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# REFLECTION OF ENERGETIC PARTICLES FROM ATOMIC OR IONIC CHAINS IN SINGLE CRYSTALS

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The channeling of p-and α-particles in Al, Au, Cu, MgO, LiF is theoretically investigated. Computer studies and analytic approximations were carried out to obtain the critical angle and the distance of closest approach to a lattice row. All calculations presented here are based upon single collisions with the lattice atoms or ions. This treatment is considered especially reliable in very close encounters, i.e. high particle energies and/or thermal vibrations of lattice atoms. Electronic stopping could be taken into account. The Lenz-Jensen potential was generalized for easier application.

## 1. Introduction

Considering the path of flight of a swift particle moving under a narrow angle against a row of atoms in a lattice (fig. 1), it becomes evident that significant scattering occurs only in the immediate vicinity of the lattice row. Furthermore, the close up, insert b) of fig. 1, shows that the scattering is mainly due to single collisions with each closest nucleus. This can also be confirmed by a more careful calculation which indicates that the neighbour atoms right and left of each closest nucleus contribute less than 0.7% to the maximum scattering angle even in the most unfavourable case (2 keV protons in Al).

* This work is a part from the thesis (D 83) by C. Varelas.

Thus, it was considered worthwhile to study the flight path of p- and α-particles by disintegrating it into a sequence of independant single collisions. Compared to the wellknown earlier treatment by means of the continuum model[1,2]), the present investigation has the advantage of being most accurate for close encounters (i.e. high particle energies and/or thermal lattice vibrations) where the validity of the continuum model breaks down.

## 2. Treatment of collisions, potentials

The scattering angle $\theta$ for each collision in the center of mass system was obtained from the first term of Lehmann-Leibfried's impuls approximation[3]) and then converted to the laboratory system by the approximaet

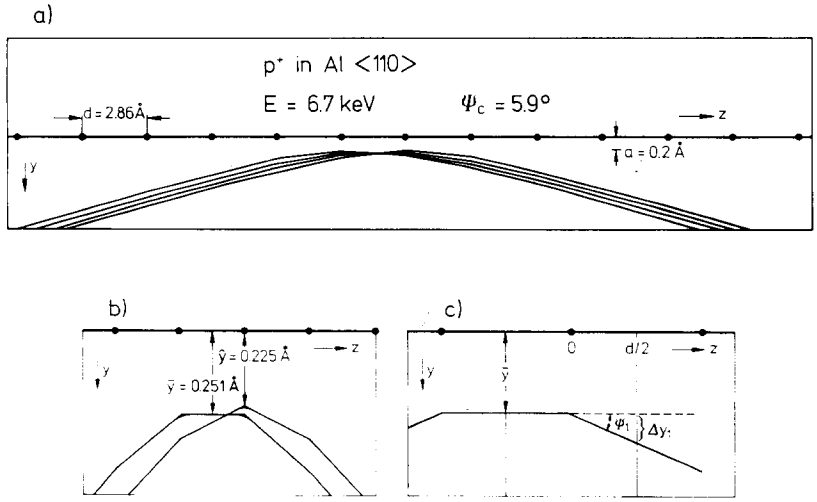


Fig. 1. a) Trajectories of 6.7 keV protons injected at the critical injection angle of $\psi_c = 5.9°$ against a <110> lattice row in Al (expanded scale in $y$ direction). Deflection predominant near the lattice row. b) Excerpt of a) with further tenfold increased $y$-scale, showing the two distinct trajectories which yield the minimum and maximum distance of closest approach. The black filled corners indicate the difference between the true and the polygonal trajectory. This difference becomes completely unvisible at higher energies. c) Construction for interpreting the criticality condition eq. (8).

relation $\varphi \simeq \theta M_2/(M_1+M_2)$, where $M_1$, $M_2$ denote the masses of the projectile and the lattice atoms respectively. Both approximations yield an overall error of $< 2\%$ for 1 keV protons and an entirely negligible error for particle energies of more than 10 keV.

For collisions with the atoms of a metal the Thomas-Fermi potential

$$V(r) = (Z_1 Z_2 e^2/r)\Phi(r/a)\,, \qquad a = 0.47\,\text{Å}\cdot Z_2^{-\frac{1}{2}}\,, \tag{1}$$

was used with Molière's screening function $\Phi(x)$[4]). ($Z_1 e$, $Z_2 e$ denote the charges of the projectile and the atom resp., $r$ being the nuclear separation of the collision partners.)

