Volume Reflection in Arbitrary Interplanar Potential

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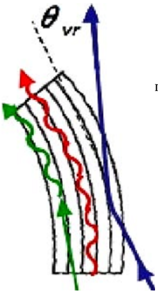
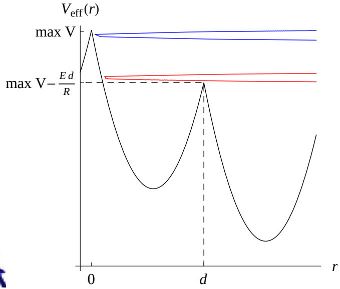
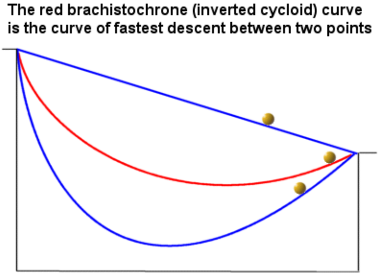
Volume reflection as transverse acceleration







The temporal pattern of VR in the non-inertial frame connected with the bent crystal:
At its passage through each interplanar interval, the longer the particle is contained in it, to the greater angle the crystal will turn during that time, and so the greater the particle aggregate deflection angle will be to the side of the bending. But the influence of the intra-crystal potential, on the contrary, is accelerating, so the particle passes the interplanar intervals faster than it would do in the absence of the crystal (in the pure centrifugal potential). For this reason, in VR, vice versa, the deflection proceeds to the side opposite to that of the crystal bending.
N.B.: The effect of acceleration of the particle passage of a given distance due to the presence of a potential well on its way is known since the brachistochrone problem of Johann Bernoulli. The essential difference, though, is that in VR there is no competing vertical ("diving") motion, only the effectively 1-dimensional radial motion. Thence, the deeper the interplanar potential, the greater the VR angle.

Benchmarks of the theory development

Taratin, Vorobiev, 1987 [1]

1. The continuous potential of a uniformly bent crystal in planar orientation may be viewed as being axially symmetric.
2. For a small crystal bending angle (attainable under elastic deformation), the centrifugal potential may be linearized within the crystal volume.

Therewith,

$$\varphi = \frac{1}{R}\int_{r_0}^{r} \frac{dr}{\sqrt{2\frac{E_\perp + V(r_0) - V(r)}{E} + 2\frac{(r-r_0)}{R}}}. \quad (1)$$

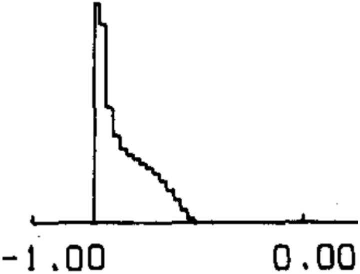


Figure: Simulated angular distribution of volume reflected positively charged particles, in units of the critical channeling angle [1].

Maisheev, 2007 [2]:

$$\alpha = \frac{2}{R}\int_{r_0}^{r_c} dr \left\{ \frac{1}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}} - \frac{1}{\sqrt{2\frac{E_\perp - V(r_c)}{E} + 2\frac{r}{R}}} \right\}. \qquad (2)$$

Handling of this representation is facilitated by assuming statistical equilibrium, i.e., uniform distribution in $E_\perp$. The integral (2) is still to be computed numerically.

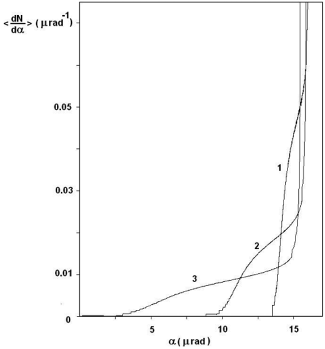


FIG. 7. Distributions of particles over the angle of volume reflection. Curves 1, 2, and 3 correspond to $R = 25$, 10, and 5 m.

