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Ion Channeling in Direct Dark Matter Detection

A dissertation submitted in partial satisfaction of the
requirements for the degree Doctor of Philosophy
in Physics

by

Nassim Bozorgnia

2012

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ABSTRACT OF THE DISSERTATION

Ion Channeling in Direct Dark Matter Detection

by

Nassim Bozorgnia

Doctor of Philosophy in Physics

University of California, Los Angeles, 2012

Professor Graciela B. Gelmini, Chair

The channeling of the ion recoiling after a collision with a WIMP changes the ionization signal in direct detection experiments, producing a larger signal than otherwise expected. We give estimates of the fraction of channeled recoiling ions in NaI (Tl), Si, Ge, CsI, and solid Xe, Ar and Ne crystals using analytic models produced since the 1960's and 70's to describe channeling and blocking effects. We find that the channeling fraction of recoiling lattice nuclei is smaller than that of ions that are injected into the crystal and that it is strongly temperature dependent. Channeling is a directional effect which depends on the velocity distribution of WIMPs in the dark halo of our Galaxy and could lead to a daily modulation of the signal. We compute upper bounds to the expected amplitude of daily modulation due to channeling using our estimates of the channeling fractions. After developing the general formalism, we examine the possibility of finding a daily modulation due to channeling in the data already collected by the DAMA experiment. We find that even the largest daily modulation amplitudes would not be observable for WIMPs in the standard halo in the 13 years of data taken by the DAMA collaboration. For these to be observable the DAMA total rate should be $1/40$ of what it is or the total DAMA exposure should be 40 times larger. The daily modulation due to channeling will be difficult to measure in future experiments.

The dissertation of Nassim Bozorgnia is approved.

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2012

*To my mother, Mahasty,
whose love and support gave me the courage
to follow my dreams*

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CHAPTER 1

Introduction

The nature of dark matter is still one of the fundamental problems of cosmology and astrophysics today. One of the well-motivated candidates for dark matter is the Weakly Interacting Massive Particle (WIMP), with interaction cross sections at the weak scale and large masses in the GeV-TeV range. Several experiments such as DAMA [14], XENON100 [15], CDMS [16], CoGeNT [2, 17], CRESST [3] and EDELWEISS [18] aim at directly detecting WIMPs.

Direct dark matter experiments search for energy deposited by the scattering of WIMPs in the dark halo of our galaxy. The recoil energy goes into phonons, scintillation, or ionization. If a signal is observed, it is desirable to have unmistakable signatures that it is due to dark matter. Two such signatures are the annual modulation of the signal due to the motion of the Earth around the Sun, extensively studied since [19, 20], and the daily modulation due to the spinning of the Earth around its axis.

Data from three direct dark matter experiments point to the region of low mass (~ 10 GeV) WIMPs: DAMA, CoGeNT and CRESST-II. The DAMA experiment uses NaI (Tl) crystals to detect the scintillation signal. In the 13 years of data, the DAMA collaboration has found a 8.9σ annual modulation signal compatible with the signal expected from dark matter particles bound to our Galactic halo. Recently, a possible dark matter signal for 7-12 GeV WIMPs has been found by the CoGeNT collaboration which is using ultra low-noise germanium detectors. CRESST-II observes an excess of events above their background, which may be interpreted as due to dark matter WIMPs.

Fig. 1.1.a (reproduced from Ref. [3]) shows the regions in cross section versus mass compatible with the CRESST results as well as the exclusion limits from CDMS-II, XENON100,

