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ENR116 Engineering Materials

Module 1 Introduction to Materials

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Atomic structure

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Intended Learning Outcomes

At the end of this section, students will be able to:-

- Identify the two atomic models and their differences.
- Describe the principle components of atomic structure.
- Describe the electronic structure of elements using quantum numbers.

The intended learning outcomes from this presentation are to be able to identify the two atomic models and their differences, describe the principle components of atomic structure and the electronic structure of elements using quantum numbers.

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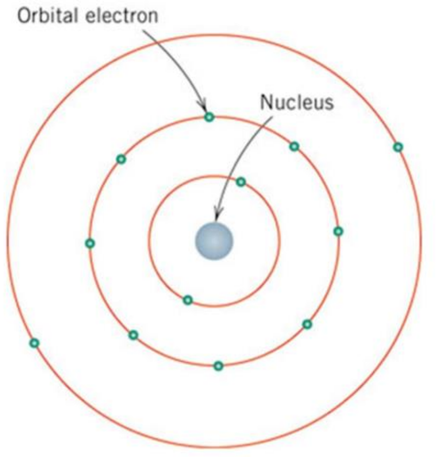
Atomic Structure

Atom:

Protons, Neutrons } 1.67×10^{-27} kg

Electrons – 9.11×10^{-31} kg

Fig. 2.01 *Callister & Rethwisch 8e.*



Electrons are negatively charged

Protons are positive

Neutrons carry no charge

Materials are made out of atoms. The atoms are made of small particles such as neutrons and electrons that revolve around a nucleus. The nucleus itself is made of even smaller particles which are the protons and the neutrons. These particles are very, very small, so you can see here that the mass of the protons and the neutrons is 1.67×10^{-27} kg and the electrons are even smaller or lighter and their mass is 9.11×10^{-31} kg. The number of protons in the nucleus is equal to the number of electrons. The electrons are negatively charged and the protons positively charged. The neutrons have no charge and are neutral. So the nucleus of the atom is positively charged and the electrons are negatively charged, but since the number of electrons is the same as the number of protons, the atom is electrically neutral.

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Atomic Structure

Atomic number: (Z) = number of protons in nucleus of atom
(= number of electrons)

Atomic mass: (A) = the sum of the masses of protons (Z) and neutrons (N) within the nucleus

Atomic weight: the weighted average of the atomic masses of the atom's naturally occurring isotopes

Isotope: an atom where number of protons ≠ number of neutrons

Now, the atomic number is equal to the number of protons in the nucleus of an atom. The atomic mass on the other hand will be the sum of the masses of the protons and the neutrons within the nucleus, so A will be equal to Z plus N. The atomic weight of an element will be the weighted average of the atomic masses of the atom's naturally occurring isotopes. An isotope is an atom where the number of protons is different to the number of neutrons.

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Atomic Structure

Atomic mass unit:

$[A]$ = amu = 1/12 mass of ^{12}C.

Mole:

In one mole of a substance there are 6.023×10^{23} atoms or molecules

Avogadro's number, N_A:

Equal to 6.023×10^{23} atoms or molecules

The measure for the atomic mass and atomic weight is the atomic mass unit or AMU, which is 1/12th of the mass of carbon 12, and one atomic mass unit/atom is equal to one g/mole where 1 mole of a substance equals 6.023×10^{23} atoms or molecules, and this is known as the Avogadro Number.

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Electronic Structure

Bohr Atomic Model: Electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital.

Quantum-mechanical Principles:

Electrons are permitted to have only specific values of energy.

Electron energies are associated with *energy levels or states.*

Electrons can change energy level but this needs to be associated with absorption or emission of energy.

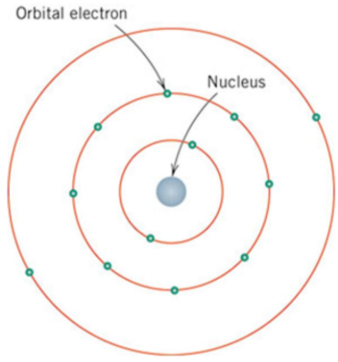

Fig. 2.01 *Callister & Rethwisch 8e.*

So, how are the electrons distributed around the nucleus? Late in the 19th Century scientists realised that some of the properties of the electrons and the behaviour of the electrons could not be explained by the classic mechanical principle, which led to the development of a new set of rules and principles called ‘quantum mechanics’. It was the scientist Niels Bohr who first proposed this model and he stated that electrons revolve around the nucleus, shown here, in discrete orbitals, and further, that the position of any particular electron is more or less defined in terms of an orbital. So the electrons will revolve around the nucleus, as the planets around the sun. Bohr stated a few important quantum mechanical principles where the electrons are permitted to have only specific values of energy. The electron energy is associated with energy states or energy levels. The electrons can change energy level but this needs to be associated with the absorption or emission of energy.

