Achievements

VESTA plotting of crystal structures

How to describe a crystal structure

-- Crystal lattice

-- Basis

How to resolve crystal structures

-- Reciprocal space

-- Scattering theory (Form and Structure Factor)

-- Resolving the crystal structure of a superconductor

Lecture 5: How crystals bind together

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Tasks for Next week

(1) Read chapter 3: Crystal Binding (less than 20 pages)

Crystals of Inert Gases
Van der Waals-London Interaction
Repulsive Interaction
Equilibrium Lattice Constants
Cohesive Energy
Ionic Crystals
Electrostatic or Madelung Energy + Evaluation of Madelung Constant
Covalent Crystals
Metals
Atomic Radii + Ionic Crystal Radii

(2) Start Reading chapter 4: Phonons / Lattice Vibrations

(3) Solve next exercise sheets

(4) Summary:

Exercise 1 *Binding energy*

a) Show that for a potential of the form $U(R) = -\frac{A}{R^m} + \frac{B}{R^n}$ an equilibrium can only be reached if $n > m$.

b) For a pure van der Waals attraction the potential is often written as

$$U(R) = 4\epsilon \left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6} \right].$$

Calculate the binding energy (cohesive energy) E_B and the equilibrium distance R_0.

c) Calculate the effect of thermal expansion, $\Delta R_0(T)/R_0$, on a linear chain of atoms with the potential of part b. Assume that the thermal energy $k_B T \ll E_B$ allows motion of the atoms around the equilibrium position. Think about in what boundaries the atoms can move. From this deduce the average position and compare the result with R_0.

Hint: Use the expansion $1/(1 \pm \epsilon) \approx 1 \mp \epsilon + \epsilon^2 + \ldots$ up to the second order and $\sqrt[n]{1+\epsilon} = 1 + \epsilon/n + \ldots$ for $\epsilon \to 0$.

Exercise 2 *Madelung constant*

Calculate the Madelung constant for an infinitely long, evenly spaced, linear chain of ions with alternating anions and cations of charge $\pm e$.

Exercise 3 *Linear ionic crystal*

Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbours.

a) Show that the expression for the potential energy can be approximated by

$$U(R) = N\left[\frac{2A}{R^n} - \frac{2\ln 2q^2}{4\pi\epsilon_0 R}\right].$$

b) Show that at the equilibrium separation

$$U(R_0) = -\frac{2Nq^2\ln 2}{4\pi\epsilon_0 R_0}\cdot\left(1-\frac{1}{n}\right).$$

c) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. Show that the work done in compressing a unit length of the crystal has the leading term $\frac{1}{2}C\delta^2$, where

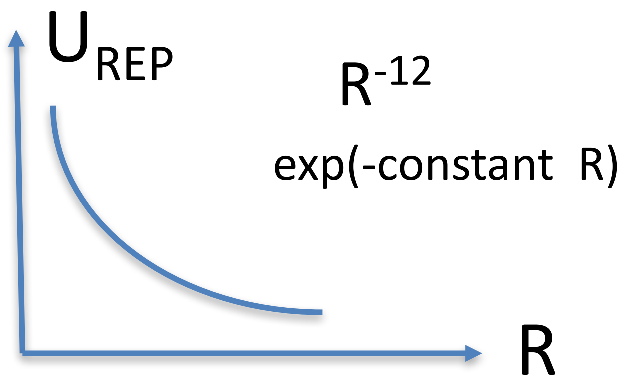
$$C = \frac{(n-1)q^2\ln 2}{4\pi\epsilon_0 R_0}.$$

Note: Use the complete expression for $U(R)$ instead of $U(R_0)$.

