SEMI AUX022-0611
CONVERSION OF UNITS FOR IMPURITY CONCENTRATIONS IN SILICON

semi

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1 Introduction

1.1 Concentrations of impurities in Si are frequently given in differing units in SEMI Standards, depending on the subject of the corresponding standard. Impurity concentrations are mainly provided in absolute units of at/cm^3 or relative units such as ppma or ppba, respectively, in specifications, whereas in chemical analytics mainly units of ppmw or ppbw are common.

1.2 Therefore equations for converting the respective units are provided in the following as well as a table illustrating the conversion for common impurity elements in Si as help for users of SEMI Standards.

1.3 The equations provided may also be used for converting concentration units in other substances. Then the atomic mass and specific gravity, respectively, of Si have to be replaced by the appropriate atomic/molecular mass and specific gravity of the substance under investigation.

2 Definitions

2.1 at/cm^3 — atoms per cubic centimeter

2.2 ppba — parts per billion atoms, 1 ppba is a fraction of 1 in 10^9 atoms

2.3 ppbw — parts per billion by weight, 1 ppbw is a fraction of 1 in 10^9 weight units, e.g., 1 ng/g

2.4 ppma — parts per million atoms, 1 ppma is a fraction of 1 in 10^6 atoms

2.5 ppmw — parts per million by weight, 1 ppmw is a fraction of 1 in 10^6 weight units, e.g., 1 µg/g

2.6 ppta — parts per trillion atoms, 1 ppta is a fraction of 1 in 10^{12} atoms

2.7 pptw — parts per trillion by weight, 1pptw is a fraction of 1 in 10^{12} weight units, e.g., 1 pg/g

NOTE 1: In fact, NIST recommends not to use ppm, ppb and ppt, but to use, e.g., µg/g, ng/g and pg/g, respectively[1].

3 Conversion Between Relative Units

3.1 Concentration $[x]_a$ of an impurity element x with atomic mass M_x given in relative units of ppya (where y denotes m, b, or t) can be converted in concentrations $[x]_w$ in relative units of ppyw using the following equations:

$$[x]_w = \frac{M_x}{M_{Si}}[x]_a \tag{1}$$

or vice versa

$$[x]_a = \frac{M_{Si}}{M_x}[x]_w \tag{2}$$

where M_{Si} is the atomic mass of Si.

3.2 The ratios $M_x/M_{Si} = [x]_w/[x]_a$ are listed in Table 1 for some common impurity elements in silicon.

[1] http://physics.nist.gov/Pubs/SP811/sec07.html

Table 1 Conversion factors $[x]_w/[x]_a$

Impurity Element x	*Atomic Mass*[#1]	$[x]_w/[x]_a$ [#2]
B	10.81	0.38
C	12.01	0.43
O	16	0.57
Na	22.99	0.82
Al	26.98	0.96
P	30.97	1.10
K	39.1	1.39
Ca	40.08	1.43
Ti	47.9	1.71
Cr	52	1.85
Fe	55.85	1.99
Ni	58.71	2.09
Cu	63.55	2.26
Zn	65.38	2.33
As	74.92	2.67
Mo	95.94	3.42
Sb	121.75	4.33

#1 Handbook of Chemistry and Physics, CRC Press Inc., Boca Raton, 1980, R.C. Weast, M.J. Astle, Eds.; rounded to two decimal digits

#2 With M_{Si} = 28.086, according to footnote 1

4 Conversion between relative units (ppma, ppba or ppta) and absolute units (atoms/cm^{3}*)

4.1 Concentration $[x]_a$ of an impurity element x with atomic mass M_x given in relative units can be converted in concentrations $[x]_c$ in absolute units of atoms/cm^3 using the following equations:

$$[x]_c = \frac{N_A D_{Si}}{M_{Si}} 10^{-6} [x]_a \approx 5 \times 10^{16} [x]_a \tag{3}$$

for ppma,

$$[x]_c = \frac{N_A D_{Si}}{M_{Si}} 10^{-9} [x]_a \approx 5 \times 10^{13} [x]_a \tag{4}$$

for ppba,

$$[x]_c = \frac{N_A D_{Si}}{M_{Si}} 10^{-12} [x]_a \approx 5 \times 10^{10} [x]_a \tag{5}$$

for ppta, with the Avogadro Constant N_A and the specific gravity of bulk Si D_{Si}.