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Electronic Structure

Wave-mechanic Model: Electrons have wave-like and particulate properties.

Electrons are in orbitals defined by a probability.

Every electron is characterised by four quantum numbers

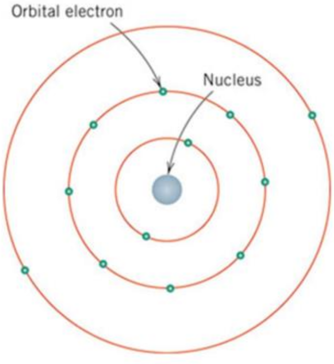

Fig. 2.01 *Callister & Rethwisch 8e.*

Later it was discovered that the Bohr model could still not explain all the behaviour of electrons which led to the development of another model known as the Wave Mechanical Model. In this model the position of the electron is not defined by a specific orbital but it is defined by the probability to find the electron somewhere around the nucleus. Additionally the position of the electron could be defined by four quantum numbers.

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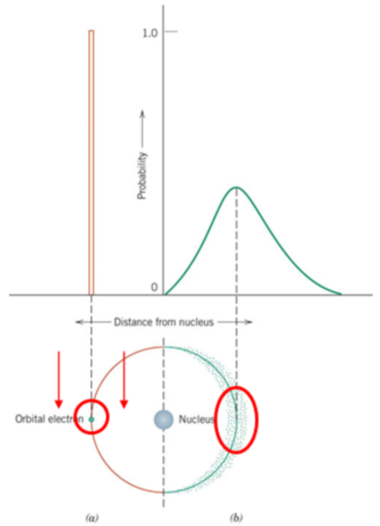
Electronic Structure

