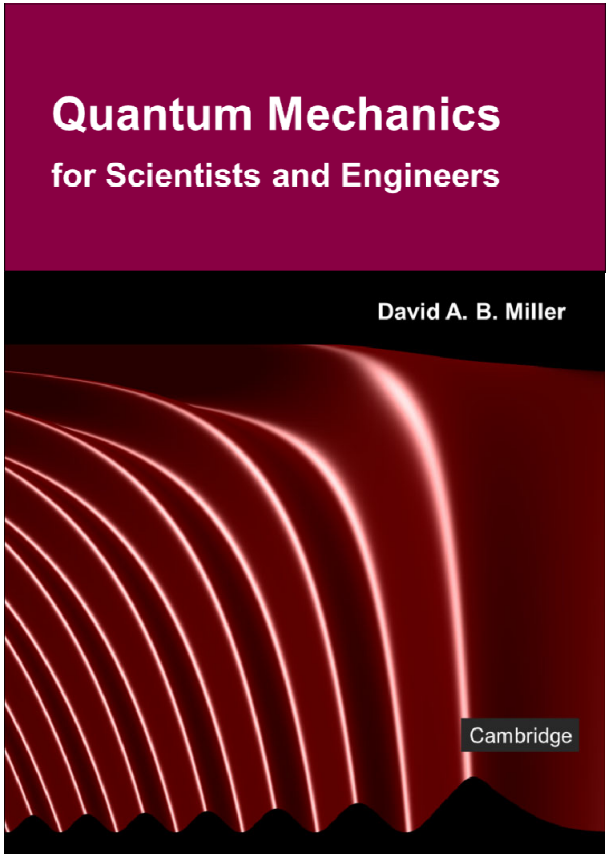
27 Quantum mechanics in crystals

Slides: Lecture 27a Introduction to quantum mechanics in crystals

Text reference: Quantum Mechanics for Scientists and Engineers

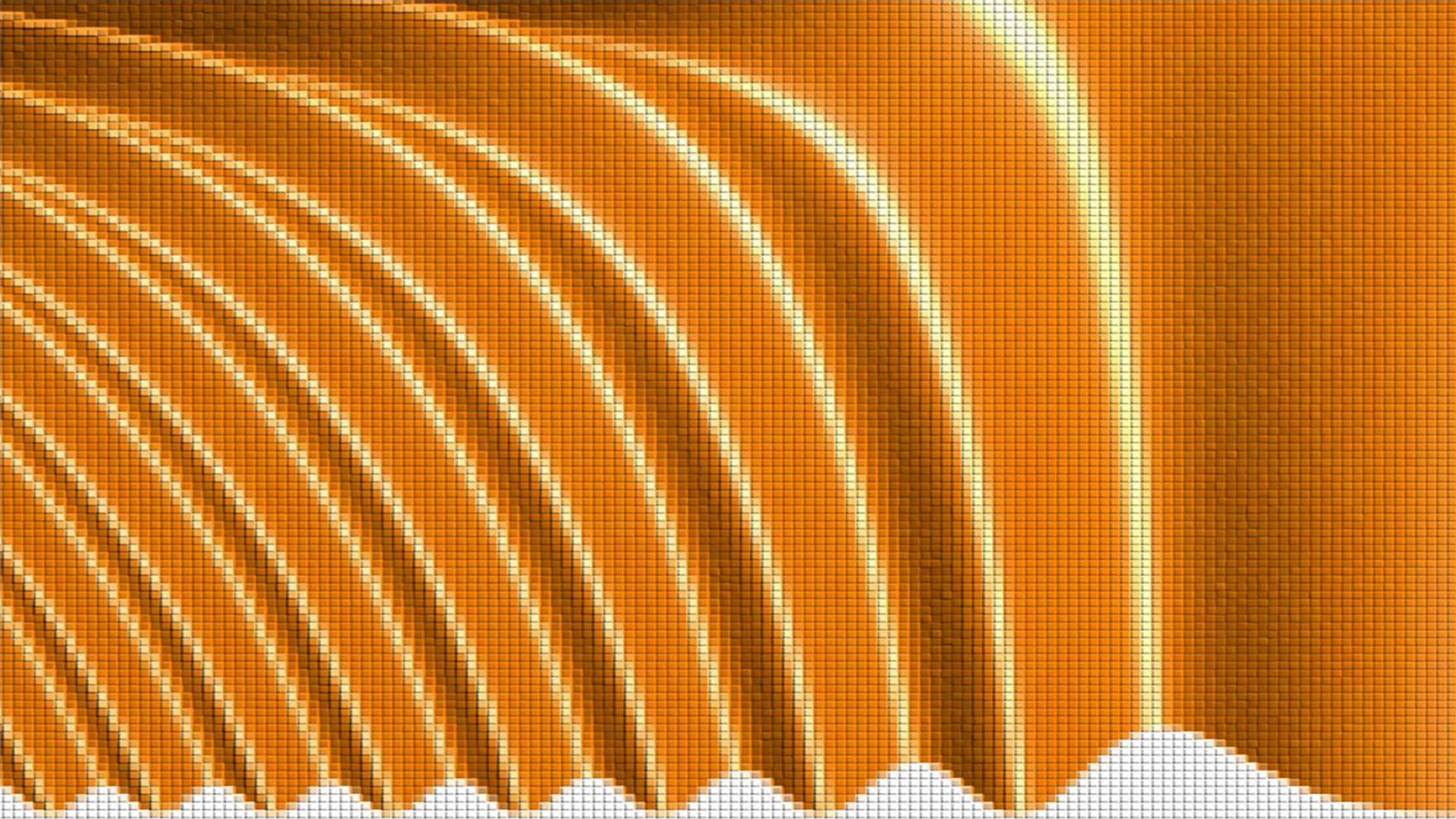
Chapter 8 Introduction



Quantum mechanics in crystals

