Concentration units (density, ppm, ppb, molarity)

In Solids (Solid-state Photonics)

- *Atonic concentration (Number density)*

The atomic concentration (number density) N (in SI units of m^{-3}, however, most of the publications use more practical units [cm^{-3}]) is one of the frequently used concentration units used in solid-state photonics. The use of number density N_t results in the simplest form for photonics related applications sus as : Rate Equations describing laser dynamic or absorption properties. For example, a transmission T_0 (attenuation) of the light propagated through the sample with thickness, L could be calculated using *Beer-Lambert-Bouguer law*.

$$T_0 = exp(-\sigma_{ab}NL)$$

, where, σ_{ab} is absorption cross-section (in this equation we neglect possible reflection from the sample surfaces for simplicity). Usage of another concentration unit will result in additional numerical factor in these equations.

The examples below estimate concentration of Zn ions in ZnSe and ZnS crystals:

Parameter	**ZnSe**	**ZnS**
Molar mass (m_μ)	65.38(Zn)+ 78.96(Se)=144.3 g/mol (ZnSe)	65.38(Zn)+ 32.06(S)=97.445 g/mol (ZnS)
Density (ρ)	5.27 g/cm³	4.09 g/cm³
Molar volume $V_\mu=m_\mu/\rho$	(144.3 g/mol):(5.27 g/cm³)=27.4 cm³	(97.445 g/mol): (4.09 g/cm³)=23.825 cm³
Zn concentration $N_{zn}=N_a/V_\mu$	(6.022×10^{23}atom/mol):(27.4 cm³)=$2.20x10^{22}$ cm^{-3}	(6.022×10^{23}atom/mol):(23.825 cm³)=$2.53x10^{22}$ cm^{-3}
	Diamond	**Yttrium Aluminum Garnet ($Y_3Al_5O_{12}$)**
Molar mass (m_μ)	12.01 g/mol	593.6180 g/mol
Density (ρ)	3.5 g/cm³	4.55 g/cm³

Molar volume $V_{\mu}=m_{\mu}/\rho$	(12.01 g/mol):(3.5 g/cm³)=3.43 cm³	(593.6180 g/mol):(4.55 g/cm³)=130.46 cm³
C concentration $N=N_a/V_{\mu}$	(6.022×10^{23}atom/mol):(3.43 cm³)=$1.8\text{x}10^{23}$ cm^{-3} [C]	($3\times6.022\times10^{23}$atom/mol):(130.46 cm³)=$1.38\text{x}10^{22}$ cm^{-3} [Y]

- *Ratio units in solids (%, ppm, ppb)*

Ratio units (such as percent (%), ppm (parts per million), ppb (part per billion)) require additional clarification. It could be a fraction of weight, or fraction of volume, molar ratio, or atomic ratio. Unfortunately, this clarification is missing often even in scientific publications.

For example, the ppm usually means fraction by weight in solids, because a total mass of the sample could be easy to measure, and it does not require knowledge of sample composition or volume (which is difficult to measure for bulk solids). For soil, 1 ppm_m is equal to 1 mg of the contaminant in 1 kg of solids, and 1

ppb_m is 1 ug/kg. However, the 1 ppm concentration of color centers (or impurity) in diamond is usually defined as an atomic ratio to C atom without any notes in the many publications. The using carbon concentration in the diamond, the 1 ppm_{at} could be calculated as ~$1.8\text{x}10^{17}$ cm³ (see Table above)

Similarly, an atomic percent (at.% gives the percentage of one kind of atom relative to the total number of atoms) could be confused atomic ratio (a measure of the ratio of atoms of one element A to another element B) in the complex crystals. For example, Rare-Earth (Nd, Ho, Tm, Er) doped materials are the most frequently used as an active media for solid-state lasers. In the crystals, based Yttrium compound (such as YAG, YAP, LYF), the rare-earth atoms substitute yttrium in the crystal structure. As a result, most of the authors and manufacturers use "at %" units without notice that it is an atomic ratio to yttrium ions. For example, Er(50%):YAG crystal is a crystal where 50% of yttrium is substituted by erbium ions. It is the typical concentration for flash-lamp pumped laser with an oscillation wavelength at 2.94 µm. The correlation between atomic ratio and density for some important solid state gain media are summarized in the table below.

Since "ratio units" notation often does not state which quantity is used, it is better to write the unit as µg/kg, or nmol/mol, even though they are dimensionless.

Crystal	at, %	Density
RE:$Y_3Al_5O_{12}$ (Yttrium Aluminum Garnet, YAG)	1%	1.38×10^{20} cm^{-3}
RE:$LiYF_4$ (YLF)	1%	1.4×10^{20} cm^{-3}
RE:YAl_2O_3 (Yttrium Aluminum Perovskite, YAP)	1%	2×10^{20} cm^{-3}
Ti:Al_2O_3 (Sapphire)	0.035%	1.7×10^{19} cm^{-3}
Cr:Al_2O_3 (Ruby)	0.067%	3.16×10^{19} cm^{-3}
Cr:$BeAl_2O_4$ (Alexandrite)	0.05%	1.8×10^{19} cm^{-3}
Cr(Fe):ZnSe	0.1%	$2.20x10^{19}$ cm^{-3}
Cr(Fe):ZnS	0.1%	$2.53x10^{19}$ cm^{-3}

in Liquids

Aqueous solutions (solution in which the solvent is water) are widely used in scientific and environmental studies. The water density at normal ambient conditions is closed to 1 mg/mL or 1kg/L, therefore 1 ppm ≈ 1 mg/L of a contaminant in water, and 1 ppb = 1 ug/L. However, you cannot use these relations if the solvent density is not 1 mg/mL.

- Molarity

The molarity (M) of a solution is the number of moles of solute dissolved in one liter of solution [mol/L].

Ratio Units in Gases

The common units of concentration of volatile components in the air(gases) are *volume mixing ratios*: ppm_v, ppb_v. These units express the concentration of a pollutant as the ratio of its volume, to the volume of the air(gases) in which it is contained at the same pressure and temperature. Ideal gas laws assume that this ratio does not dependent upon temperature and pressure as it effects on both the pollutant and the air to the same extent.

Another common unit is mass per unit volume, where mass is usually measured in µg(mg) and volume in cubic meter [m^3]. This concentration in these units depends on the pressure and temperature of the sample. Usually, conversions for chemicals in the air are made assuming a pressure of 1 atmosphere (101.325 kPa or 1.01325 bar) and a temperature of 25 degrees Celsius (298K). For these conditions, the equations to convert from concentration in parts per million to concentration in milligrams per cubic meter (mg/m³) and inverse relation are as follows:

$$C[ppm_V] = C\left[\frac{mg}{m^3}\right] \times \frac{24.45}{m_\mu} \qquad C\left[\frac{mg}{m^3}\right] = C[ppm_V] \times \frac{m_\mu}{24.45}$$

Using ideal gas law, the above relations could be adopted for varied temperature as follows

$$C[ppm_V] = C\left[\frac{mg}{m^3}\right] \times \frac{(0.082057338 \cdot \mathrm{T})}{m_\mu} \qquad C\left[\frac{mg}{m^3}\right] = C[ppm_V] \times \frac{m_\mu}{(0.082057338 \cdot \mathrm{T})}$$

, where T is temperature in [K].

References

- David N. Nikogosyan "Properties of Optical and Laser-Related Materials: A Handbook" John Wiley & Sons (1997)