Comparison between

Wave-mechanical model

and

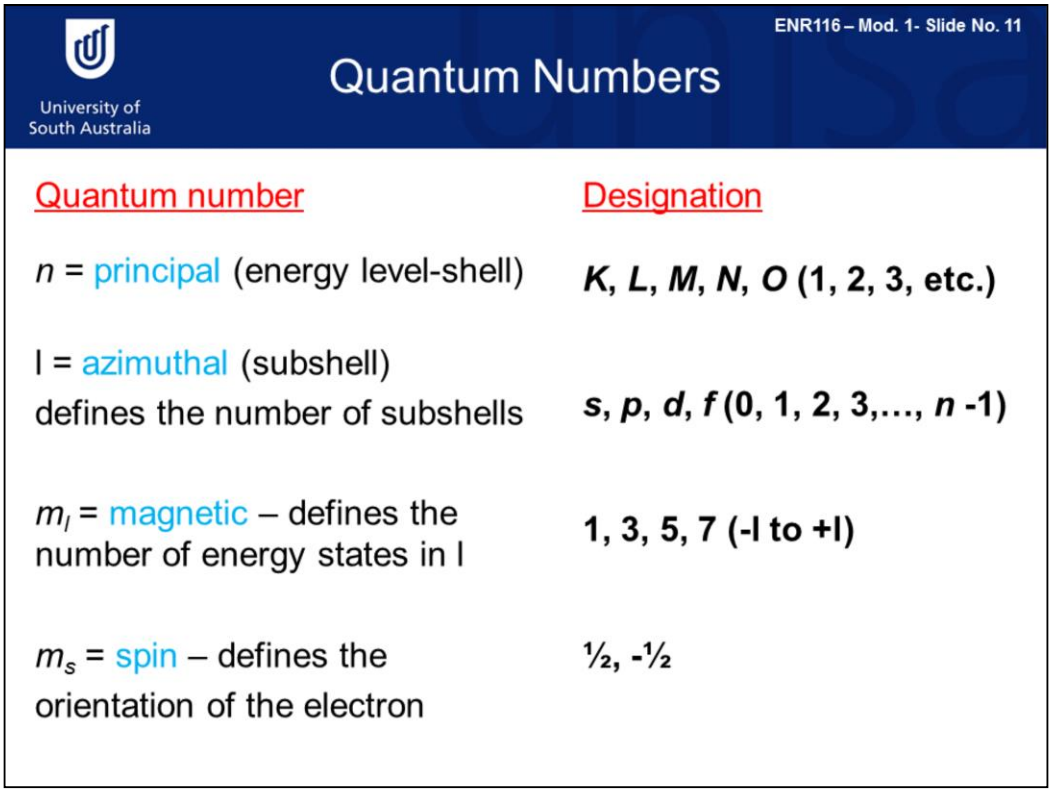
Bohr atomic model



Bohr atomic model   Wave-mechanical model

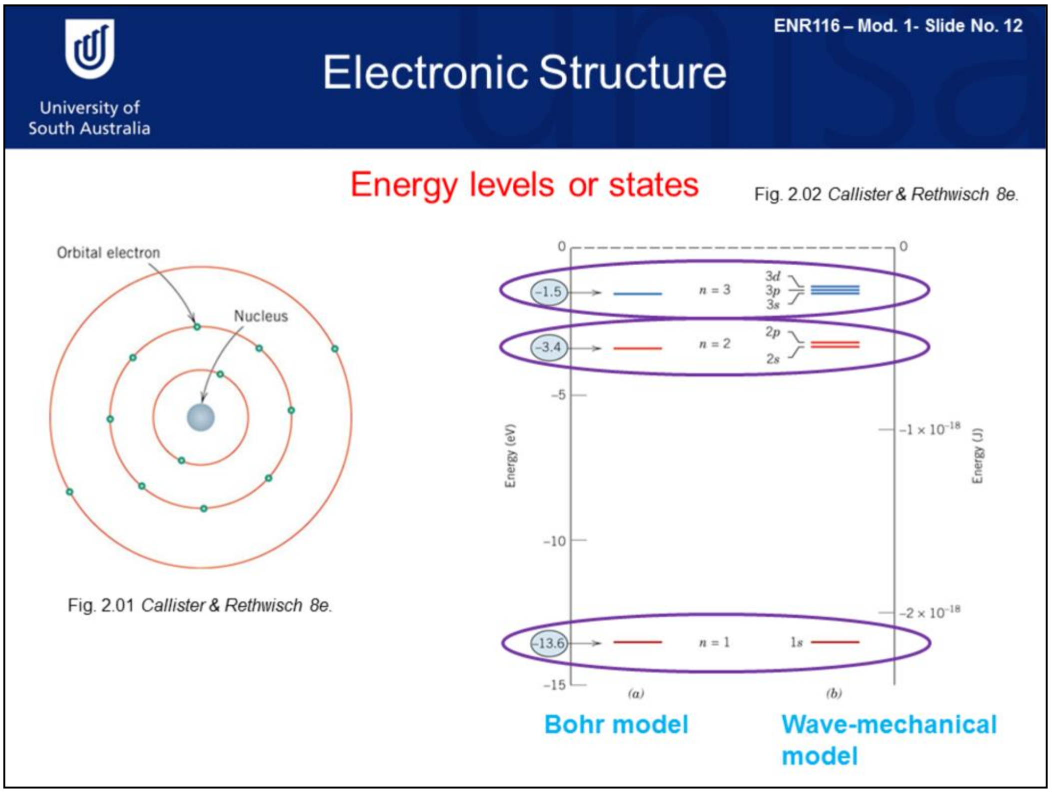
Fig. 2.03 *Callister & Rethwisch 8e.*

Let’s compare both models. For the Bohr model the electron is fixed here, at a particular distance from the nucleus. By comparison in the wave mechanical model the electron can be found somewhere here; so this is the probability to find the electron somewhere here, like the green dots.