Collisions inside an ionic crystal were treated by means of the Lenz-Jensen potential[5,6])

$$V(r) = [Z_1(Z_2-N_2)e^2/r] + (Z_1 N_2 e^2/r)\,e^{-t}\sum_{i=0}^{4} k_i t^i\,, \qquad t = (gZ_2^{\frac{1}{2}} r/0.529\,\text{Å})^{\frac{1}{2}}\,, \tag{2}$$

where $N_2$ is the number of electrons of the considered ion and

$$\begin{aligned} k_0 &= k_1 = 1\,,\\ k_2 &= (27c^3+15c^2+3c)/q\,,\\ k_3 &= (7c^3+3c^2)/q\,,\\ k_4 &= c^3/q\,,\\ q &= 60c^3+36c^2+9c+1\,. \end{aligned}$$

The two primarily unknown parameters $g$ and $c$ until now had to be determined individually for each ion by requiring minimum total energy. This procedure, however, is not feasible for a rapid computation. Thus, for easier application the approximative formulae

$$c = 0.632 - 0.367\cdot N_2/Z_2\,, \qquad g = 31.93 - 21\cdot N_2/Z_2\,, \tag{3}$$

were established by a least square fit to a number of individually calculated $c$ and $g$. These simple expressions reveal an accuracy of about 1% for all mono and divalent ions.

## 3. Computation and results

An electronic computer (S 2002) was programmed to follow the trajectory of the incident particle by successive steps, each treating one binary collision with a lattice atom (or ion). The computation stopped whenever the projectile penetrated the atomic (or ionic) lattice row, or when it returned to the channel axis. In the latter case it was registered as channelled particle, provided that the transversal momentum (component in $y$-direction, fig. 1) was not increased compared to its initial value. At present only static lattice rows (without thermal vibrations) and complanar trajectories are treated*. In order to obtain the largest possible injection angle $\psi_c$ for the channeling effect, only such particles were considered which entered the lattice near the channel axis. By slightly shifting the point of injection, two distinct shapes of the trajectory could be observed, cf. insert b) of fig. 1, which yielded the minimum and maximum distance between the lattice row and the particle at its closest approach. These two values, denoted by $\hat{y}$ and $\bar{y}$ as in fig. 1b, differ appreciably even at the highest energies and therefore are both given in the compilation of results, tables 1 and 2; they correspond to the so called $\varrho_{\min}$ in the continuum theory.

## 4. Influence of energy losses

One purpose of the present work was to study the influence of energy losses which could easily be introduced into the computation.

### 4.1. Nuclear stopping of the channelled particles

In each collision by a small angle $\varphi$, a momentum $\Delta p \approx p\varphi$, and an energy

$$\Delta E_n = \Delta p^2/2M_2 \approx E\varphi^2\ M_1/M_2$$

is transferred to the lattice atom. Although these individual energies are extremely small ($\Delta E_n \ll 1$ eV) they can be accepted by the lattice: since many momenta $\Delta p$ are simultaneously† transferred and are all correlated, in fig. 1 going upwards over the length of a $\lambda/2$ – motion of the channelled particle, they can give rise to phonons of wavelengths of the same order of magnitude as $\lambda/2$ (the total transferred energy was found sufficient for the creation of a great number of such phonons).

* The influence of lattice vibrations in three dimensions will be described shortly in a forthcoming paper.

† Speed of sound is negligible compared to the velocity of the projectile.

TABLE 1

Critical angle $\psi_c$, and distances of closest approach $\hat{y}$, $\bar{y}$ (cf. fig. 1b) for various particle energies $E$. Computation without (left) and with energy losses (right). $\overline{\Delta E_n}$, $\overline{\Delta E_e}$ denote the averaged nuclear, respect. electronic energy loss per collision; $n$ is the number of collisions along the $\lambda/2$-motion of the particle (start and endpoint on the middle line between two next neighbour rows).