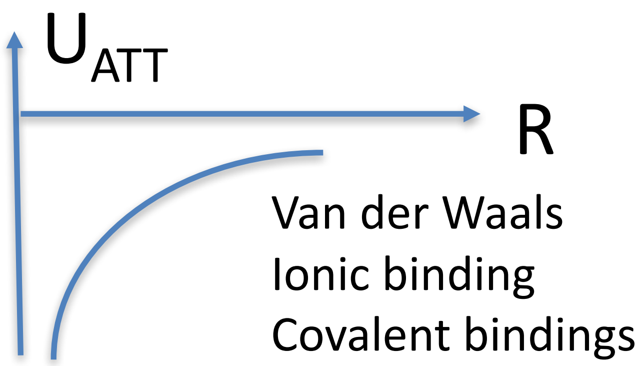
Crystal bindings

Total crystal potential: $U(R) = U_{REP} + U_{ATT}$

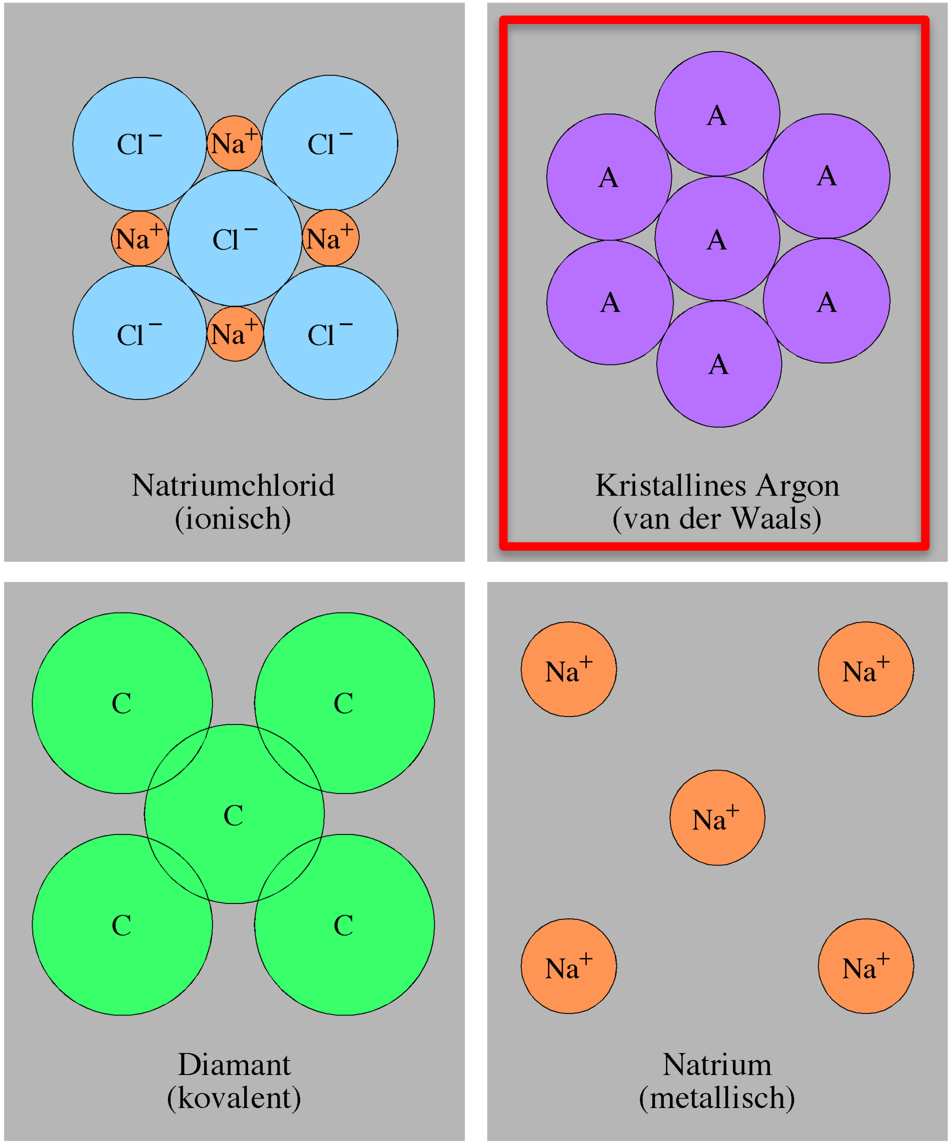
Repulsive Potential U_{REP}



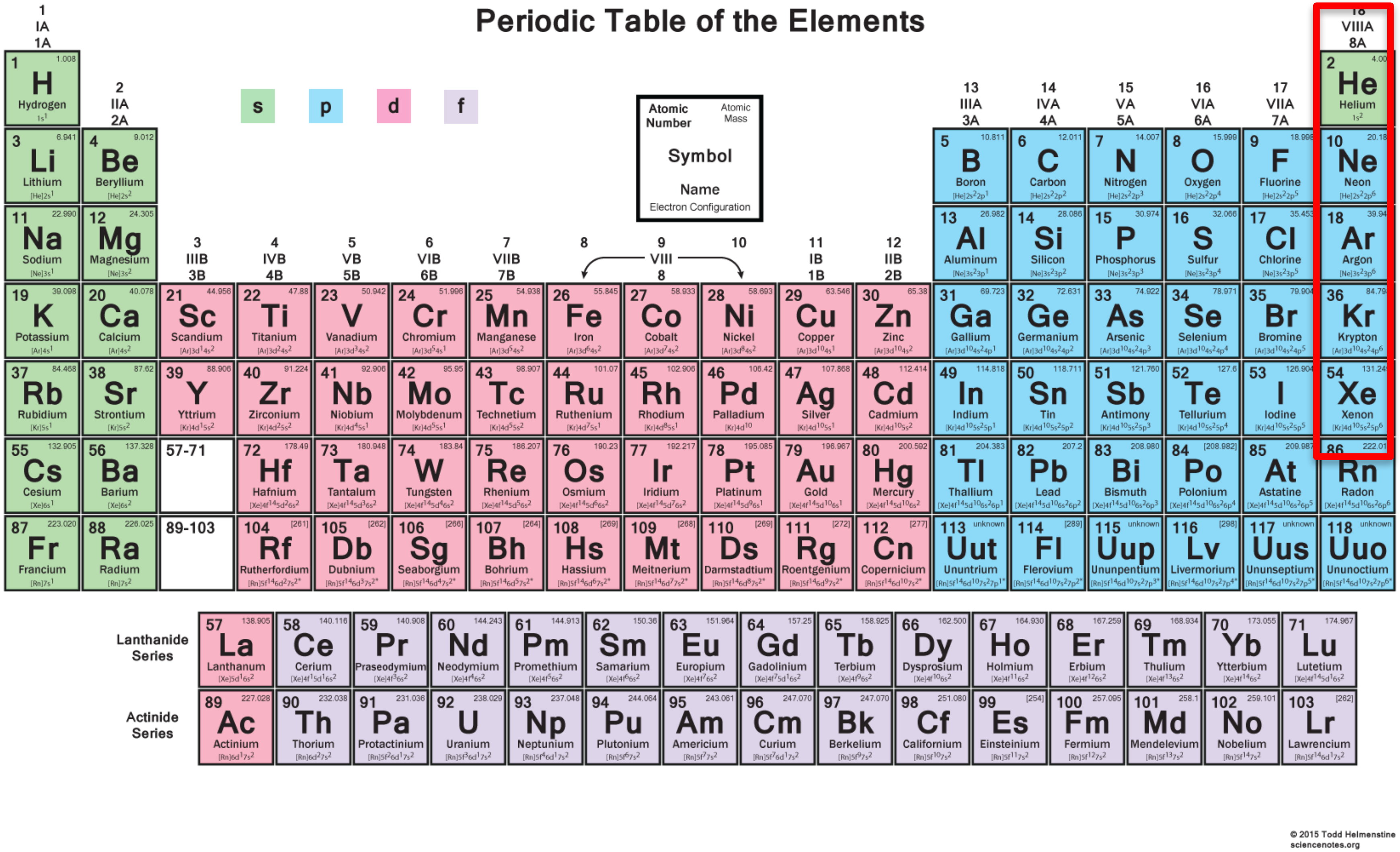