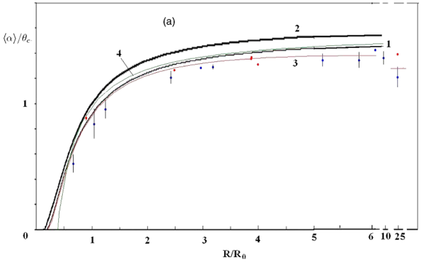


Figure: a). Angular distribution of volume reflected positively charged particles, in units of the critical channeling

The present author, 2010 [5].
A complete calculation was performed for a model of purely harmonic interplanar potential. By evaluating the trajectory in each interplanar interval exactly, and then replacing the summation over the intervals by another integration, an asymptotic analysis at $R/R_c \to \infty$ was carried out up to the next-to leading order (NLO).

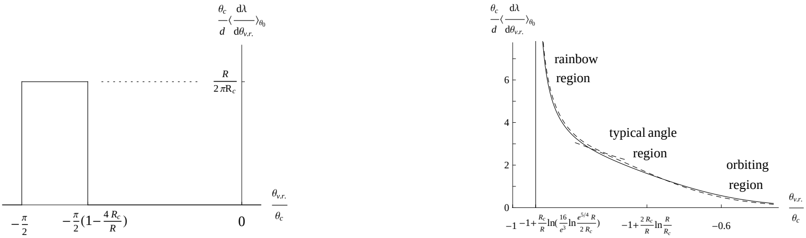


Figure: Angular distribution of positively (a) and negatively (b) charged volume reflected particles in the NLO [5].

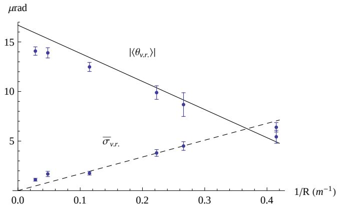


Figure: Dependence of the mean volume reflection angle $\bar{\theta}_{VR} = \frac{\pi}{2}\theta_c\left(1 - \frac{2R_c}{R}\right)$ (solid line) and variance (dashed line) in the NLO, according to [5]. Points – experimental data [3].

Remaining issues:

1. In numerical calculations, there is a significant skewedness of the angular distribution for positively charged particles, as well.
2. In the angular distribution, the contribution NNLO in R_c/R appears to be $\mathcal{O}\left[(R_c/R)^{3/2}\right]$. Compared to the NLO $\mathcal{O}(R_c/R)$, it gives a sizable correction, which in addition is non-uniform (blows up near the top of the potential barrier).
3. For germanium crystals, the interplanar potential is far from parabolic.

A closed-form representation for the $E_\perp$-dependent VR angle

$$\theta_{VR} = 2\lim_{r\to\infty}\left\{\sqrt{2\frac{r}{R}} - \frac{1}{R}\int_{r_{\min}(E_\perp)}^{r}\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}}\right\}. \quad (3)$$

In order to separate generic volume reflection effects from the dependence on the interplanar continuous potential, interchange the order of integration and summation over the intervals.

To this end, exploit the periodicity of $V(r)$. Therewith, the integral in (3) can be partitioned into a sum of integrals over single inter-planar intervals:

$$\int_{r_{\min}(E_\perp)}^{r}\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}} = \int_{r_{\min}(E_\perp)}^{d}\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}} + \sum_{n=1}^{\lfloor r/d\rfloor}\int_0^d\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r+nd}{R}}}. \quad (4)$$

The first integral in the rhs of (4) can as well be extended to the same interval $0 < r \le d$, provided thereat we take only its real part:

$$\int_{r_{\min}(E_\perp)}^{d}\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}} = \Re\mathfrak{e}\int_0^d\frac{dr}{\sqrt{2\frac{E_\perp - V(r)}{E} + 2\frac{r}{R}}}.$$

That leads to the limiting form

$$\theta_{VR} = 2\lim_{r\to\infty}\left\{\sqrt{2\frac{r}{R}} - \frac{1}{\sqrt{2Rd}}\Re\mathfrak{e}\sum_{n=0}^{\lfloor r/d\rfloor}\int_0^d\frac{dr}{\sqrt{\frac{R}{d}\frac{E_\perp - V(r)}{E} + \frac{r}{d} + n}}\right\}. \quad (5)$$

