

It is worth noting that this sampling method is essentially independent of the adopted form factor, and is directly applicable to molecules. The efficiency of the algorithm (*i.e.*, the fraction of generated values of  $\cos\theta$  that is accepted) increases with photon energy. At low energies, it equals 2/3 (exactly) for all elements. For  $E = 100$  keV, the efficiencies for hydrogen and uranium are 100% and 86%, respectively.

## 2.2 Photoelectric effect

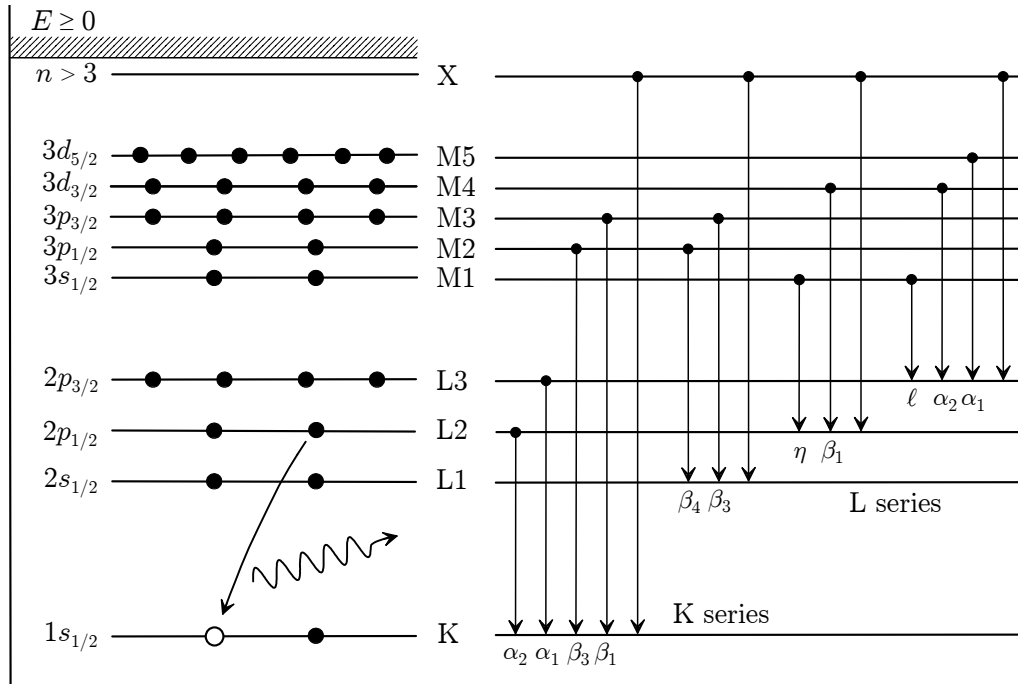
In the photoelectric effect, a photon of energy  $E$  is absorbed by the target atom, which makes a transition to an excited state. The photon beams found in radiation transport studies have relatively low photon densities and, as a consequence, only single-photon absorption is observed<sup>1</sup>. To represent the atomic states, we can adopt an independent-electron model, such as the Dirac-Hartree-Fock-Slater self-consistent model (see, *e.g.*, Pratt *et al.*, 1973), in which each electron occupies a single-particle orbital, with well-defined ionisation energy. The set of orbitals with the same principal and total angular momentum quantum numbers and the same parity constitute a shell. Each shell  $i$  can accommodate a finite number of electrons, with characteristic ionisation energy  $U_i$ . Notice that the shell ionisation energies are positive; the quantity  $-U_i$  represents the “binding” energy of each individual electron. Figure 2.3 (left diagram) shows the various notations used to designate the innermost atomic electron shells (*i.e.*, those with the largest ionisation energies) as well as their ordering in energy and allowed occupancies. In our simulations, we use the experimental ionisation energies given by Lederer and Shirley (1978), which pertain to free, neutral atoms. Ionisation energies of K-, L- and M-shells are displayed in Fig. 2.4.

Considering the interaction with the photon field as a first-order perturbation (which is appropriate for fields with low photon densities) it follows that only one-electron transitions are allowed. That is, in the photoelectric effect, the photon is absorbed by an individual electron in the “active” shell  $i$ , which leaves the parent atom with kinetic energy  $E_e = E - U_i$ . Evidently, photoionisation of a given shell is only possible when the photon energy exceeds the corresponding ionisation energy; this gives rise to the characteristic absorption edges in the photoelectric cross section (see Fig. 2.5).