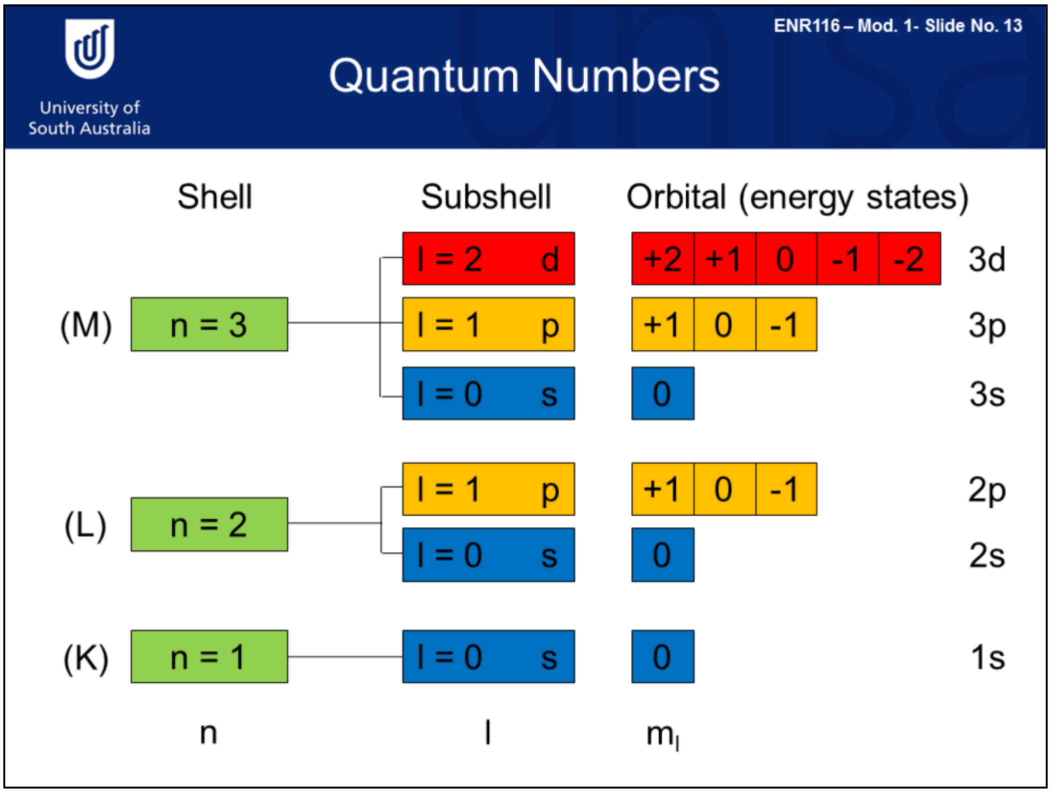


These quantum numbers are as follows. The principal quantum number is n which defines the energy level or shell. The designation of these energy levels are the capital letters K, L, M, N, O. l will be azimuthal quantum number which will define the electron subshells and the number of these subshells. The designation of the subshells will be the small letters s, p, d, f and the number of these subshells will be n, the principal quantum number, minus 1.

The third quantum number is the magnetic quantum number which defines the number of energy states in a particular subshell. This quantum number may have values of -l to +l and will therefore be 1 or 3 or 5 and so on. The final, forth quantum number is the spin of the electron or the orientation of the electron and this can only have values of plus ½ or minus ½.



Let's consider some models; so the first shell is here and the Bohr model and the wave mechanical models are roughly the same, so there is only one energy shell. Then the first shell, the K shell or n the principal quantum number of 1 will be the lowest energy, so it will be closest to the nucleus. The second shell will have a higher energy and according to the Bohr model will be only a single shell, but according to the wave mechanical model it will have two subshells with 2s and 2p. Then the third shell will have two subshells in addition to the 3s shell, the 3p and 3d.



So let's consider this from the quantum mechanics perspective. This is the first quantum number K, the principal quantum number. Now the subshells, we have n=1 so there are zero subshells, or subshell zero. Now the spacing on this subshell zero will be defined by the third quantum number m, which has a value of -l to +l, so that's zero. Hence, there is only one orbital or energy state.

As we move to a principal quantum number of 2, the second shell or l shell, there is one additional subshell. The subshell values can be zero and 1, the s and p subshells. They are designated as 2s and 2p. The principal quantum number m will define the energy state, so on the l=zero subshell there will be only one state, zero. On the subshell which is designated 1 there will be three energy states or +1, zero and -1. On the third shell or the m shell we have a principal quantum number of 3 and so there are three subshells; zero, 1 and 2. These will, in turn, have 1, 3 and 5 energy states.

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How many orbitals are in the N-shell, n=4?