In fact, the summation over n can be performed in closed form, employing the standard limit

$$\lim_{n_{\max}\to\infty}\left(\sum_{m=0}^{n_{\max}}\frac{1}{\sqrt{\eta+m}}-2\sqrt{n_{\max}}\right)=\zeta\left(\frac{1}{2},\eta\right), \tag{6}$$

which is generalized Riemann zeta function with parameter $\frac{1}{2}<1$. As a result, for a generic potential $V(r)$, the limiting volume reflection angle can be expressed as

$$\theta_{VR}=-\frac{2}{\sqrt{2Rd}}\mathfrak{Re}\int_0^d dr\zeta\left(\frac{1}{2},\frac{R}{d}\frac{E_\perp-V(r)}{E}+\frac{r}{d}\right). \tag{7}$$

In practice, for all $\eta>-1$, function (6) may be approximated by

$$\zeta\left(\frac{1}{2},\eta\right)\approx\frac{1}{\sqrt{\eta}}+\frac{1}{\sqrt{\eta+1}}+\frac{1}{2\sqrt{\eta+2}}-2\sqrt{\eta+2}. \tag{8}$$

This is not the end of the theory, but just the beginning

Exact representation for the mean VR angle. Model results to all orders in R_c/R

Under the assumption of statistical equilibrium (uniform distribution of initial particles in $E_\perp$ within the relatively small interval $\Delta E_\perp = \frac{Ed}{R}$ [2]), the beam average may be obtained by averaging (7) over $E_\perp$ in the interval $[-\Delta E_\perp, 0]$. Employing the identity

$$\int_s^{s+1} ds' \zeta\left(\frac{1}{2}, s'\right) = -2\sqrt{s},$$

we are led to an exact representation for the mean VR angle:

$$\bar{\theta}_{VR}(R) = \frac{1}{\Delta E_\perp}\int_{-\Delta E_\perp}^{0} dE_\perp \theta_{VR}(R, E_\perp) = \frac{2}{d}\sqrt{\frac{2}{E}}\mathfrak{Re}\int_0^d dr\sqrt{\max_{r'>r} V_{\text{eff}}(r') - V_{\text{eff}}(r)}, \tag{9}$$

$V_{\text{eff}}(r) = V(r) - Er/R$. For harmonic interplanar potential, it yields explicit expressions valid through all orders in R_c/R:

$$\frac{\bar{\theta}_{VR}}{\theta_c} = \frac{\pi}{2}\left(1 - \frac{R_c}{R}\right)^2 \qquad \text{[positively charged particles, orientation (110)],} \tag{10}$$

$$\frac{\bar{\theta}_{VR}}{\theta_c} = 1 - \frac{R_c}{R}\left(1 + \ln\frac{R}{R_c}\right) \qquad \text{[negatively charged particles, orientation (110)],} \tag{11}$$

$$\bar{\theta}_{VR} = \frac{\pi}{2d}\left\{d_1\theta_{c1}\left(1 - \frac{R_{c1}}{R}\right)^2 + d_2\theta_{c2}\left(1 - \frac{R_{c2}}{R}\right)^2\right\} \qquad \text{[positively charged particles, or-n (111)],} \tag{12}$$

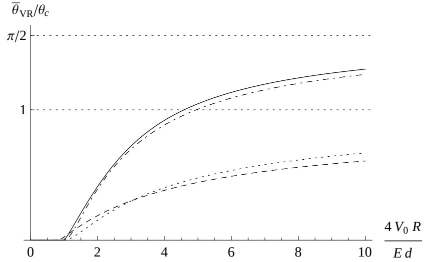


Figure: Dependence of the mean VR angle on the crystal bending radius: a). for silicon in orientation (110); b). for tungsten in the same orientation. Solid curves – calculation with a realistic interplanar potential for positively charged particles; dashed curves – for negatively charged particles. For comparison, dot-dashed and dotted curves indicate the corresponding dependencies for a harmonic interplanar potential, Eqs. (**??**) and (**??**).

Limiting VR angle ($R/R_c \to \infty$)

For applications of volume reflection, the most important case is when $R \gg R_c \sim Ed/V_0$. Then,

$$\theta_{VR} \approx \theta_{VR\infty} = \sqrt{\frac{2}{E}}\frac{2}{d}\int_0^d dr\sqrt{\max V - V(r)}, \qquad (13)$$

i.e., the leading-order approximation appears to be independent of R and $E_\perp$ (i.e., of impact parameters).