| $E$(keV) | $\psi_c$(°) | $\bar{y}$ (Å) | $\hat{y}$ (Å) | $n$ | $\psi_c$ (°) | $\bar{y}$ (Å) | $\hat{y}$(Å) | $\overline{\Delta E_n}$(eV) | $\overline{\Delta E_e}$(eV) | $n$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Protons in Al ⟨110⟩ | | | | | | | | | | |
| 3500 | 0.58 | 0.0163 | 0.0151 | 110 | 0.59 | 0.0157 | 0.0144 | 0.040 | 34.8 | 107 |
| 3000 | 0.63 | 0.0168 | 0.0153 | 102 | | | | | | |
| 2800 | 0.64 | 0.0175 | 0.0164 | 98 | | | | | | |
| 2500 | 0.67 | 0.0196 | 0.0182 | 95 | | | | | | |
| 2000 | 0.74 | 0.0206 | 0.0193 | 86 | 0.75 | 0.0196 | 0.0180 | 0.053 | 49.3 | 84 |
| 1600 | 0.82 | 0.0215 | 0.0202 | 79 | | | | | | |
| 1400 | 0.86 | 0.0238 | 0.0223 | 74 | 0.88 | 0.0222 | 0.0197 | 0.066 | 61.0 | 72 |
| 1300 | 0.89 | 0.0245 | 0.0225 | 72 | | | | | | |
| 1200 | 0.92 | 0.0250 | 0.0234 | 71 | | | | | | |
| 1000 | 1.00 | 0.0260 | 0.0242 | 64 | 1.01 | 0.0252 | 0.0230 | 0.075 | 72.0 | 63 |
| 900 | 1.04 | 0.0287 | 0.0257 | 62 | | | | | | |
| 800 | 1.08 | 0.0309 | 0.0286 | 60 | 1.11 | 0.0274 | 0.0250 | 0.083 | 79.5 | 58 |
| 600 | 1.24 | 0.0323 | 0.0290 | 53 | 1.25 | 0.0320 | 0.0279 | 0.095 | 81.5 | 51 |
| 500 | 1.31 | 0.0375 | 0.0343 | 50 | | | | | | |
| 400 | 1.43 | 0.0420 | 0.0379 | 46 | 1.49 | 0.0367 | 0.0312 | 0.12 | 95.0 | 43 |
| 300 | 1.59 | 0.0480 | 0.0444 | 43 | | | | | | |
| 200 | 1.87 | 0.0554 | 0.0512 | 36 | 1.99 | 0.0455 | 0.0407 | 0.16 | 117.5 | 33 |
| 100 | 2.45 | 0.0740 | 0.0670 | 28 | 2.61 | 0.0585 | 0.0527 | 0.21 | 147.0 | 25 |
| 50 | 3.09 | 0.1080 | 0.0962 | 24 | 3.4 | 0.0857 | 0.0701 | 0.26 | 161.0 | 20 |
| 33.5 | 3.59 | 0.1210 | 0.1100 | 21 | | | | | | |
| 20 | 4.20 | 0.1600 | 0.1430 | 17 | 4.7 | 0.111 | 0.103 | 0.33 | 128.0 | 15 |
| 13.4 | 4.80 | 0.1870 | 0.1670 | 16 | | | | | | |
| 10 | | | | | 5.8 | 0.165 | 0.148 | 0.30 | 84.5 | 12 |
| 6.7 | 5.90 | 0.2510 | 0.2250 | 13 | | | | | | |
| 5 | | | | | 7.1 | 0.233 | 0.206 | 0.28 | 52.0 | 10 |
| 2 | 8.70 | 0.3600 | 0.3300 | 9 | 9.2 | 0.361 | 0.301 | 0.26 | 25.4 | 8 |
| Protons in Au⟨110⟩ | | | | | | | | | | |
| 3500 | 1.07 | 0.0349 | 0.032 | 60 | 1.09 | 0.0314 | 0.0298 | 0.061 | 121 | 57 |
| 1000 | 1.66 | 0.0619 | 0.058 | 40 | 1.71 | 0.0568 | 0.0532 | 0.075 | 201 | 37 |
| 500 | 2.09 | 0.083 | 0.079 | 32 | 2.21 | 0.0749 | 0.0673 | 0.090 | 331 | 29 |
| 200 | 2.80 | 0.121 | 0.114 | 24 | 3.17 | 0.0964 | 0.0845 | 0.150 | 808 | 20 |
| 100 | 3.35 | 0.172 | 0.158 | 20 | 3.9 | 0.142 | 0.120 | 0.147 | 2540 | 16 |
| 50 | 4.3 | 0.196 | 0.186 | 16 | 4.7 | 0.187 | 0.164 | 0.126 | 1410 | 13 |
| 20 | 5.3 | 0.297 | 0.277 | 14 | 5.9 | 0.266 | 0.238 | 0.107 | 721 | 11 |
| 10 | 6.5 | 0.364 | 0.338 | 12 | 7.0 | 0.355 | 0.317 | 0.092 | 395 | 9 |
| 5 | 7.7 | 0.455 | 0.419 | 9 | 8.2 | 0.448 | 0.392 | 0.081 | 209 | 8 |
| 2 | 9.6 | 0.601 | 0.541 | 8 | | | | | | |
| α-particles in Au ⟨110⟩ | | | | | | | | | | |
| 10.000 | 0.87 | 0.0345 | 0.0327 | 72 | | | | | | |
| 1000 | 2.0 | 0.0851 | 0.0795 | 34 | | | | | | |
| 50 | 4.7 | 0.269 | 0.256 | 16 | | | | | | |
| 20 | 6.1 | 0.359 | 0.332 | 12 | | | | | | |
| 10 | 7.4 | — | 0.339 | 10 | | | | | | |
| 5 | 8.2 | 0.565 | 0.513 | 8 | | | | | | |
| Protons in Cu ⟨110⟩ | | | | | | | | | | |
| 100 | | | | | 3.7 | 0.074 | 0.065 | 0.365 | 1035 | 17 |
| 50 | | | | | 4.5 | 0.110 | 0.090 | 0.327 | 648 | 15 |
| 20 | | | | | 5.9 | 0.173 | 0.141 | 0.295 | 344 | 11 |
| 10 | | | | | 7.1 | 0.239 | 0.198 | 0.263 | 210 | 10 |
| α-particles in Cu ⟨110⟩ | | | | | | | | | | |
| 10.000 | 0.68 | 0.0201 | 0.0194 | 94 | | | | | | |
| 1000 | 1.70 | 0.0525 | 0.0475 | 40 | | | | | | |
| 200 | | | | | 3.5 | 0.0714 | 0.0682 | 1.95 | 740 | 19 |
| 100 | 3.60 | 0.145 | 0.135 | 20 | 4.4 | 0.1105 | 0.0869 | 2.00 | 485 | 15 |
| 50 | 4.55 | 0.185 | 0.167 | 16 | 5.4 | 0.164 | 0.132 | 1.96 | 299 | 12 |
| 20 | 5.9 | 0.259 | 0.236 | 13 | 7.0 | 0.218 | 0.203 | 1.75 | 152 | 10 |
| 10 | 7.2 | 0.331 | 0.297 | 11 | 8.4 | 0.317 | 0.276 | 1.7 | 99 | 8 |