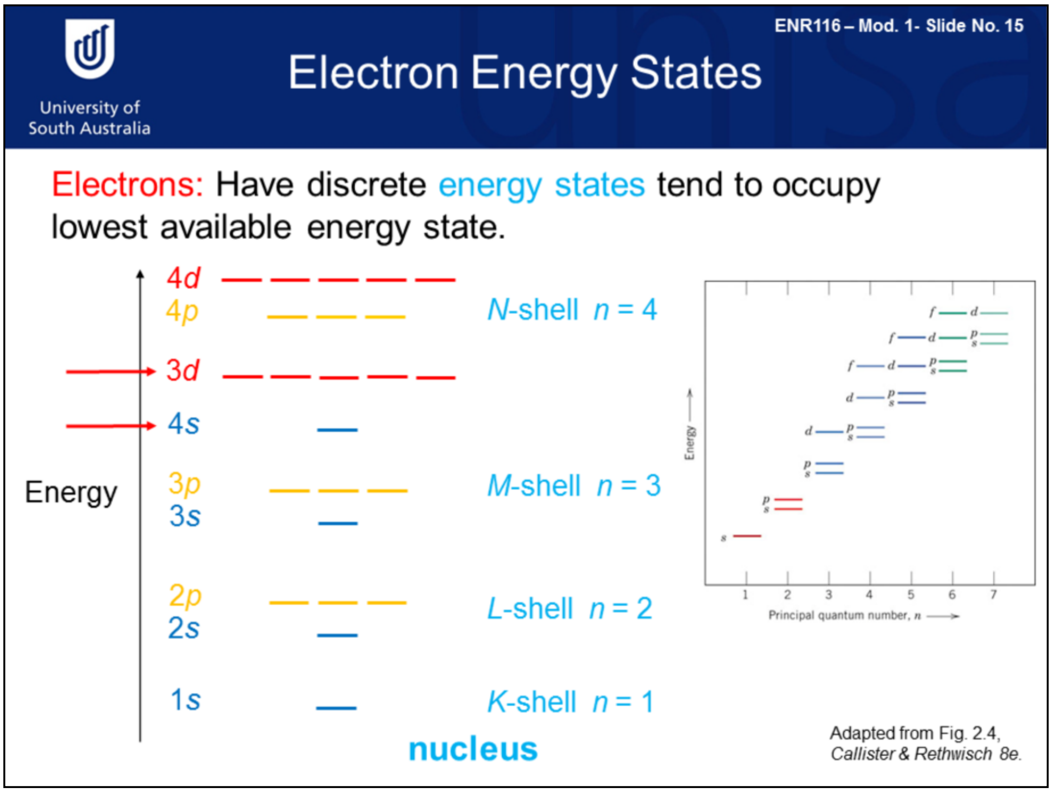
If n=4 there are four subshells **l** = 0, 1, 2, 3

One ***s*** orbital	0							4s
Three ***p*** orbitals	+1	0	-1					4p
Five ***d*** orbitals	+2	+1	0	-1	-2			4d
Seven ***f*** orbitals	+3	+2	+1	0	-1	-2	-3	4f

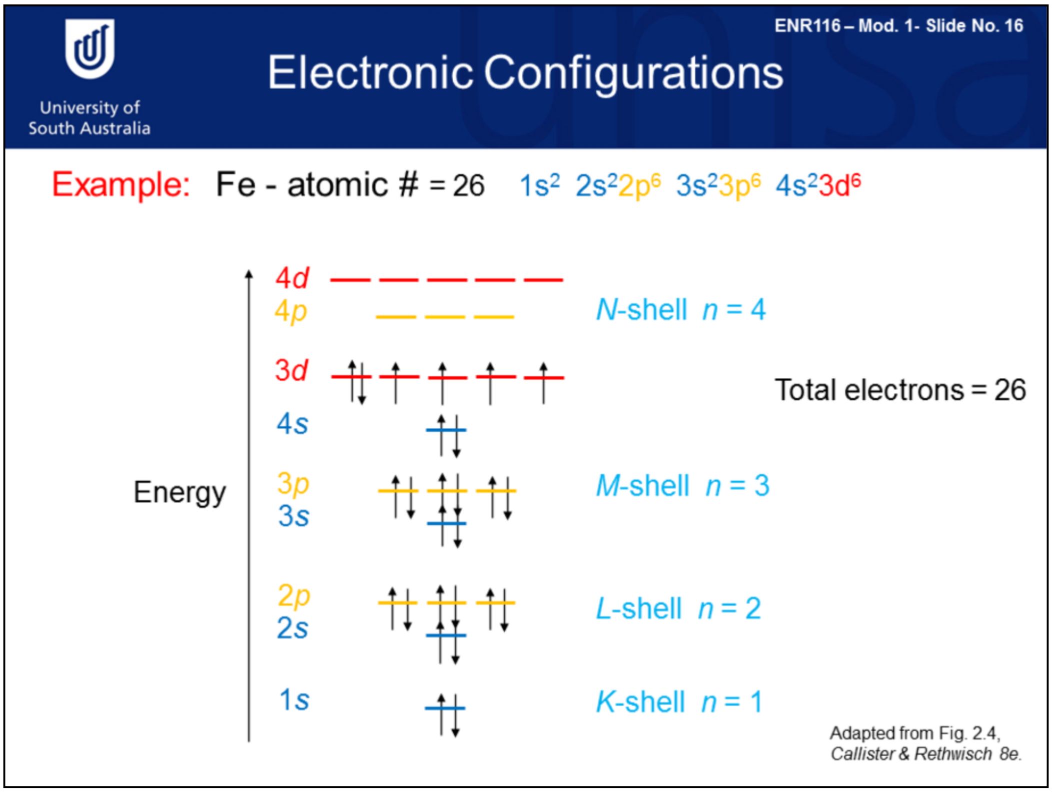
In total there are 16 orbitals

How many orbitals or energy states do we have on the n shell with a principal quantum number of 4?

