3.091: Introduction to Solid State Chemistry
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Recitation 1

1 Balancing reactions

A *chemical reaction* involves rearranging elements in compounds to make different substances. They are usually written as a sum of *reactants*, which when combined yield a sum of *products*:

$$A + B \rightarrow C + D$$

Here, A, B, C, and D represent chemical compounds. The fundamental principle guiding the process of balancing a reaction is *conservation of mass*: a chemical reaction cannot create or destroy mass! This has several implications that can be used to determine whether a reaction is valid:

1. The mass of the reactants must equal the mass of the products
2. Every element that is in a reactant must be in a product
3. The number of each type of atom in the reactants must equal the number of each type of atom in the products

Example: Ethylene and oxygen gas are combined to make water and carbon dioxide. If you start with 4 moles of O_2 gas, how many moles of water and carbon dioxide can you make? The unbalanced equation is given below:

$$C_2H_4 + O_2 \rightarrow CO_2 + H_2O$$

First, we must balance the reaction. One method to do this is by using a table:

	C	H	O	C	H	O
Initial (unbalanced):	2	4	2	1	2	3
Need: even number of oxygens Try: 2 × H_2O on the right	2	4	2	1	4	4
Need: even number of carbons Try: 2 × CO_2 on the right:	2	4	2	2	4	6
Need: more oxygen on the left Try: 3 × O_2 on the left	2	4	6	2	4	6

Once there are the same number of each elements on both sides of the reaction, we're done balancing! The final reaction is

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$$

The greatest common factor between the coefficients in front of each compound is 1, so this is the simplest form.

2 Yield

The *yield* of a reaction is the maximum amount of products that can be made with the reactants that are put in. For example, consider a s'more, which consists of a marshmallow, a piece of chocolate, and two graham crackers. If you had 5 marshmallows, 4 pieces of chocolate, and 6 graham crackers, you could make 3 full s'mores (with 2 extra marshmallows and 1 extra marshmallow). We combine chemical compounds in the same way!

Example: Ammonia (NH_3) is produced when nitrogen gas (N_2) is combined with hydrogen gas (H_2). Write a balanced equation for this reaction, and determine how much ammonia can be produced if you start with 5 moles of hydrogen gas.

First, let's balance the reaction. We can try some coefficients by inspection and verify they satisfy conservation of mass:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

This balanced reaction tells us that for every three moles of H_2 gas, we can make two moles of ammonia. Therefore, if we start with 5 moles of H_2:

$$5 \text{ moles of } H_2 \times \frac{2 \text{ moles of } NH_3}{3 \text{ moles of } H_2} = 3.33 \text{ moles of } NH_3$$

3 Limiting reagents

If we don't start with the right stoichiometric ratios of reagents, there might be some reactant left over after we have formed the products. If we go back to the s'mores example, we were able to make three full s'mores, with extra chocolate and marshmallow. Since all of the graham crackers were used before the other reactants, they are the *limiting reagent*. The limiting reagent is specific to the initial amount of reactants available.

Example: The Kroll process for making titanium metal out of titanium chloride is:

$$\text{TiCl}_4 + \text{Mg} \rightarrow \text{MgCL}_2 + \text{Ti}$$

You react 25kg of Mg with 200kg of $TiCl_4$.
a) Balance the reaction, b) determine the limiting reagent, and c) determine the yield of Ti in this reaction.

a) To balance the reaction, we can start by looking at the Cl atoms: we need to double the $MgCl_2$ on the right to equal the left. Then, we just need to balance the Mg atoms: we need double on the right to account for the extra we just created on the left. The balanced reaction is therefore

$$TiCl_4 + 2Mg \rightarrow 2MgCl_2 + Ti$$

b) To find the limiting reagent, we need to find the molar mass of the reactants:

$$TiCl_4\text{: } 47.87 + 4 \times 25.45 = 189.7 g/mol$$

$$Mg\text{: } 24.3 g/mol$$

Next, we can convert from grams to moles:

$$200 \text{ kg } TiCl_4 \times \frac{1000 \text{ g } TiCl_4}{1 \text{ kg } TiCl_4} \times \frac{1 \text{ mol } TiCl_4}{189.7 \text{ g } TiCl_4} = 1054 \text{ mol } TiCl_4$$

$$15 \text{ kg Mg} \times \frac{1000 \text{ g Mg}}{1 \text{ kg Mg}} \times \frac{1 \text{ mol Mg}}{24.3 \text{ g Mg}} = 1029 \text{ mol Mg}$$

The balanced reaction tells us we need twice as many moles of magnesium as moles of titanium chloride. We don't have enough Mg to react with all of the $TiCl_4$, so Mg is the limiting reagent.
c) The yield is determined by the initial amount of the limiting reagent. The balanced reaction tells us we get two moles of $MgCl_2$ and 1 mole of Ti per mole of Mg we react, so the yield is

$$1029 \text{ mol Mg} \times \frac{1 \text{ mol Ti}}{2 \text{ mol Mg}} \times \frac{47.87 \text{ g Ti}}{1 \text{ mol Ti}} = 24.7 \text{ kg of Ti}$$

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