### 4.2. Electronic stopping interpolation formula for intermediate energies

Energy losses due to electronic excitation are of the order of 1 keV/collision, and thus are more effective in slowing down the projectile. The universal electronic stopping power formulas which take into account the dependence on the collision parameter $b$, are:

1. that of Firsov[7])

$$\Delta E_F = v \frac{4.3\times 10^{-8}(Z_1+Z_2)^{\frac{5}{3}}}{[1+0.31\,b(Z_1+Z_2)^{\frac{1}{3}}]^5}, \quad (v \text{ in cm/s},\ b \text{ in Å}) \tag{4}$$

being valid for velocities $v < v_0 Z_1^{\frac{2}{3}}$, $v_0 = e^2/\hbar$, and

2. that of Bethe-Bloch, modified by Lindhard[1]),

$$\Delta E_L = B(b)\frac{\ln\varepsilon}{\varepsilon} \text{ with } \varepsilon = \frac{2m_e v^2}{Z_2 \cdot 10\,eV} \text{ and} \tag{5}$$

$$B(b) = \frac{8\pi Z_1^2 e^4}{10\,eV}\left[\tfrac{1}{2}Nd + \tfrac{1}{2}\int_{-d/2}^{+d/2}\frac{\varrho\{\sqrt{(b^2+z^2)}\}\,dz}{Z_2}\right],$$

which is valid only if $v > v_0 Z_1^{\frac{2}{3}}$ *and also* $v > v_0 Z_2^{\frac{1}{2}}$. The factors $\frac{1}{2}$ are the result of applying Lindhard's "equipartition rule" which gives the same weight to close and distant electrons. Here $N$ denotes the number of atoms per cm$^3$, $d$ the spacing of subsequent atoms in the lattice row, and $\varrho(r) = Z_2\{\sqrt{\Phi(r/a)}/(r/a)\}^3/4\pi a^3$ the variable electronic density within the traversed atom; for $\Phi$ and $a$ cf. eq. (1)*.