There are four subshells of zero, 1, 2 and 3. For these subshells there is 1 s orbital, 3 p orbitals, 5 d orbitals and 7 f orbitals. So in total there are 1 plus 3 plus 5 plus 7 orbitals or 16 orbitals.



What energy states do these shells and subshells have? The first shell will have lowest energy and subsequent shells will have higher energies however the differences between these energies will become smaller as the principle quantum number increases. Beyond n = 3 the energy levels of the higher level subshells overlap with those of lower and so the order in which the subshells are filled with electrons becomes discontinuous. For example, the 4s subshell is filled with electrons before the 3d subshell.



How do electrons populate the subshells? Well - the Pauli exclusion principle says that each energy state can hold only two electrons with opposite spins. Let's look at the electronic configuration of iron which has 26 electrons. These electrons start by occupying the lowest energy states and continue occupying energy states with increasing energy until there are no more electrons. Where there are subshells with the same energy the electrons occupy an unpaired position prior to pairing-up.

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Quantum Numbers

Quantum number	Designation
n = principal (energy level-shell)	K, L, M, N, O (1, 2, 3, etc.)
l = azimuthal (subshell)	s, p, d, f (0, 1, 2, 3,…, n -1)
m_l = magnetic	1, 3, 5, 7 (-l to +l)
m_s = spin	½, -½

Table 2.1 The Number of Available Electron States in Some of the Electron Shells and Subshells

Principal Quantum Number n	Shell Designation	Subshells	Number of States	Number of Electrons: Per Subshell	Number of Electrons: Per Shell
1	K	s	1	2	2
2	L	s	1	2	8
		p	3	6	
3	M	s	1	2	18
		p	3	6	
		d	5	10	
4	N	s	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

Table 2.1 *Callister & Rethwisch 8e.*

This table summarises the quantum numbers and shows that for each shell there are a maximum number of electrons for the shell to be completely filled. For the first shell this number is 2, for the second 8 and so on. The number of electrons in the outermost shell is very important since it is these electrons which will participate in chemical reactions and be involved with any bonding between atoms. These electrons are known as the valence electrons.

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Electron Configurations

Valence electrons: Those that occupy the outermost shell

Filled shells are more stable

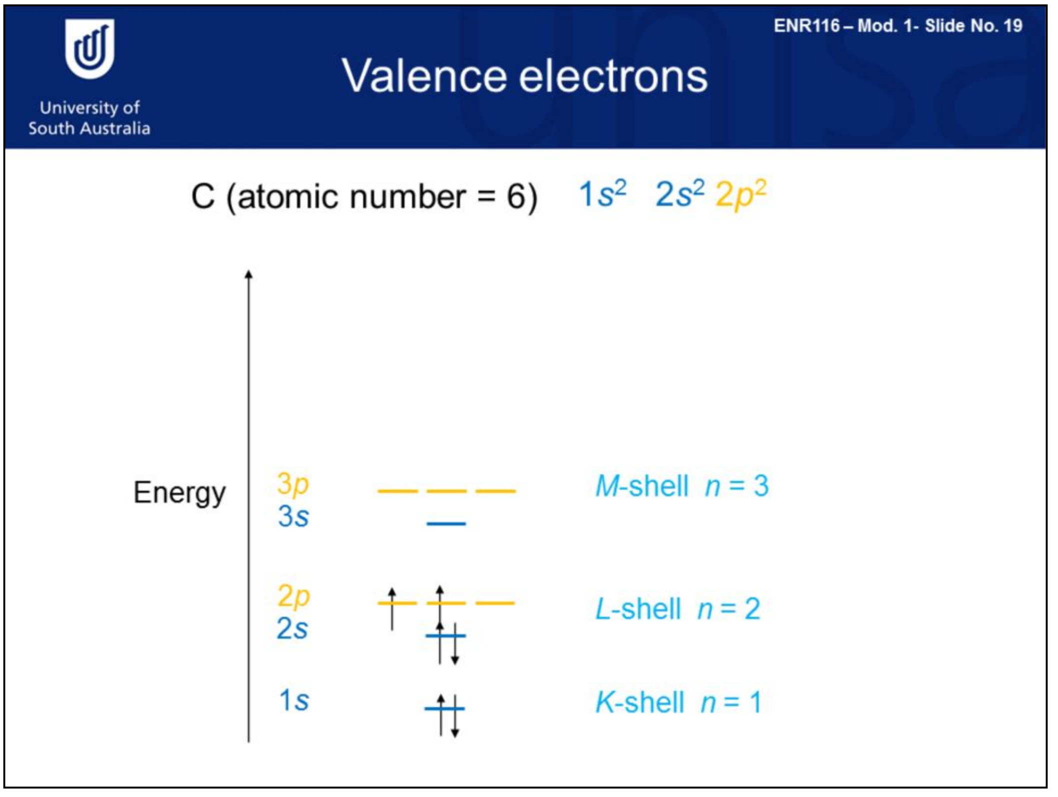
Valence electrons are most available for bonding and tend to control the chemical properties