Attractive Potential U_{ATT}



Today's lecture



Periodic Table

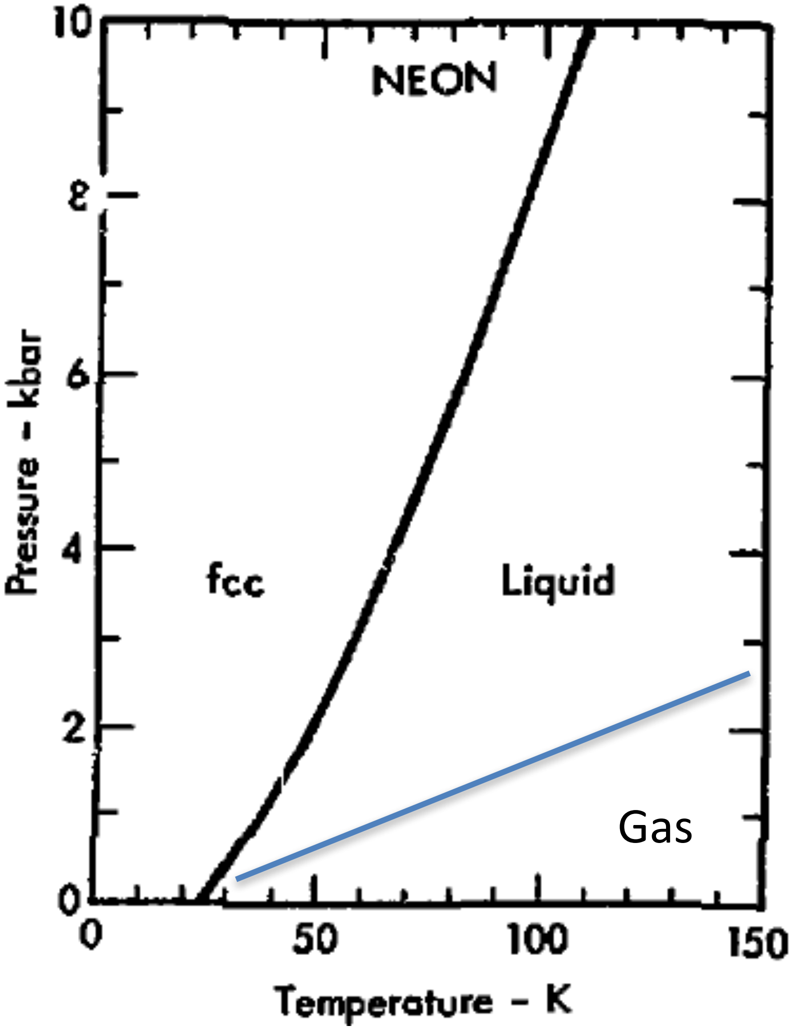


http://sciencenotes.org