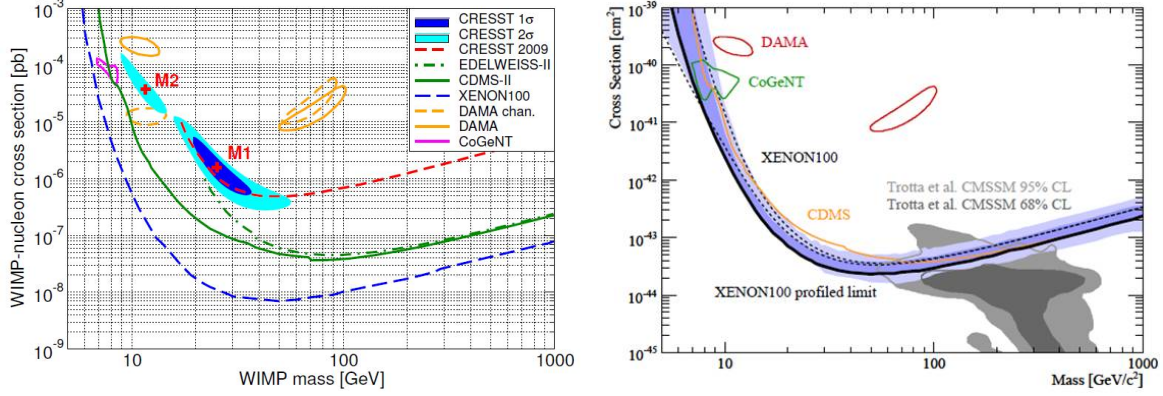


Figure 1.1: Parameter space of spin-independent elastic WIMP-nucleon cross section as a function of WIMP mass. (a) The region compatible with the CRESST results together with the exclusion limits from CDMS-II, XENON100, and EDELWEISS-II, as well as the CRESST limit obtained in an earlier run. The 90% confidence regions favored by CoGeNT and DAMA (without and with ion channeling) are also shown. (b) Upper limit from XENON100 at 90% CL shown in thick (black) line, as well as the sensitivity for the data set analyzed shown as light and dark (blue) shaded areas at 1σ and 2σ CL, respectively. Two limits from the same data set, derived for two assumptions of the behavior of the scintillation efficiency factor are shown as dotted lines, and a limit from CDMS is shown as thin (orange) line. Expectations from a theoretical model [1], and the areas (at 90% CL) favored by CoGeNT (green) [2] and DAMA (red, without channeling) are also shown. Figs. 1.1.a and 1.1.b are reproduced from Ref. [3], and Ref. [4], respectively.

EDELWEISS-II, and CRESST (obtained in an earlier run). The 90% confidence regions favored by CoGeNT and DAMA is also shown. Fig. 1.1.b (reproduced from Ref. [4]) shows the upper limits from XENON100 at 90% confidence level (CL) and the sensitivity as the one sigma and two sigma bands. Limits from XENON100 derived for two assumptions of the behavior of the scintillation efficiency, limits from CDMS, expectations from a theoretical model [1], and the regions (at 90% CL) favored by CoGeNT and DAMA are also shown.

Ion channeling in crystals has received a large amount of attention in the interpretation of experiments designed to search for dark matter WIMPs through their scattering in a low-