Quantum mechanics for scientists and engineers

David Miller

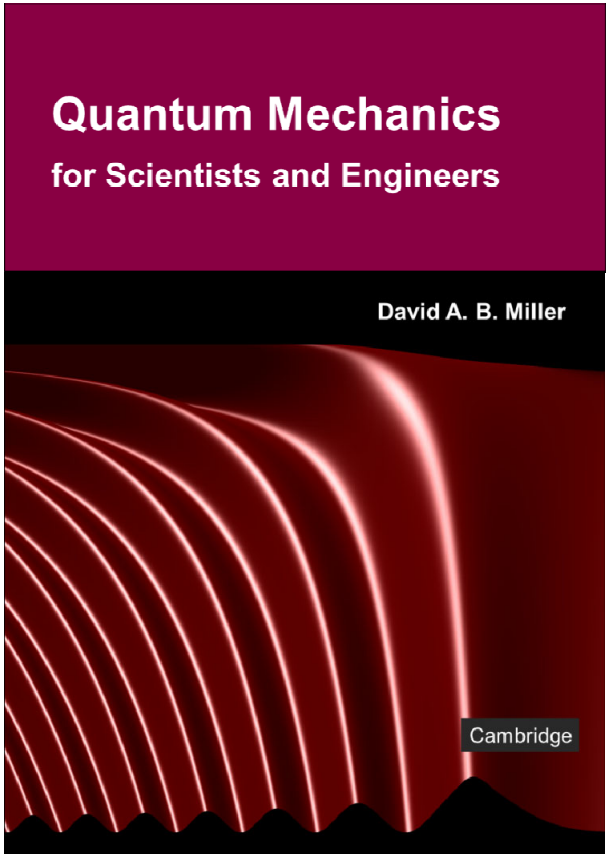


27 Quantum mechanics in crystals

Slides: Lecture 27b Crystal structures

Text reference: Quantum Mechanics for Scientists and Engineers

Section 8.1



Quantum mechanics in crystals

Crystal structures