For example, for a harmonic potential $V(r) = V_0(1 - 2r/d)^2$, in the case of positively charged particles [$V(r) > 0$],

$$\theta_{VR\infty} = \sqrt{\frac{2V_0}{E}}\int_{-1}^{1} dx\sqrt{1 - x^2} = \frac{\pi}{2}\theta_c,$$

whereas in the case of negatively charged particles [$V(r) < 0$],

$$\theta_{VR\infty} = \sqrt{\frac{2V_0}{E}}\int_{-1}^{1} dx\sqrt{0 - (-x^2)} = \theta_c,$$

where $\theta_c = \sqrt{\frac{2V_0}{E}}$ is the critical channeling angle [5].

Higher orders in R_c/R in the angular distribution

Retaining higher orders in R_c/R, one acquires the $E_\perp$ dependence, which gives rise to a finite angular spread. In the NLO, in such a way there were calculated the angular distributions for positively and negatively charged VR particles [5], the difference between the nuclear inelastic or elastic incoherent scattering rates for VR particles and particles in a corresponding straight crystal or amorphous matter [6], etc.

NLO – rectangular shape

In the next-to-leading order (NLO), the angular distribution of positively charged VR particles for arbitrary interplanar potential appears to be rectangular:

$$\begin{aligned}\theta_{VR} &\approx \sqrt{\frac{2}{E}}\frac{2}{d}\mathfrak{Re}\int_0^d dr\sqrt{-V(r)+E_\perp+\frac{E}{R}\left(r-\frac{d}{2}\right)} \\ &\underset{R\gg R_c}{\simeq} \sqrt{\frac{2}{E}}\left[\frac{2}{d}\int_0^d dr\sqrt{-V(r)}+\frac{1}{d}\int_0^d dr\frac{E_\perp+\frac{E}{R}(r-d/2)}{\sqrt{-V(r)}}\right] \\ &= \sqrt{\frac{2}{E}}\left[\frac{2}{d}\int_0^d dr\sqrt{-V(r)}+\frac{E_\perp}{d}\int_0^d\frac{dr}{\sqrt{-V(r)}}\right]. \end{aligned} \quad (14)$$

I.e.,

$$\frac{dw}{d\theta_{VR}}=\frac{R}{\int_0^d dr\sqrt{\frac{2E}{-V(r)}}}=\text{const} \quad (15)$$

within the finite interval
$\frac{2}{d}\int_0^d dr\sqrt{-\frac{2V(r)}{E}}-\frac{1}{R}\int_0^d dr\sqrt{-\frac{2E}{V(r)}}\leq\theta_{VR}\leq\frac{2}{d}\int_0^d dr\sqrt{-\frac{2V(r)}{E}}$.

NNLO – sail-like shape

$$\theta_{VR}(R, E_\perp) = a\mu + b\sqrt{\mu} + c, \tag{16}$$

where $\mu = 1 + \frac{E_\perp}{\Delta E_\perp}$, $0 < \mu \leq 1$,

$$a(R) = \sqrt{\frac{2}{E}} \frac{\Delta E_\perp}{d} \left[\int_0^d \frac{dr}{\sqrt{-V(r)}} - 2c_1 \frac{\sqrt{\Delta E_\perp}}{F_{\max}} \right], \tag{17}$$

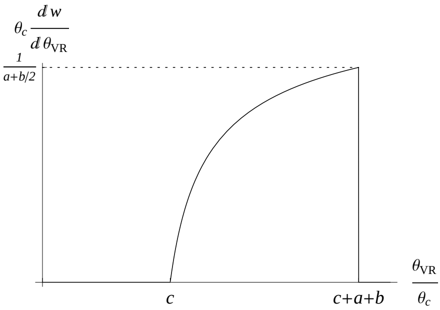
$$b(R) = 4\sqrt{\frac{2}{E}} \frac{(\Delta E_\perp)^{3/2}}{F_{\max} d}, \tag{18}$$