/periodic-table-showing-shells/

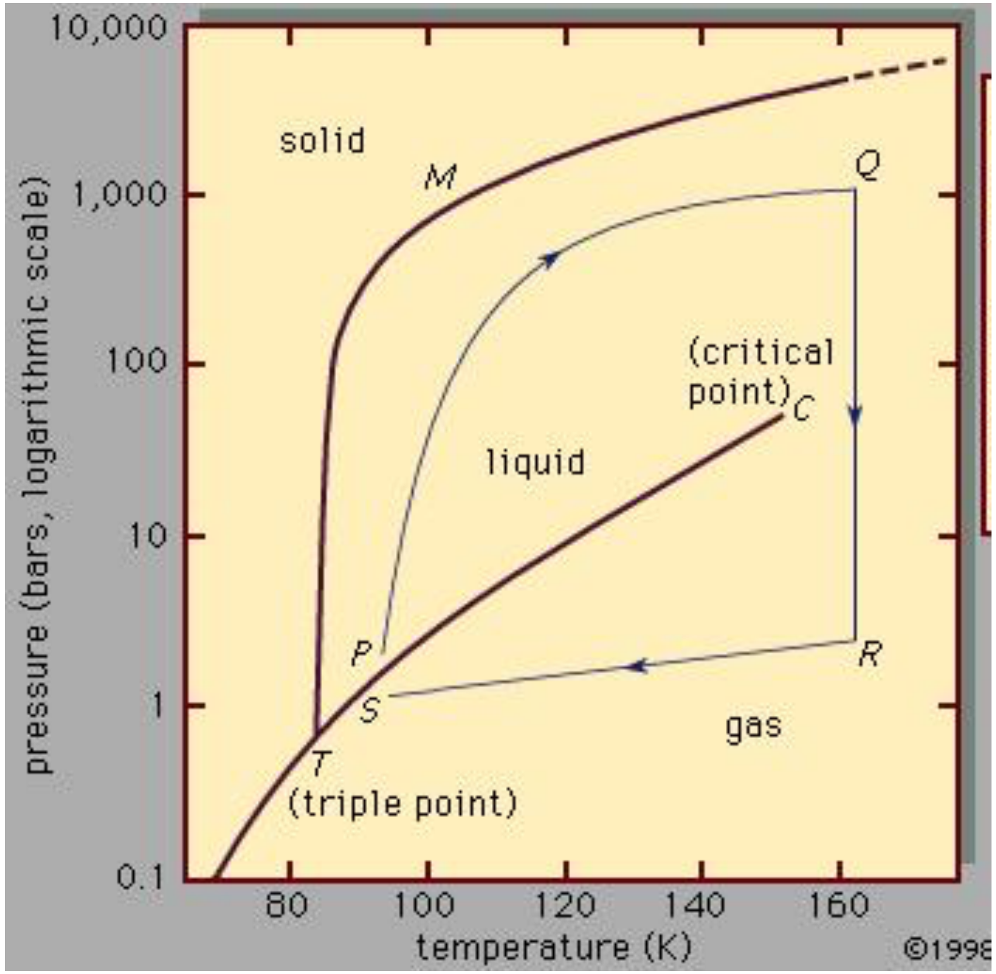
See also table 3 in Kittel.

Phase diagrams:

