_{3h}, C_{6h}, D_6, C_{6v}, D_{3h}, D_{6h}$	168-194
cubic (5, 36)	T, T_h, O, T_d, O_h	195-230