Quantum mechanics for scientists and engineers

David Miller

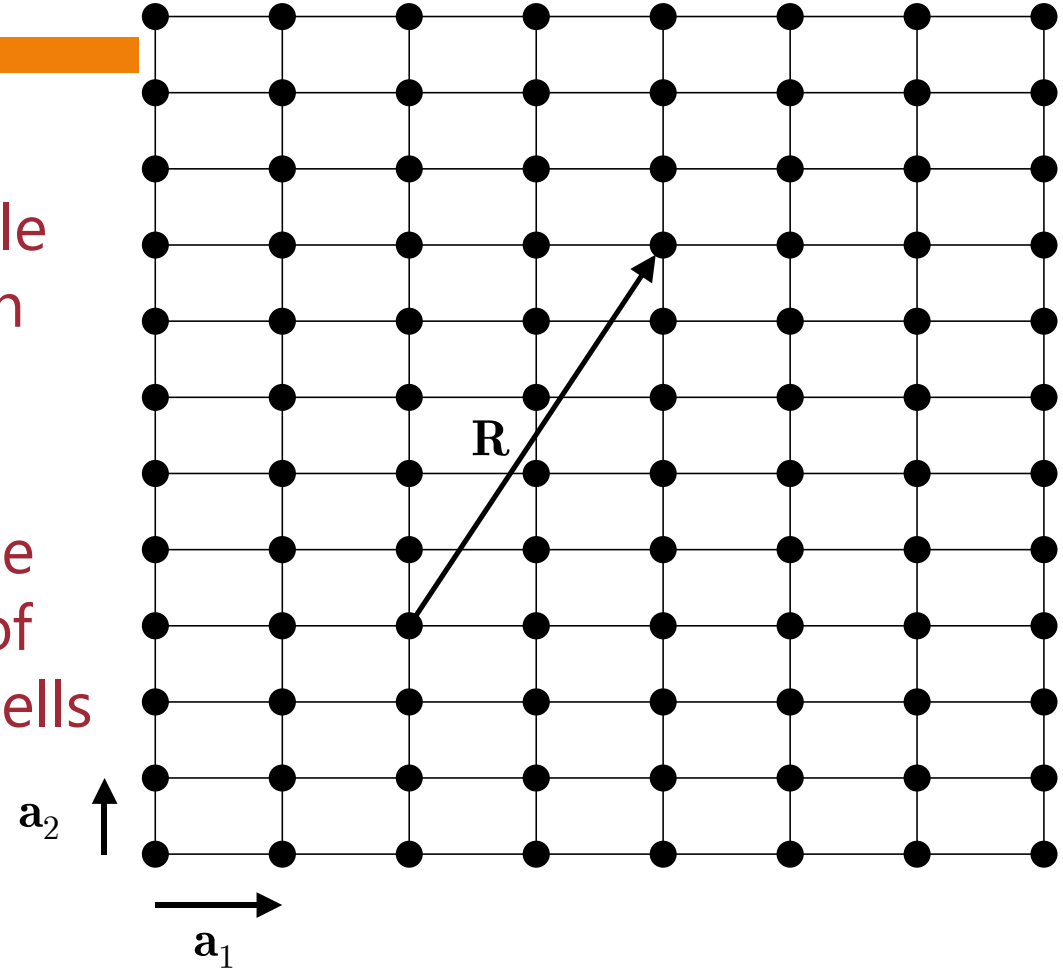
Crystal structures

Crystal

material whose measurable properties are periodic in space

Crystal structure

is one that can fill all space by the regular stacking of identical blocks or unit cells