– example: C (atomic number = 6)

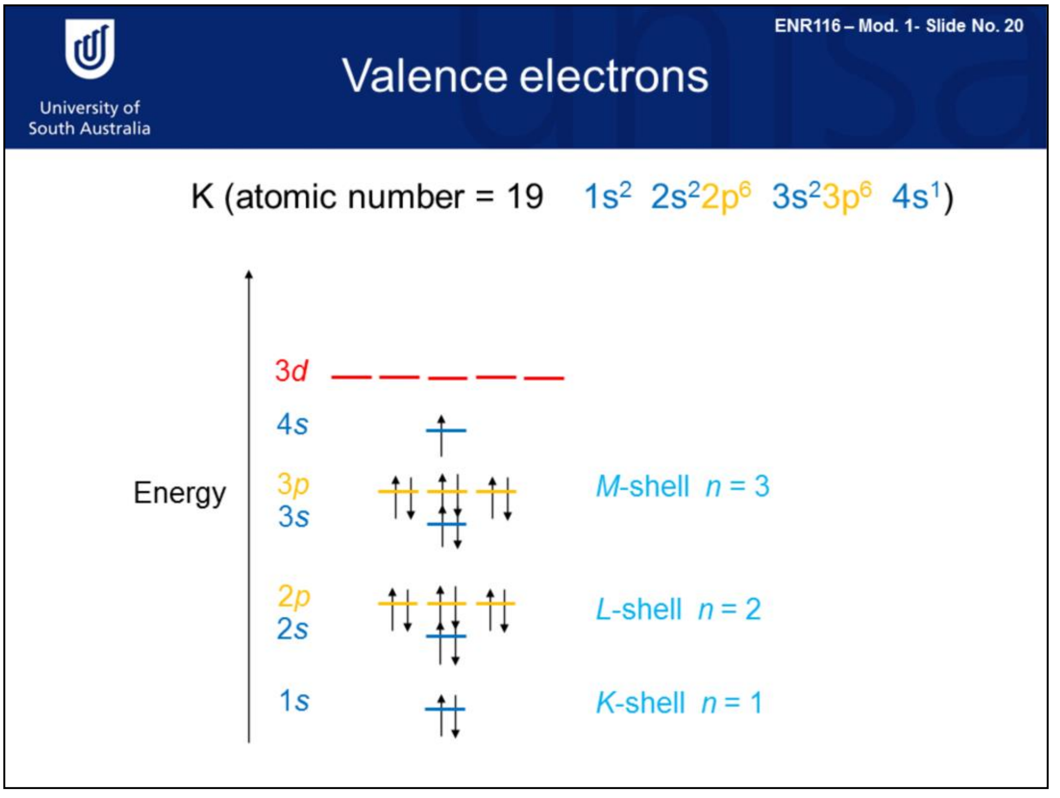
$1s^2 \; \boxed{2s^2 \; 2p^2}$

valence electrons

For example here is the electron configuration of carbon. Carbon has an atomic number of 6 with 6 electrons – 2 in the 1s subshell which is the complete 1s level, 2 in the 2s subshell and 2 in the 2p subshell. So, the 4 electrons of the 2s and 2p subshell are the valence electrons and carbon has a valence number of 4.



Diagrammatically we can see here how the subshells are occupied for carbon. The K-shell is complete and there are 4 electrons in the L-shell; 2 in the complete 2s subshell and 2 in the partially filled 2p subshell.



By comparison potassium has 19 electrons. We can see these diagrammatically with the lone valence electron in the 4s subshell.