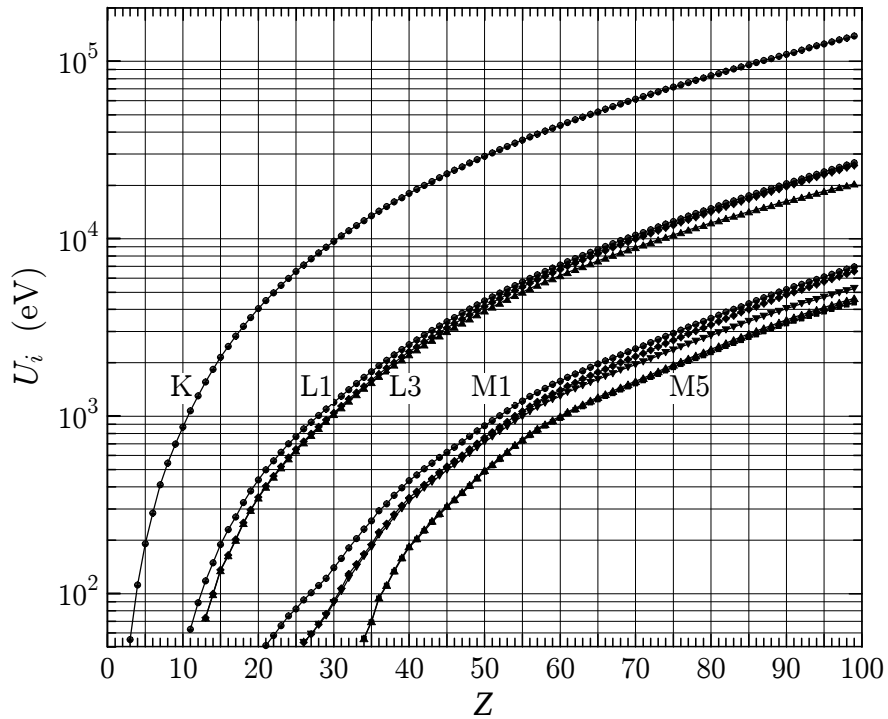
The photoelectric cross sections used in PENELOPE are obtained by interpolation in a numerical table that was extracted from the LLNL Evaluated Photon Data Library (EPDL; Cullen *et al.*, 1997). This library contains photoelectric cross sections for all shells of the elements  $Z = 1 - 100$  and photon energies from 1 eV to 1000 GeV, derived from Scofield’s theoretical calculations of shell cross sections (Saloman *et al.*, 1988) and Hubbell’s total cross sections (Hubbell *et al.*, 1980; Berger and Hubbell, 1987). The PENELOPE database for photoelectric absorption (a subset of the EPDL) consists of tables of the total atomic cross section  $\sigma_{\text{ph}}(E)$  and the cross sections for the K, L and M shells,  $\sigma_{\text{ph},i}(E)$  ( $i = \text{K, L1, L2, L3, and M1 to M5}$ ) for the elements  $Z = 1 - 99$ ,

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<sup>1</sup>In intense low-energy photon beams, such as those from high-power lasers, simultaneous absorption of several photons is possible.

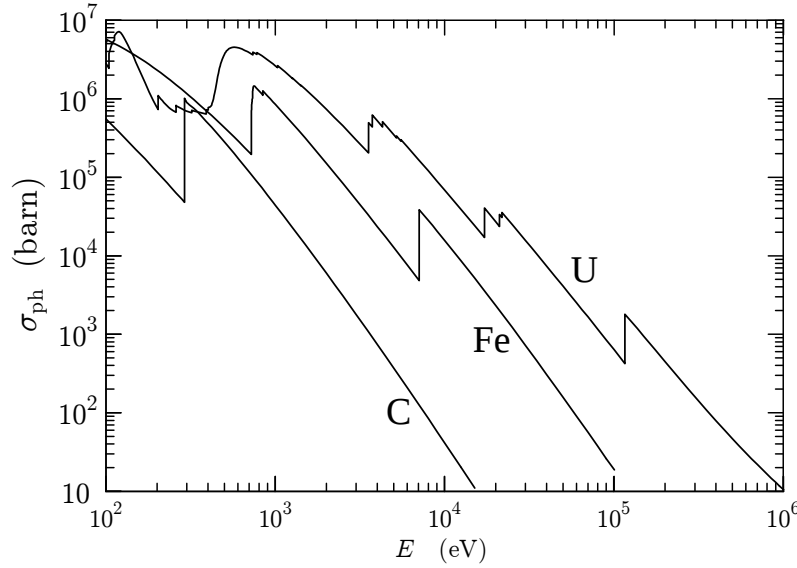


**Figure 2.3:** Various notations for inner atomic electron shells (left) and allowed radiative transitions (right) to these shells. Transitions that are different from the ones indicated in the diagram (*e.g.*, K-M4) are also possible, but their transition probabilities are extremely small.



**Figure 2.4:** Ionisation energies of the innermost shells of free atoms, as given by Lederer and Shirley (1978).

which span the energy range from 50 eV to 1000 GeV. These tables are estimated to be accurate to within a few percent for photon energies above 1 keV (Cullen *et al.*, 1997). At lower energies, uncertainties in the data are much larger, of the order of 10–20% for  $0.5 \text{ keV} < E < 1 \text{ keV}$ , 100–200% for  $0.1 \text{ keV} < E < 0.5 \text{ keV}$ , and 1000% for  $E < 100 \text{ eV}$ . Notice that the cross sections in the EPDL are based on free-atom theoretical calculations and, therefore, near-edge absorption structures produced by molecular or crystalline ordering (*e.g.*, extended x-ray absorption fine-structure) are ignored.



**Figure 2.5:** Atomic photoelectric cross sections for carbon, iron and uranium as functions of the photon energy  $E$ .

For compound materials (and also for mixtures) the molecular cross section  $\sigma_{\text{ph}}(E)$  is evaluated by means of the additivity approximation, that is, as the sum of the atomic cross sections of the elements involved. In the energy range between successive absorption edges, the photoelectric cross section is a continuous function of the photon energy (see Fig. 2.5). In PENELOPE, the molecular cross section is defined by means of a table of numerical values  $\sigma_{\text{ph}}(E_i)$  for a logarithmic grid of energies  $E_i$ , which is stored in memory. Photon mean free paths are determined by linear log-log interpolation in this table. Knowledge of the atomic cross sections is needed only when a photoabsorption event has effectively occurred in order to select the element that has been ionised (whose probability is proportional to the atomic cross section).

### 2.2.1 Simulation of photoelectron emission

Let us consider that a photon with energy  $E$  is absorbed by an atom of the element  $Z$ . The “active” shell  $i$  that is ionised is considered as a discrete random variable with PDF

$$p_i = \sigma_{\text{ph},i}(Z, E) / \sigma_{\text{ph}}(Z, E), \quad (2.18)$$