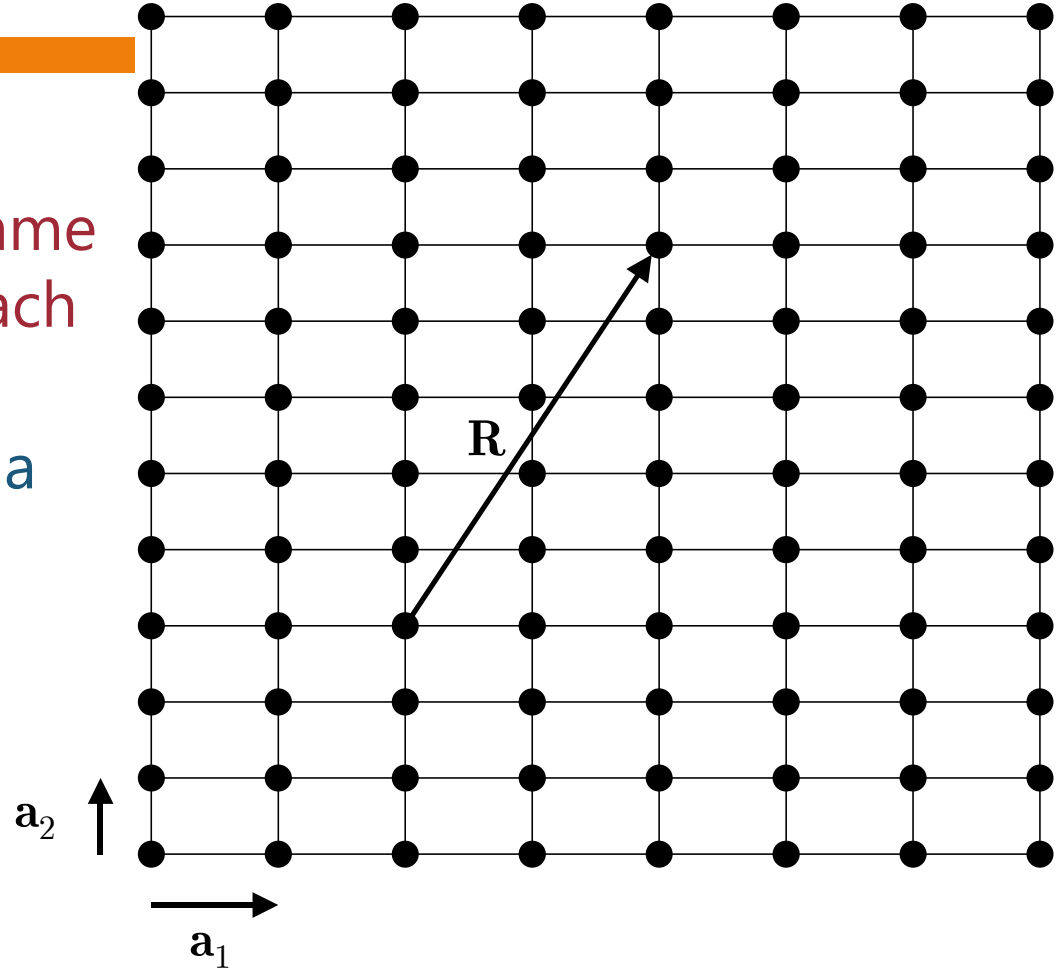


Crystal structures

Crystal lattice

If we put a mark on the same spot on the surface of each block

these spots would form a crystal lattice



Lattice vectors

The set of lattice vectors

consists of all of the vectors

