

Distorted Wave Theory of Elastic Scattering of Electrons by Atoms

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Short Communication

As is known, the process of electron scattering on the atoms of solids makes it possible to study not only the properties of individual atoms, but also the influence of neighboring atoms on the properties of the target atom. The standard expression for the differential electron scattering cross section has the form:

$$\frac{d\sigma_{if}}{d\Omega} = \frac{E_i E_f}{(2\pi)^2} \cdot \frac{k_f}{k_i} \cdot \frac{1}{2J_i + 1} \sum_{\sigma_i \sigma_f} \sum_{M_i M_f} \left| T_{if} \right|^2, \quad (1)$$

where the matrix element of the transition of the target atom from the initial state (i) to the final state (f) is represented as:

$$T_{if} = -4\pi Z e^2 \langle J_f M_f | \int dx \frac{g(x)}{q_{eff}^2(x)} \exp \{i[qx + \varphi(x)]\} \rho(x) | J_i M_i \rangle \quad (2)$$

As can be seen from (2), the distortion in the wave functions of the rescattered electrons in the field of the target atom occurs both in amplitude and in phase. Due to the fact that the electrostatic potential for an individual atom is approximated by the superposition of the spherically symmetric Yukawa potential, the expression for the density takes the form [1]:

$$\rho(x) = \frac{1}{4\pi} \sum_{\mu=1}^3 A_{\mu} \alpha_{\mu}^2 \frac{e^{-\alpha_{\mu} x}}{x}. \quad (3)$$

Here, the parameters A_{μ} and α_{μ} are determined by an analytical fitting procedure to the potential values found by the Dirac-Hartree-Fock-Slater self-consistent field method.

In order to study the elastic scattering of electrons on an individual atom, we express the distorted-wave differential cross section in terms of the form factor of the atom [2]:

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega} \right)_0 |F(q)|^2, \quad (4)$$

here $\left(\frac{d\sigma}{d\Omega}\right)_0 = \left(\frac{2Ze^2k}{q^2}\right)^2 \cos^2 \frac{\theta}{2}$ - differential cross section for electron scattering on a point atom.

With the help of the proposed mathematical method, the atom form factor is expressed in terms of the plane-wave Born form factor $F(q)$:

$$F(q) = 2\pi i(qR) \sum_{n=0}^{\infty} [Re\beta_n F_{(B)}^{(n)}(q) + Im\beta_{(B)} F_{(B)}^{(n)}(q)]. \quad (5)$$

Here $F_{(B)}^{(n)}(q) = \frac{\partial^n F_{(B)}(q)}{\partial q^n}$. Theoretical calculations of the differential cross section for electron scattering by In, Ga, Se, and Yb atoms were carried out at incident electron energies of 80 eV and compared with experimental data. The results of theoretical calculations agree with the experiment for radii: $R_{In} = 2.5A^0$, $R_{Ga} = 4.0A^0$, $R_{Se} = 1.4A^0$, $R_{Yb} = 1.4A^0$. It should be noted that taking into account distortions in the wave functions of the incident and scattered electrons makes it possible to fill the diffraction minima and shifts them towards small scattering angles.

References

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