Chapter 6
Interatomic Potentials, Scattering and Nuclear Stopping

Abstract This chapter focuses on interatomic potentials of interest in single and multiple scattering of heavy charged particles and the associated energy loss. In the keV energy range and above it is commonly assumed that binary elastic scattering on central potentials makes up an adequate description. Limitations of this description are mentioned. Classical scattering for screened-Coulomb interaction is outlined, and special attention is given to scaling properties, in particular for Thomas-Fermi-type interaction. Power-law scattering is mentioned as a convenient tool for rough estimates. Comparisons between different theoretical estimates as well as between measured and calculated cross sections are presented, and attempts to directly invert a measured cross section into the underlying potential are reported. The chapter concludes with explicit results for nuclear stopping and straggling including pertinent experiments.

6.1 Introductory Comments

Elements of classical and quantal scattering theory for central-force potentials have been presented in Chap. 3, Vol. 1, with applications mainly to Coulomb interaction between point charges. The present chapter addresses interactions between screened ions and atoms as well as between neutral atoms. In the field of radiation physics such screened-Coulomb forces are most often expressed in terms of central pairwise potentials, but more sophisticated descriptions may be appropriate, in particular for collisions at energies in the eV and lower-keV range.

A simple estimate presented in Sect. 2.3, Vol. 1 suggests the stopping cross section for electronic collisions to exceed that for elastic nuclear collisions by 3–4 orders of magnitude. This result holds for interactions between practically free point charges within an energy regime where stopping cross sections decrease monotonically with increasing energy. You have seen in Chap. 4 that the electronic stopping cross section actually experiences a maximum and, from there, decreases monotonically toward zero with decreasing energy. We shall see that the nuclear stopping
cross section exhibits a similar behaviour, but at a lower energy and with a different height. In general there exists a cross-over point between electronic and nuclear stopping at some energy which, for not too light ions, lies in the keV or lower-MeV range. For collision cascades governing radiation effects such as defect formation and sputtering, discussed briefly in Chap. 1, Vol. 1, nuclear stopping is most often the dominating process.

At higher beam energies, where electronic stopping dominates energy loss, angular deflections are governed by the interaction with the nuclei, as you have seen in Chap. 2, Vol. 1. For small-angle deflections—which determine multiple scattering—it is essential that screening of the interaction be taken properly into account.

6.2 Potentials

Calculating the interaction force between two (neutral or charged) atoms is in principle a problem of quantum chemistry, but the type of questions asked in radiation physics is different from standard problems treated in quantum chemistry. Most of all, the range of internuclear distances of interest in scattering problems differs from that in molecular physics: Atoms moving with kinetic energies in the keV regime or above may approach each other to internuclear distances much smaller than those of atoms bound in a molecule. From this follows that interaction forces of interest are predominantly repulsive, while in traditional quantum chemistry it is more the equilibrium range that is of interest.

Moreover, the range of relative velocities of interacting atoms may lie several orders of magnitude above what is of interest in molecular spectroscopy and chemical reaction kinetics. In quantum chemistry and molecular-beam physics, adiabatic potentials, based on the ground-state configuration of the combined electron cloud of two collision partners, are typically a good first estimate. Conversely, once the relative speed between the colliding nuclei exceeds characteristic orbital velocities of the target and projectile electrons, it may be more appropriate to consider the opposite extreme, ignore any deformation of the electron clouds during collision and, instead, determine the interaction between undisturbed atomic-electron configurations.

Within the scope of this book, more emphasis will be laid on general behaviour than on element-specific details. Therefore, scaling laws valid for a wide range of elements and their experimental verification will receive attention. This, in fact, is dictated by necessity: There are about $10^4$ ion-target systems if only atomic beams and elemental targets are taken into consideration. If molecular and cluster beams are allowed for as well as alloyed and compound targets, the variety of systems to be treated ab initio becomes rapidly prohibitive from the point of view of computational capacity and manpower.

The main justification of various adopted screening functions and screening radii is their ability to accurately describe pertinent experimental results. Those include measurements of elastic ion-atom scattering distributions under single- and/or