Ion induced radiation damage on the molecular level

Alvarado Chacon, Fresia

Atomic units and conversion factors

The atomic units (a.u.) originate from the typical dimensions of the hydrogen atom. The length is the classical Bohr radius a_0 of the ground state electron, the velocity αc is the classical velocity of the electron in the ground state of hydrogen, and the time is the ratio of the length and velocity. The charge in atomic units is the charge of the electron, the mass is the mass of the electron and the energy is the sum of the kinetic and the potential energy of the hydrogen 1s electron, 2×13.6 eV. An overview of the most important quantities is given in the following table 1. The atomic unit system is based on the following definition:

$$\bar{h} = m_e = e = 4\pi\varepsilon_0 = 1, \tag{1}$$

where $\bar{h}$ is Planck's constant divided by 2π, m_e and $-e$ are the mass and the charge of the electron, respectively, and ε_0 the permittivity of free space.

Throughout this thesis both the projectile velocity in a.u. and its kinetic energy in keV/amu are used. For non-relativistic collision energies the relation between them is given by:

$$\text{v (a.u.)} = 0.20\sqrt{E(\text{keV/amu})} \tag{2}$$

Some conversion factors of interest are given in table 2 in the backside of this page.

Table 1: *Atomic units*

length	a_0	5.292×10^{-11}	m
time	$a_0/\alpha c$	2.419×10^{-17}	s
velocity	αc	2.188×10^{6}	m/s
mass	m_e	9.109×10^{-31}	kg
charge	e	1.602×10^{-19}	C
energy	$m_e(\alpha c)^2$	4.359×10^{-18}	J
angular momentum	$\bar{h}$	1.054×10^{-34}	J s

Table 2: *Conversion factors*

1 amu	1.660×10^{-27}	kg
	1822.888	m_e
1 a.u.	27.2116	eV
energy	627.5095	kcal/mol
1 cal	4.184	J