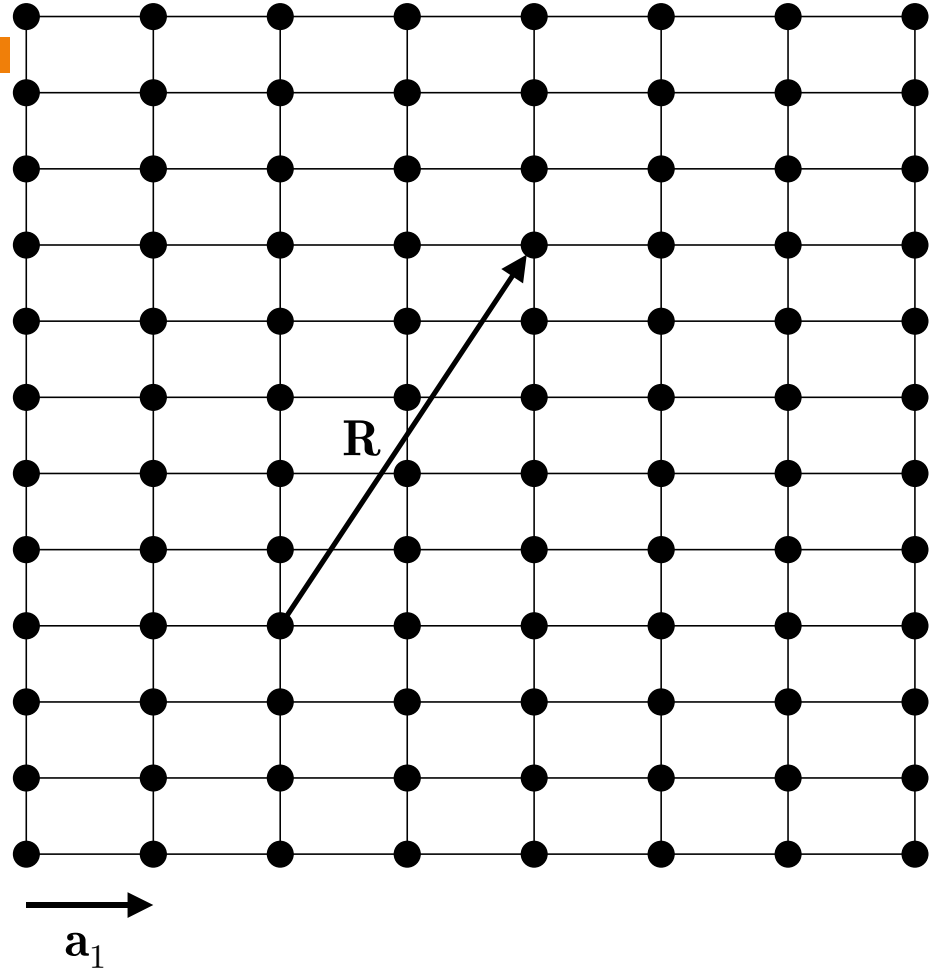
$$\mathbf{R}_L = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

with integer n_1, n_2, and n_3

linking the same point in two different "unit cells"

"Translating" (moving) by a lattice vector makes no difference

"translational symmetry"