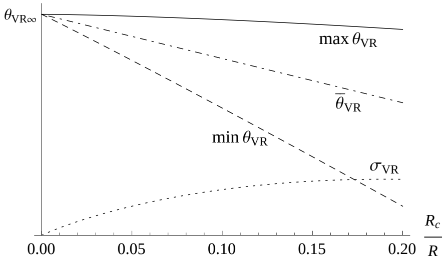
$$c(R) = \sqrt{\frac{2}{E}} \frac{2}{d} \left\{ \int_0^d dr \sqrt{-V(r)} - \frac{\Delta E_\perp}{2} \int_0^d \frac{dr}{\sqrt{-V(r)}} + (c_0 + c_1) \frac{(\Delta E_\perp)^{3/2}}{F_{\max}} \right\} \tag{19}$$

($c_0 \approx -2.3$, $c_1 \approx 2$), we may solve the quadratic equation (16) wrt μ, and differentiating it by θ_{VR}, obtain the angular distribution:

$$\frac{dw}{d\theta_{VR}} = \frac{d\mu}{d\theta_{VR}} = \frac{1}{a} \left[1 - \frac{1}{\sqrt{1 + \frac{4a}{b^2}(\theta_{VR} - c)}} \right] \vartheta(\theta_{VR} - c)\vartheta(c + a + b - \theta_{VR}) \tag{20}$$

[assuming that $a > 0$, so that (16) has only one root]. Thus, at $R \gg R_c$ the angular distribution of volume reflected particles assumes a universal “sail-like" form for any interplanar potential having non-vanishing derivatives at the interval ends.





The mean volume reflection angle corresponding to the angular distribution (20) equals

$$\bar{\theta}_{VR} = \int_c^{c+a+b} d\theta_{VR}\theta_{VR}\frac{dw}{d\theta_{VR}} = c + \frac{a}{2} + \frac{2b}{3}. \tag{21}$$

The shape of the distribution (20) could be regarded as parameter-free, if we use $\frac{4a}{b^2}(\theta_{VR} - c)$ as the scaling variable. But the genuine parameter is the value of this scaling variable at the end of the interval $\theta_{VR} = a + b + c$:

$$\frac{4a}{b^2}(a+b) = \frac{(2a+b)^2}{b^2} - 1.$$

If the latter ratio is large ($2a \gg b$), the distribution at typical θ_{VR} would be flat. However, the square root dependence on it indicates that this will happen only rather remotely.

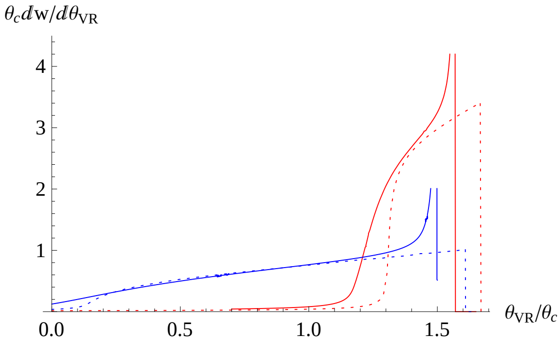


Figure: Angular distributions of VR particles in a continuous potential of Si (110) crystal at room temperature (solid curves) and for a static lattice (dotted curves). Red: $R = 4R_c$, blue: $R = 16R_c$.

With the account of the smoothness of the interplanar potential near the atomic planes, in addition to the linear and square root dependencies on μ in Eq. (16) there emerge logarithmic dependencies singular at $\mu \to 0$, and also $\mu \to 1$ [5]. That gives rise to effects of orbiting and rainbow scattering, which for positively charged particles are relatively small and temperature dependent. The resulting behavior of the angular distribution for a realistic interplanar potential is shown in Fig. 6.

Summary

- There exist exact representations for the generic VR angle, mean VR angle and (asymptotically) the angular distribution of VR in an arbitrary continuous potential.
- For model (piecewise parabolic) potentials, the integrals can be taken exactly, and VR angle be expressed in closed form, to all orders in R_c/R.
- For description of the angular distribution, a NNLO analysis in R_c/R is required.
- For VR of negatively charged particles (and to a lesser degree for positively charged VR particles), there are pronounced rainbow and orbiting effects, which can be handled as in [5].
- Tilted periodical ("washboard") potentials similar to the effective potential of a bent crystal are encountered as well in other areas of physics.

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