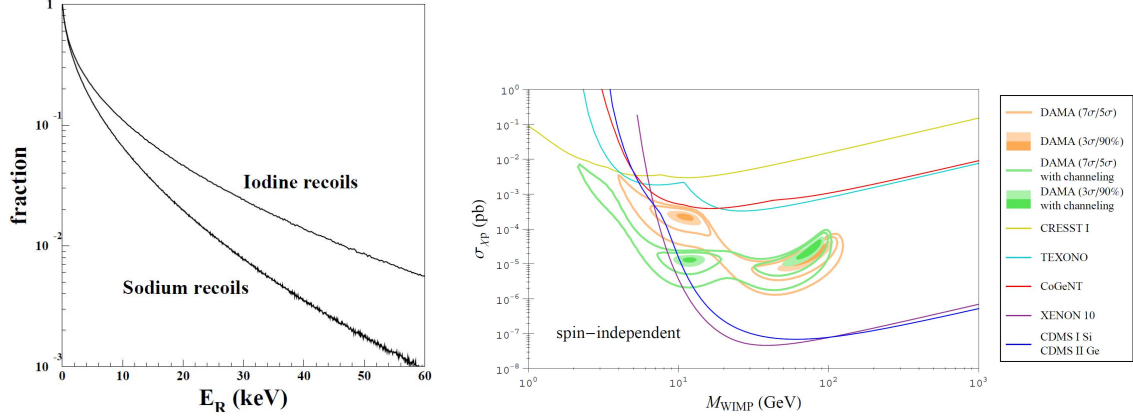


Figure 1.2: (a) Fraction of channeled recoils as a function of the recoil energy in NaI (Tl) crystals, and (b) experimental constraints as well as the DAMA best fit parameters for spin-independent only scattering. The DAMA best fit regions are determined using a likelihood ratio method with (green) and without (orange) the channeling effect as evaluated by the DAMA collaboration. Figs. 1.2.a and 1.2.b are reproduced from Ref. [5], and Ref. [6], respectively.

background detector. Channeling would occur when the nucleus that recoils after being hit by a dark matter particle moves off in a direction close to a symmetry axis or symmetry plane of the crystal. Channeled ions lose their energy predominantly to electrons, while non-channeled ions transfer their energy to lattice nuclei. In scintillators like NaI (Tl), which are sensitive to the electronic energy losses, channeling increases the fraction of recoil energy that is observed as scintillation light. The DAMA collaboration [5] evaluated the fraction of channeled recoils and found it to be large for low recoiling energies in the keV range. This effect shifts the regions in cross section versus mass of acceptable WIMP models in agreement with the DAMA data towards lower WIMP masses [6]. Fig. 1.2.a (reproduced from Ref. [5]) shows the channeling fraction of Na and I recoils evaluated by the DAMA collaboration as a function of the recoil energy. Fig. 1.2.b (reproduced from Ref. [6]) shows the experimental constraints and DAMA best fit parameters determined using a likelihood ratio method with and without the channeling effect as evaluated by the DAMA collaboration.

Another aspect of channeling is that it could give rise to a daily modulation due to the

preferred direction of the dark matter flux arriving on the Earth (“WIMP wind”). Earth’s daily rotation naturally changes the direction of the WIMP wind with respect to the crystal axes and planes, thus changing the amount of recoiling ions that are channeled vs. non-channeled. This amounts to a daily modulation of the dark matter signal detectable via scintillation or ionization. If this daily modulation could be measured, it would be a signature of dark matter without background. This was pointed out by Avignone, Creswick, and Nussinov [21, 22] for NaI (Tl) crystals, although their estimates of the amplitude of the daily modulation were simplistic.

Given the importance of channeling in the interpretation of direct detection experiments, and the need to refine the previous calculations of a possible daily modulation due to channeling, it has been worthwhile to take a deeper look at channeling in the context of dark matter detection. We evaluate the upper bounds on the channeling fractions for different crystalline detectors used in dark matter experiments through analytical means. Our calculations are based on classical analytic models developed since the 1960’s and 70’s (e.g. by Lindhard [23]). We find that the channeling fractions for all the crystals we study would never be larger than a few percent, and the result of our work has had important consequences on the compatibility of the DAMA results with other experiments. We also compute the daily modulation amplitudes expected in the data already collected by the DAMA experiment and find large modulation amplitudes of the signal rate, of the order of 10% in some instances, which are not observable at the 3σ level.

This dissertation is based on [9, 10, 11, 12, 13] (see also [24, 25, 26, 27, 28, 29]). In Chapter 2 we give the definitions and a brief history of ion channeling and blocking. In Chapter 3 we present our analytic calculations of the channeling fraction in NaI (Tl). We present our results for Si and Ge crystals in Chapter 4, CsI in Chapter 5, and solid Xe, Ar, and Ne in Chapter 6. Our calculations of the daily modulation due to channeling is presented in Chapter 7, and the conclusions are given in Chapter 8.

