

# Schottky Defect and Structures and Physical Properties of Period 3 Elements

## Schottky Defect

Lattice structures are not perfect; in fact most of the time they experience defects. Lattice structures (or crystals) are prone to defects especially when their temperature is greater than 0 K [1]. One of these defects is known as the Schottky defect, which occurs when oppositely charged ions vacant their sites [1].

## Introduction

Like the human body, lattice structures (most commonly known as crystals) are far from perfection. Our body works hard to keep things proportional but occasionally our right foot is bigger than our left; similarly, crystals may try to arrange its ions under a strict layout, but occasionally an ion slips to another spot or simply goes missing. Realistically speaking, it should be expected that crystals will depart itself from order (not surprising considering defects occurs at temperature greater than 0 K). There are many ways a crystal can depart itself from order (thus experiences defects); these defects can be grouped in different categories such as Point Defects, Line Defects, Planar Defects, or Volume or Bulk Defects [2]. We will focus on Point Defects, specifically the defect that occurs in ionic crystal structures (i.e. NaCl) called the Schottky Defect.

## Point Defects

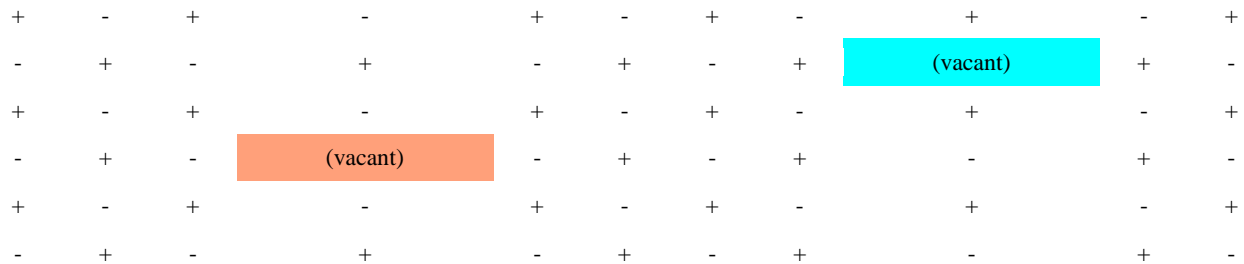
Lattice structures (or crystals) undergoing point defects experience one of two types:

1. atoms or ions leaving their spot (thus creating vacancies) [3].
2. atoms or ions slipping into the little gaps in between other atoms or ions; those little gaps are known as interstitials-- since atoms or ions in the crystals are occupying interstitials, they inherently become (create) interstitials [3].

By the simplest definition, the Schottky defect is defined by type one. For anyone interested, type two is known as the Frenkel defect.

# Schottky Defect

The Schottky Defect is often visually demonstrated using the following layout of anions and cations:



The positive symbols represents cations (i.e. Na<sup>+</sup>) and the negative symbol represents anions (i.e. Cl<sup>-</sup>). In addition, this layout is applicable only for ionic crystal compounds of the formula MX--layout for ionic crystals with formula MX<sub>2</sub> and M<sub>2</sub>X<sub>3</sub> will be discussed later--where M is metal and X is nonmetal. Notice the figure has exactly one cation and one anion vacating their sites; that is what defines a (one) Schottky Defect for a crystal of MX formula--for every cation that vacates its site, the same number of anion will follow suit; essentially the vacant sites come in pairs. This also means the crystal will neither be too positive or too negative because the crystal will always be in equilibrium in respect to the number of anions and cations [3].

It is possible to approximate the number of Schottky defects (n<sub>s</sub>) in a MX ionic crystal compound by using the equation:

$$a) n_s = N e^{-\frac{\Delta H}{2RT}} \quad [3]$$

Where  $\Delta H$  is the enthalpy of defect formation, R is the gas constant, T is the temperature in K, and N can be calculated by:

$$b) N = \frac{\text{density of the ionic crystal compound} \times N_A}{\text{molar mass of the ionic crystal compound}} \quad [3]$$