Apparently there remains a gap between the ranges of validity of the two formulae, just where the maximum energy loss is expected.

For the present work an interpolation formula was used

$$\frac{1}{\Delta E_e} = \frac{1}{\Delta E_F} + \frac{1}{B\ln(\varepsilon+1+5/\varepsilon)/\varepsilon}, \tag{6}$$

which includes the above formulae (4) and (5) as limiting cases. In the transition region it was fitted to various empirical stopping power curves (after integrating over $b$) by proper choice of the two additive terms under the logarithm†.

* Both energy loss formulae are based upon Thomas-Fermi distributions of electrons and neglect therefore any oscillating dependence on $Z_1$ and $Z_2$.

† The quality of this fit will be shown graphically in a forthcoming HMI report.

The results of the computation with energy losses are added for comparison to table 1 which contains in the first columns the former results (neglecting energy losses). Evidently, the characteristic channeling quantities $\psi_c$, $\bar{y}$, $\hat{y}$, are well influenced by energy losses, especially in the region of maximum electronic stopping power. This can also be seen in the following pictures, figs. 2 and 3.

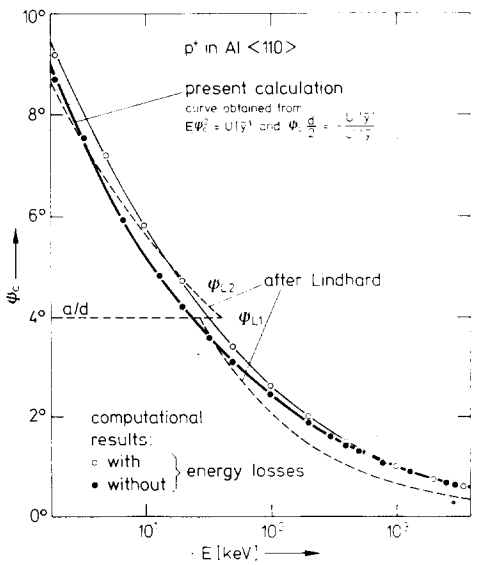


Fig. 2. The relation between $\psi_c$ and $E$ for protons in aluminium, as obtained here from eqs. (7) and (9), and by Lindhard[1]), in comparison with the numerical results. The change of $\psi_c$ to higher values in consequence of energy losses is also depicted.

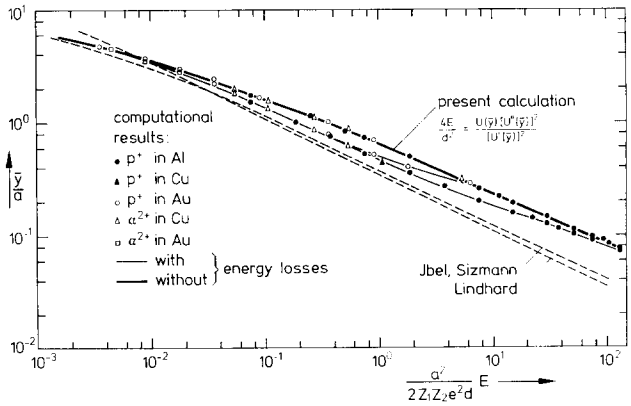


Fig. 3. The distance of closest approach $\bar{y}$ in dependence of the particle energy $E$ in generalized coordinates. The present analytic formula (9), together with the other existent formulae of Lindhard[1]) and of Ibel and Sizmann[8]) are compared with the computational results. The influence of energy losses shifts the numerical points slightly down at medium energies ($E \approx Z_1 Z_2 e^2 d/a^2$).