Lattice vectors

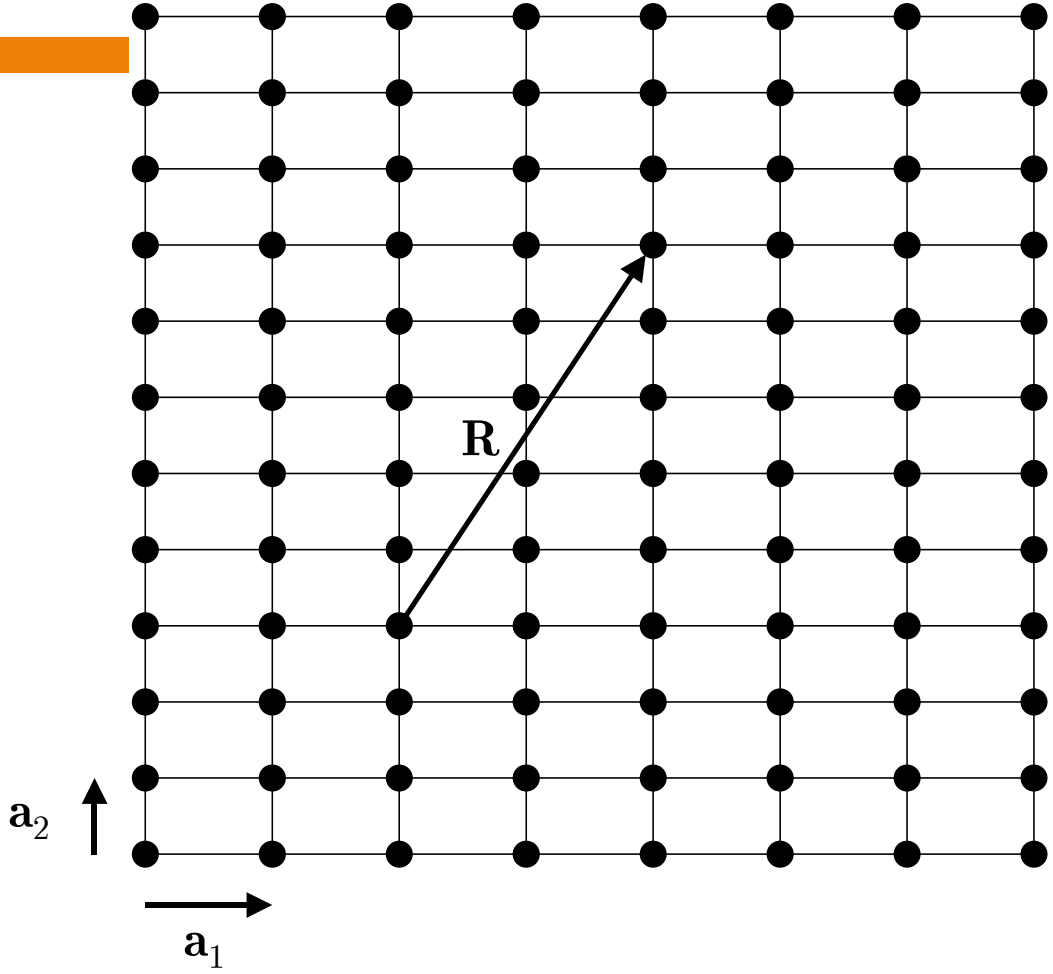
In

$$\mathbf{R}_L = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

$\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the three linearly independent vectors that take us

from a point in one unit cell

to the equivalent point in the adjacent unit cell



Bravais lattices

In a given dimensionality, e.g., 1D, 2D, 3D

there are only specific finite numbers of different types or symmetries of lattices of points

Bravais lattices

1D – only one kind of lattice is possible

equally spaced points

2D – 5 are possible

note no 5-sided object can be repeated to fill all space in a plane, for example

3D – 14 are possible

Diamond and zinc-blende lattices

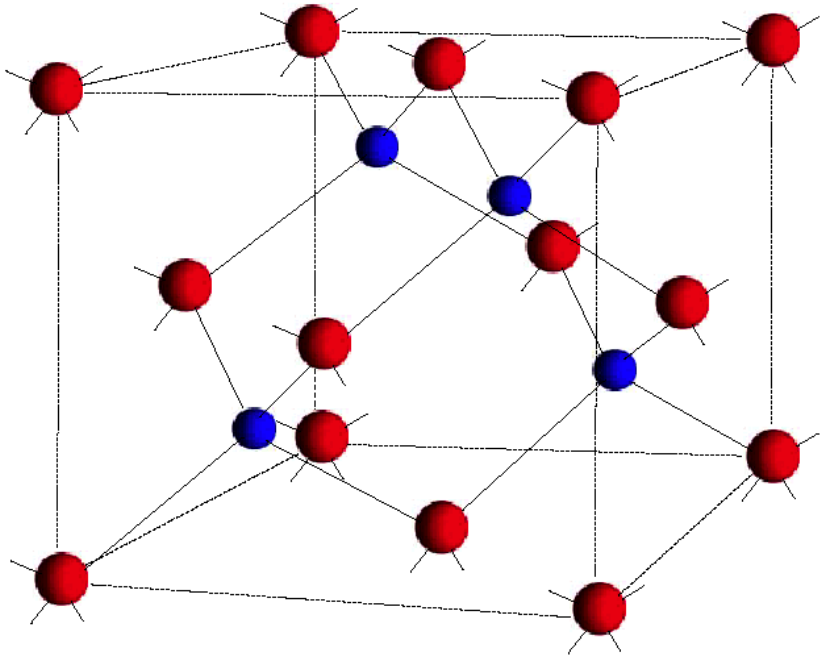
A large fraction of the semiconductor materials of practical interest

such as silicon, germanium, and most of the III-V (e.g., GaAs) and II-VI (e.g., ZnSe) materials

have a specific form of cubic lattice

Diamond and zinc-blende lattices

The Bravais lattice for these
  is “face-centered cubic”
The actual physical lattice
  has two interlocking face-centered cubic lattices
    which is the Bravais lattice with a pair of atoms associated with each lattice point