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Survey of elements

Most elements: Electron configuration not stable.

Why? Valence (outer) shell usually not filled completely.

Table 2.2 A Listing of the Expected Electron Configurations for Some of the Common Elements[a]

Element	Symbol	Atomic Number	Electron Configuration
Hydrogen	H	1	$1s^1$
Helium	He	2	$\boxed{1s^2}$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 \boxed{2s^2 2p^6}$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 \boxed{3s^2 3p^6}$
Potassium	K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium	Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium	Sc	21	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
Titanium	Ti	22	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Vanadium	V	23	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
Chromium	Cr	24	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Manganese	Mn	25	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$
Iron	Fe	26	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
Cobalt	Co	27	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
Nickel	Ni	28	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
Copper	Cu	29	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
Zinc	Zn	30	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
Arsenic	As	33	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$
Selenium	Se	34	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$
Bromine	Br	35	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$
Krypton	Kr	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \boxed{4s^2 4p^6}$

Adapted from Table 2.02, *Callister & Rethwisch 8e.*

If we look at a table of the elements and their electronic configurations we can see that most are unstable since they do not have a filled outermost shell. The elements helium, neon, argon and krypton outlined in blue are stable as they all have completely filled shells. These then are known as the inert gases as they are unlikely to participate in chemical reactions. The other elements all have unfilled outermost shells and undergo chemical reactions in order to gain a filled outermost shell.

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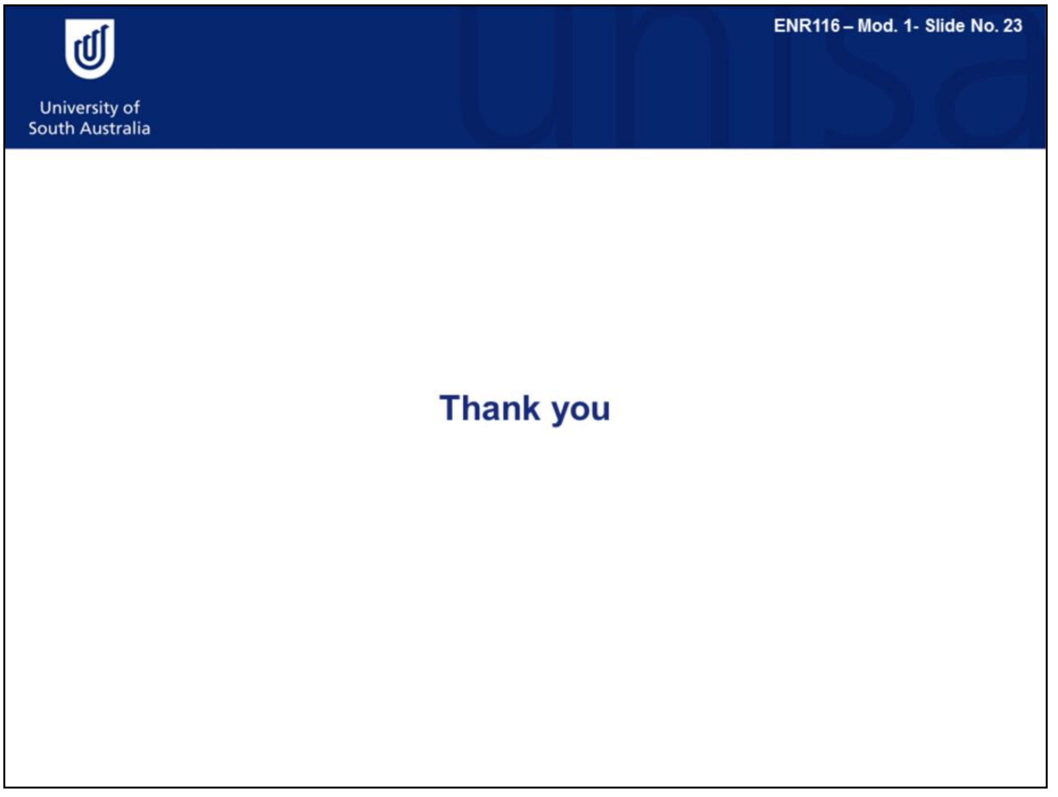
Summary

- In describing atomic structure there are two models which differ in how electrons are described.
- Electron energies can only have specific values.
- The four quantum numbers are used to specify electrons

In summary there are two models describing the atomic structure of materials. Whilst, the models differ in their description of electrons and electronic structure they both agree that electrons can only have specific energies. The wave-mechanical model describes the electronic structure of an atom using quantum numbers to identify a specific electron.



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