## 5. Analytic approximations and discussion

By checking the results $\psi_c$, $\bar{y}$ (without energy loss) against the wellknown relation of the continuum theory

$$E\psi_c^2 = U(\bar{y}),$$
$$U(y) = 1/d \int_{-\infty}^{+\infty} V\{\sqrt{(y^2+z^2)}\}\, dz\,, \tag{7}$$

a universal agreement within $\pm 1\%$ was found.

Of course, the results $\psi_c$, and $\hat{y}$ do not satisfy relation (7) as may be anticipated. (Only in the first case, where the trajectory becomes parallel to the lattice row, cf. fig. 1b, the transversal kinetic energy $E_\perp = p_y^2/2M_1 \approx E\psi^2$ *vanishes completely* over the length of one lattice spacing $d$.)

Unfortunately, no second relation from the continuum theory was found to agree with the numerical results: $\psi_c(E)$ as derived by Lindhard[1]) proved to be especially low at higher energies as shown in fig. 2; e.g. for 3.5 MeV protons in Al <110> the present result is $\psi_c = 0.585°$, whereas Lindhard's formula yields $\psi_c = 0.351°$. Even worse discrepancies occurred for the distance of closest approach $\varrho_{min}$ $(E)$ at higher energies, as depicted in fig. 3, where analytic expressions of two authors[1,8]) can be compared with the present results.

In order to obtain a valid second relation for the two quantities $\psi_c$ and $\bar{y}$ besides of eq. (7), a criticality condition of the form

$$\psi_c \cdot d/2 = -U'(\bar{y})/U''(\bar{y}) \tag{8}$$

was assumed and tested. The comparison with the numerical results for both metals and ionic crystals revealed an excellent agreement. From the two independant eqs. (7) and (8) an $E$-$\bar{y}$ relation can be derived explicitly

$$E(4/d^2) = \left[\frac{U''(\bar{y})}{U'(\bar{y})}\right]^2 \cdot U(\bar{y})\,, \tag{9}$$

while the $E$-$\psi_c$ relation is only implicitly contained in eqs. (8) and (9). Both relations are depicted as solid lines in figs. 2 and 3; they show perfect agreement with the numerical results.

The form of condition (8) was suggested by considering the most critical collision at $\bar{y}$ (point of closest approach to a lattice atom), cf. fig. 1c. If here the continuum approximation is required to hold, i.e. $\psi_1 = -d \cdot U'(\bar{y})/2E$, then the quantity $U'(y)$ along the true particle path $y(z)$ should not change by more than its own value:

$$\Delta U' \cong y_1 \cdot U''(\bar{y}) = \psi_1 (d/2)\, U''(\bar{y}) \leqslant \left|U'(\bar{y})\right|,$$

cf. fig. 1c.

By substituting $\psi_c$ for an upper limit of $\psi_1$ and replacing "$\lesssim$" by "$=$" one arrives at eq. (8).

The averaged potential functions and their derivates to be used in eqs. (7), (8) and (9) are

a. *for metals* on the basis of the Thomas-Fermi-Molière Potential, eq. (1):

$$U(y) = [Z_1 Z_2 e^2/d]\,[0.2\,K_0(6\,y/a) + 1.1\,K_0(1.2\,y/a) + 0.7\,K_0(0.3\,y/a)],$$

TABLE 2

The characteristic channeling quantities for ionic crystals neglecting energy losses (symbols as in table 1).