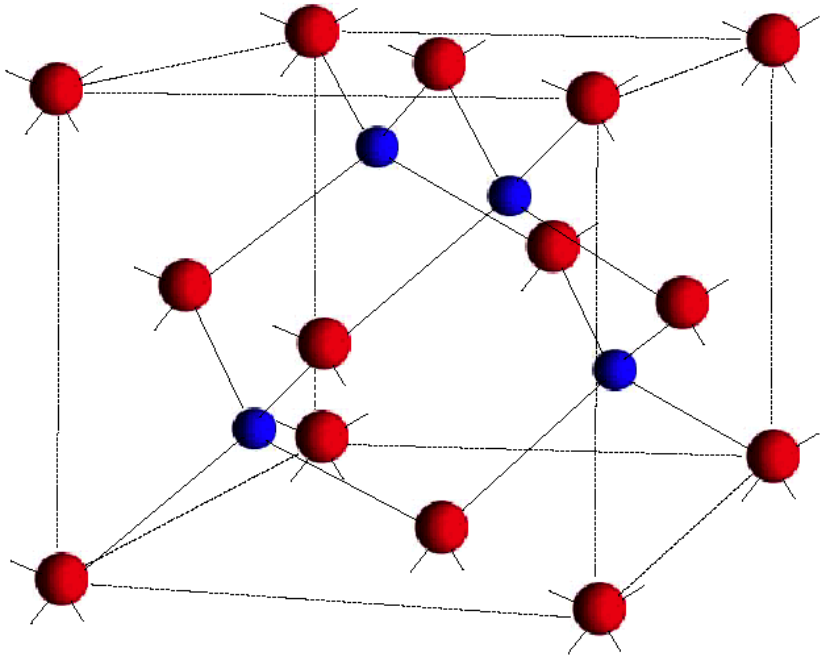
Diamond and zinc-blende lattices

"Zinc-blende" is the crystal structure for

most III-V and II-VI materials

The group III (or II) atoms lie on one such face-centered cubic lattice

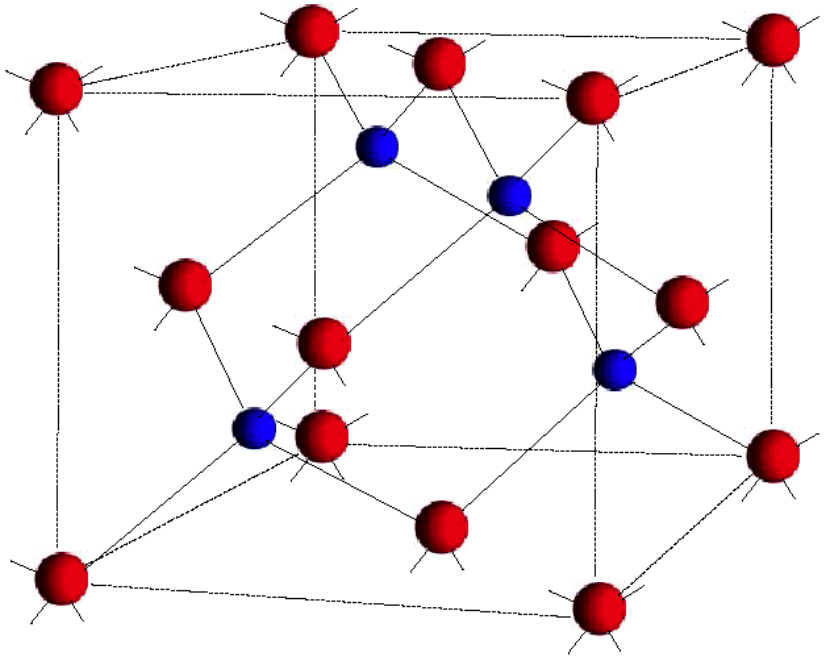
and the group V (or VI) lie on the interlocking face-centered cubic lattice



Diamond and zinc-blende lattices

"Diamond" is the lattice for
- some group IV materials
  - e.g., silicon, germanium
  - some forms of carbon (diamond itself) and tin