CHAPTER 2

Ion channeling and blocking

Channeling and blocking effects in crystals refer to the orientation dependence of charged ion penetration in crystals. In the “channeling effect” ions incident upon a crystal along symmetry axes and planes suffer a series of small-angle scatterings that maintain them in the open “channels” between the rows or planes of lattice atoms and thus penetrate much further into the crystal than in other directions. Channeled incoming ions do not get close to lattice sites, where they would be deflected at large angles. The “blocking effect” consists in a reduction of the flux of ions originating in lattice sites along symmetry axes and planes, creating what is called a “blocking dip” in the flux of ions exiting from a thin enough crystal as a function of the exit angle with respect to a particular symmetry axis or plane. Directional effects in ion penetration in crystals was first observed in 1960 [30] in the sputtering ratio for ions bombarding a single crystal and its explanation in terms of channeling was first done in 1962 [31], although the effect had been predicted to exist in 1912 [32]. Strongly anisotropic effects for positive particle trajectories originating at lattice sites were discovered in 1965, with particles emitted from radioactive atoms and wide-angle scattering of positive ions in several experiments. Immediately the relation between these blocking effects and the channeling effect was explained by Lindhard [23] in 1965. In the 1960’s and 70’s the experimental and theoretical work on channeling proceeded at a very fast pace (see for example the review by D. Gemmell [33] and references therein).

Channeling and blocking effects in crystals are used in crystallography, in the study of lattice disorder, ion implantation, and the location of dopant and impurity atoms in crystals, in studies of surfaces, interfaces and epitaxial layers, in measurements of short nuclear lifetimes, in the production of polarized beams etc (see for example [34, 35, 36]).

Channeling and blocking effects are related because the non-channeled incident ions are those which suffer a close-encounter process with an atomic nucleus in the crystal, namely those which pass sufficiently close to a lattice nucleus to be deflected at a large angle. After a close-encounter collision the deflected ion acts as if it was “emitted” from a lattice site. Channeling is many times observed as a lack of large angle deflections for ions incident at a small angle ψ with respect to a particular symmetry axis or plane. This forms a “channeling dip” in the outgoing flux as a function of the incident beam angle ψ . As first pointed out by Lindhard [23], when no slowing-down processes are involved, the “channeling” and “blocking” dips should be identical, when compared for the same particles, energies, crystals and crystal directions.

Ion channeling in NaI (Tl) was first observed in 1973 by Altman, Dietrich, Murray and Rock [37]. They observed that the scintillation output of a monochromatic 10 MeV ^{16}O beam through an NaI (Tl) scintillator shows two peaks: one at low energy due to non-channeled ions, and one at high energy due to channeled ions. The channeled ions produce more scintillation light because they lose most of their energy via electronic stopping rather than nuclear stopping.

This may be an important effect in direct dark matter detection experiments in which a scintillation signal due to the recoil of ions as a result of WIMP collisions is searched for. The potential importance of the channeling effect for direct dark matter detection was first pointed out for NaI (Tl) by Drobyshevski [38] and by the DAMA collaboration [5]. When Na or I ions recoiling after a collision with a dark matter WIMP move along crystal axes and planes, their quenching factor is approximately $Q = 1$ instead of $Q_{\text{Na}} = 0.3$ and $Q_{\text{I}} = 0.09$, since they give their energy to electrons. The DAMA collaboration [5] found that the fraction of channeled recoils is large for low recoiling energies in the keV range.

Most of the applications of channeling and blocking are at energies of MeV and higher, however some use much lower energies, up to the keV range. In particular, avoiding channeling is essential in the manufacturing of semiconductor devices, since ion implantation at a controlled depth is the primary technique. Boron, arsenic and phosphorus ions are implanted

in silicon, for example, to produce integrated circuits, at energies from 100's of eV to several MeV (see for example [39]).