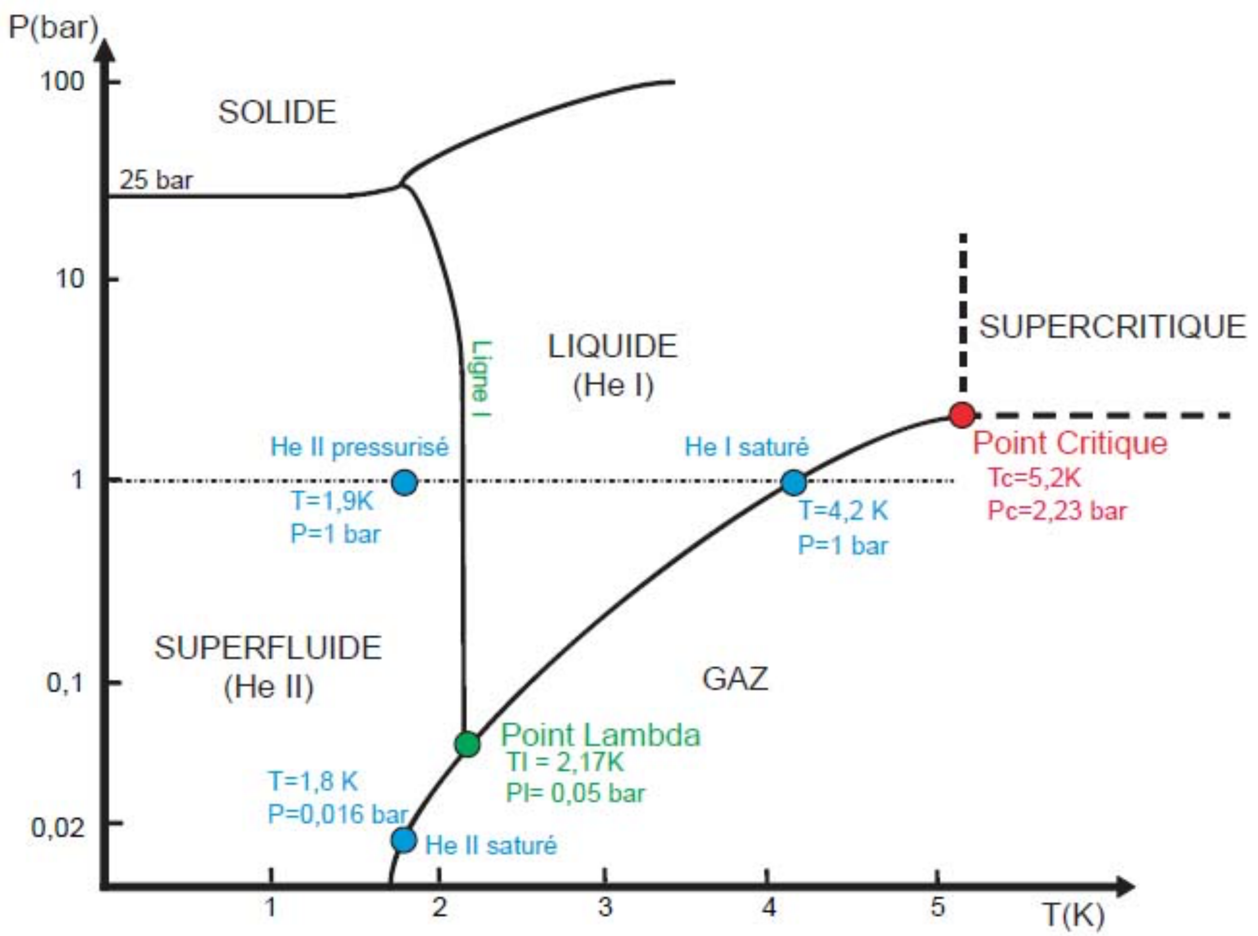
NEON



ARGON

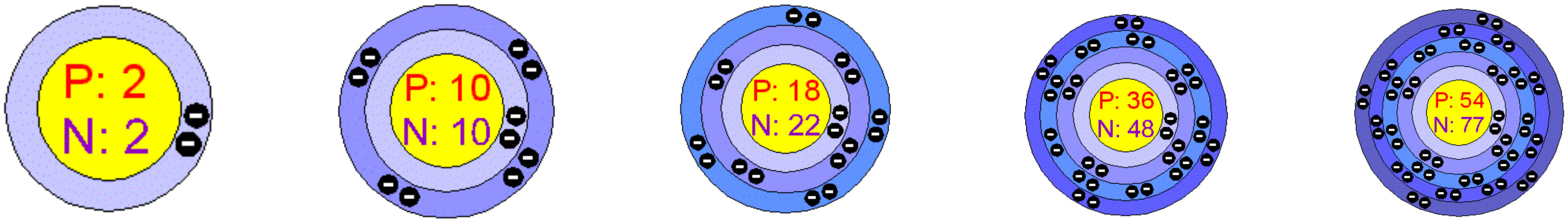


Phase diagram of Helium



Inert gasses

Helium | Neon | Argon | Krypton | Xenon

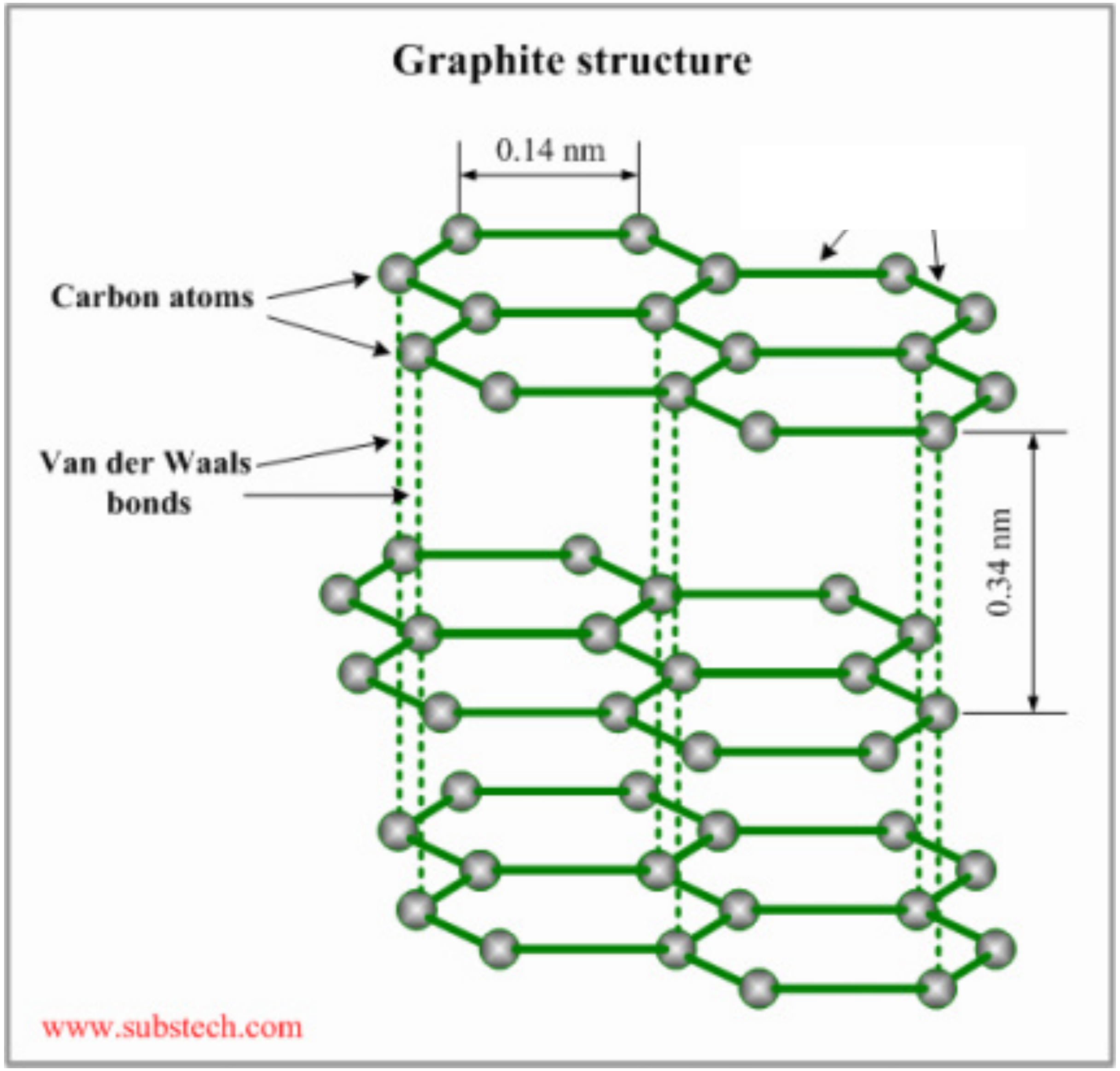


Melting point = 24 K | 84 K | 117 K | 161 K

Questions:

(1) Why are these gasses solidifying in FCC rather than BCC?
(2) What are the “glue” that binds these atoms together in the solid form?
(3) Why are the melting point rather low?
(4) Why are the inert gasses having different melting points?

Van der Waals bonds



Van der Waals bonds used Gecko’s