| $E$ (keV) | $\psi_c$ (°) | $\bar{y}$ (Å) | $\hat{y}$ (Å) | $n$ |
|---|---|---|---|---|
| Protons in LiF <100> | | | | |
| 3500 | 0.43 | 0.0141 | 0.0131 | 144 |
| 2000 | 0.51 | 0.0219 | 0.0216 | 123 |
| 1000 | 0.66 | 0.0318 | 0.0303 | 96 |
| 500 | 0.86 | 0.0420 | 0.0400 | 74 |
| 200 | 1.20 | 0.0611 | 0.0582 | 53 |
| 100 | 1.53 | 0.079 | 0.0756 | 42 |
| 50 | 1.92 | 0.105 | 0.0995 | 34 |
| 20 | 2.54 | 0.150 | 0.143 | 26 |
| 10 | 3.12 | 0.191 | 0.189 | 21 |
| 5 | 3.8 | 0.242 | 0.237 | 17 |
| 2 | 4.9 | 0.320 | 0.316 | 13 |
| Protons in MgO <100> | | | | |
| 3500 | 0.50 | 0.0195 | 0.0190 | 125 |
| 1000 | 0.82 | 0.0329 | 0.0319 | 77 |
| 200 | 1.49 | 0.0635 | 0.0617 | 44 |
| 100 | 1.91 | 0.0825 | 0.0814 | 34 |
| 20 | 3.40 | 0.142 | 0.134 | 20 |
| 10 | 4.4 | 0.167 | 0.160 | 16 |
| 5 | 5.8 | 0.193 | 0.181 | 12 |
| 2 | 8.2 | 0.227 | 0.214 | 9 |
| α-particles in MgO <100> | | | | |
| 3500 | 0.65 | 0.0277 | 0.0268 | 97 |
| 2000 | 0.83 | 0.0313 | 0.0304 | 77 |
| 1000 | 1.06 | 0.0443 | 0.0432 | 61 |
| 500 | 1.37 | 0.0593 | 0.0575 | 47 |
| 200 | 1.91 | 0.0828 | 0.0819 | 34 |
| 100 | 2.43 | 0.108 | 0.104 | 27 |
| 50 | 3.28 | 0.118 | 0.113 | 21 |
| 20 | 4.3 | 0.177 | 0.168 | 16 |
| 10 | 5.6 | 0.207 | 0.194 | 12 |
| 5 | 7.7 | 0.237 | 0.196 | 9 |

$$U'(y) = -[Z_1 Z_2 e^2/(da)]\,[1.2\,K_1(6\,y/a) + 1.32\,K_1(1.2\,y/a) + 0.21\,K_1(0.3\,y/a)],$$

$$U''(y) = [Z_1 Z_2 e^2/(da^2)]\,[7.2\,K_0(6\,y/a) + 1.584\,K_0(1.2\,y/a) + 0.063\,K_0(0.3\,y/a)] - U'(y)/y\,,$$

$K_\nu$ being the modified Hankel functions of order $\nu$,

b. *for ionic crystals* on the basis of the Lenz-Jensen Potential, eqs. (2) and (3), (approximative within $\pm 2\%$)

$$U(y) = (Z_1 e^2/d)\,[N_2 \cdot H(Z_2, N_2, y) + N_3 \cdot H(N_3, Z_3, y)],$$

$$H = (\pi/9)\,[4(1+2t)\mathrm{e}^{-2t} + (1+1.4t)\mathrm{e}^{-1.4t} + 1.4(1+1.2t)\mathrm{e}^{-1.2t} + 1.86(1+t)\mathrm{e}^{-t}],$$

$t = (g_{2,3} \cdot Z_{2,3}^{\frac{1}{3}} \cdot y/0.529\,\text{Å})^{\frac{1}{2}}$, cf. eqs. (2) and (3).

$d$ is the spacing between next neighbors which may be unequal ions (denoted by the indices 2 and 3). The derivates are trivial.

The main purpose of the present discussion was to compare the various theoretical results which have been derived from equal assumptions (static lattice, no energy losses). Although a quite satisfactory description of this idealized case could be achieved, one can not necessarily expect that the above results apply to realistic cases with the same accuracy*. The measurable effects (angular dependences of particle transmission, emission or backscattering, nuclear reactions, X-ray production etc.) are usually influenced by lattice vibrations and – at certain energies as shown above – by energy losses. A study of particle trajectories in vibrating lattices will be presented shortly.

* In a former relevant work[9]) Morgan and Van Fliet draw their main attention to a computer simulation of realistic experiments.

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## References

[1]) J. Lindhard, Mat. Fys. Medd., Dan. Vid. Selsk. **34**, no. 14 (1965).
[2]) C. Erginsoy, Phys. Rev. Letters **15** (1965) 360.
[3]) C. Lehmann and G. Leibfried, Z. Physik **172** (1963) 465.
[4]) G. Molière, Z. Naturforsch. **2a** (1947) 133.
[5]) W. Lenz, Z. Physik **77** (1932) 713.
[6]) H. Jensen, Z. Physik **77** (1932) 722.
[7]) O.B. Firsov, Soviet Phys. JETP **36** (1959) 1076.
[8]) K. Ibel and R. Sizmann, Phys. Stat. Sol. **29** (1968) 403.
[9]) D.V. Morgan and D. Van Fliet, Can. J. Phys. **46** (1968) 503.