From equation (a), it is also possible to calculate the fraction of vacant sites by using the equation:

$$c) \frac{n_s}{N} = e^{-\frac{\Delta H}{2RT}} \quad [3]$$

## Schottky defects for MX<sub>2</sub> and M<sub>2</sub>X<sub>3</sub>:

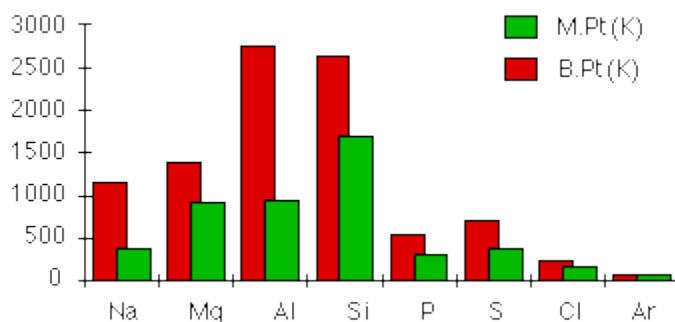
As mentioned earlier, a Schottky defect will always result a crystal structure in equilibrium--where no crystal is going to be too positive or too negative; thus in the case of:

MX<sub>2</sub>: one Schottky defect equals one cation and two anion vacancy [2].

M<sub>2</sub>X<sub>3</sub>: one Schottky defect equals two cation and three anion vacancy [3].

## Structures and Physical Properties of Period 3 Elements

### Melting and boiling points



In a moment we shall explain all the ups and downs in this graph.

### Electrical conductivity

Sodium, magnesium and aluminum are all good conductors of electricity. Silicon is a semiconductor. None of the rest conduct electricity. These trends are explained below.

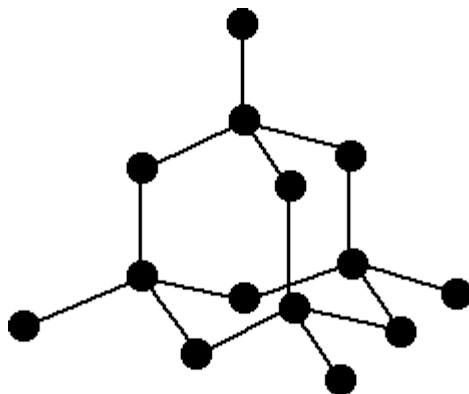
### Three metallic structures

Sodium, magnesium and aluminum all have metallic structures, which accounts for their electrical conductivity and relatively high melting and boiling points. Melting and boiling points rise across the three metals because of the increasing number of electrons which each atom can contribute to the delocalized "sea of electrons". The atoms also get smaller and have more protons as you go from sodium to magnesium to aluminum.

The attractions and therefore the melting and boiling points increase because:

- The nuclei of the atoms are getting more positively charged.
- The sea is getting more negatively charged.
- The sea is getting progressively nearer to the nuclei and so more strongly attracted.

**Silicon - a giant covalent structure**



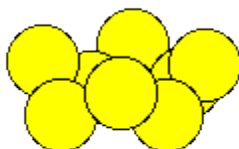
Silicon is a non-metal, and has a giant covalent structure exactly the same as carbon in diamond - hence the high melting point. You have to break strong covalent bonds in order to melt it. There are no obviously free electrons in the structure, and although it conducts electricity, it doesn't do so in the same way as metals. Silicon is a semiconductor.

## Four molecular elements

Phosphorus, sulfur, chlorine and argon are simple molecular substances with only van der Waals attractions between the molecules. Their melting or boiling points will be lower than those of the first four members of the period which have giant structures. The presence of individual molecules prevents any possibility of electrons flowing, and so none of them conduct electricity. The sizes of the melting and boiling points are governed entirely by the sizes of the molecules:



a P<sub>4</sub> molecule



an S<sub>8</sub> molecule



a Cl<sub>2</sub> molecule

Argon molecules consist of single argon atoms.

- **Phosphorus:** There are several forms of phosphorus. The data in the graph at the top of the page applies to white phosphorus which contains P<sub>4</sub> molecules. To melt phosphorus you don't have to break any covalent bonds - just the much weaker van der Waals forces between the molecules.
- **Sulfur:** sulfur consists of S<sub>8</sub> rings of atoms. The molecules are bigger than phosphorus molecules, and so the van der Waals attractions will be stronger, leading to a higher melting and boiling point.
- **Chlorine:** Chlorine, Cl<sub>2</sub>, is a much smaller molecule with comparatively weak van der Waals attractions, and so chlorine will have a lower melting and boiling point than sulfur or phosphorus.
- **Argon:** Argon molecules are just single argon atoms, Ar. The scope for van der Waals attractions between these is very limited and so the melting and boiling points of argon are lower again.