Both interlocking lattices
- have the same kinds of atoms on them



Other important semiconductor lattice structures

Hexagonal

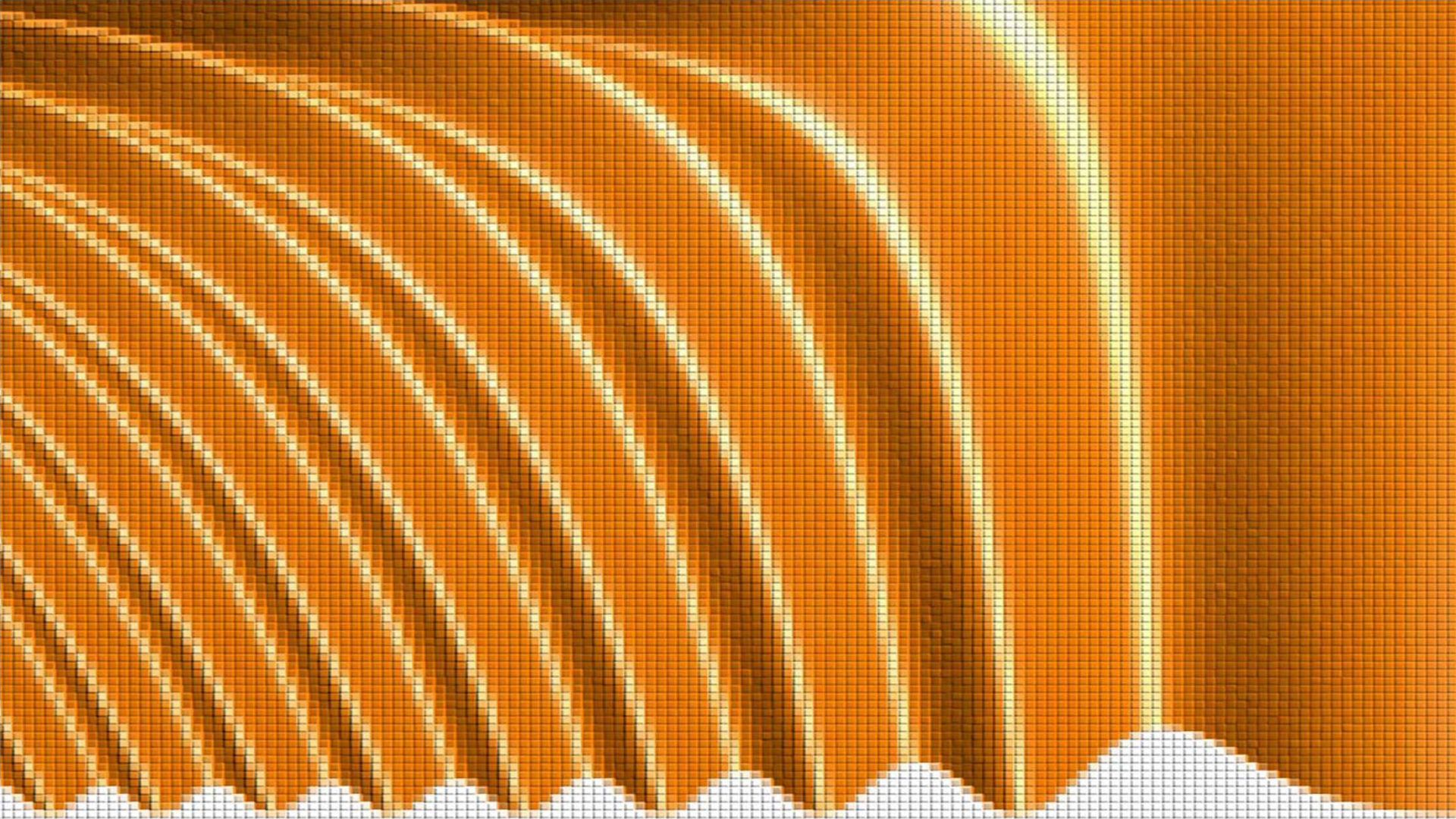
as in the graphite form of carbon

also graphene

a single sheet of hexagonal carbon atoms

and the basis of carbon nanotubes

rolled up sheets of hexagonal carbon atoms

Wurtzite

a form of hexagonal lattice with two atoms per lattice point