CHAPTER 3

Channeling fraction in NaI (Tl) crystals

3.1 Models of Channeling

3.1.1 Continuum models

There are different approaches to calculate the deflections of ions traveling in a crystal. In the “binary collision model” the ion path is computed by a computer program (see Ref. [40] for one of the first ones) in terms of a succession of individual interactions, each with one of the atoms in the crystal. Crystal imperfections and lattice vibrations are thus easily and correctly taken into account. In “continuum models”, reasonable approximations are made which allow to replace the discrete series of binary collisions with atoms by a continuous interaction between a projectile and uniformly charged strings or planes. These models allow to replace the numerical calculations by an analytic description of channeling, and provide good quantitative predictions of the behavior of projectiles in the crystal in terms of simple physical quantities. This is the approach we use here. This analytical description was initially developed mostly by J. Lindhard [23] and collaborators for ions of energy MeV and higher, and its use was later extended to lower energies, i.e. hundreds of eV and above, mostly to apply it to ion implantation in Si. This approach must be complemented by determination of parameters through data fitting or simulations. Moreover, lattice vibrations are more difficult to include in continuum models. Since we use a continuum model, our results should in last instance be checked by using some of the many sophisticated simulation programs that implement the binary collision approach or mixed approaches (e.g. [41, 42, 43, 44, 45, 46, 47, 48]).

Although the analytical description works better at higher energies (where it has been very well tested experimentally), at low and intermediate energies the critical angles for channeling predicted by analytic models have also been found to be in good agreement with experimental results. For the low energy range we found most useful the work of G. Hobler, who in 1996 [7, 49] perfected and checked experimentally previous continuum model predictions [50] for axial and planar channeling at energies in the keV to a few 100 keV range, to avoid channeling in the implantation of B, P and As atoms in Si crystals. Measurements of axial critical angles obtained in the late 1960's for light (H^+ , D^+ and He^+) and intermediate mass (B and Ar) ions propagating in various crystals (gold, tungsten, silicon) with energies between 1 and 100 keV were found to be in good agreement with the predictions of Lindhard models [51, 52, 53]. In 1999 K. M. Lui [54] and collaborators compared experimental results of 5 keV Ne^+ ions on platinum and predictions of the trajectory simulation code SARIC [47], based on the binary collision model, with the predictions of Lindhard's analytical model and the observed angular half-width of the blocking dips for axial channels were found to be in good qualitative agreement with Lindhard's critical angle (both are similar as can be seen in Table I of Ref [54]). In 2002, S. M. Hogg *et al.* [55] studied channeled implantation of 80 keV Er ions into Si and concluded that the axial measured critical angle was in excellent agreement with both computer simulations (made with the MDRANGE program [48]) and experimental results. In 2005 Lindhard's critical angle prediction was used to understand qualitative features of computational results of the SARIC program for 4 keV Ne^+ ions impinging on a Pt surface [56].

Our calculation is based on the classical analytic models developed in the 1960's and 70's, in particular by Lindhard [23, 57, 58, 59, 60, 61, 62, 63, 64]. The fact that the de Broglie wavelengths of ions in the keV-MeV range are of the order of ~ 0.01 pm (and smaller at higher energies), which is much less than the lattice constant of a crystal (~ 10 pm), justifies using a classical treatment. We use the continuum string and plane model, in which the screened Thomas-Fermi potential is averaged over a direction parallel to a row or a plane. This averaged potential U is considered to be uniformly smeared along the row or plane of atoms, which is a good approximation if the propagating ion interacts with many lattice

atoms in the row or plane by a correlated series of many consecutive glancing collisions with lattice atoms. We are going to consider just one row, which simplifies the calculations and is correct except at the lowest energies we consider, as we explain below.

There are several good analytic approximations of the screened potential. In this chapter we use Lindhard's expression, because it is the simplest and allows to find analytical expressions for the quantities we need. The transverse averaged continuum potential of a string as a function of the transverse distance r to the string, relevant for axial channeling, was approximated by Lindhard [23] as

$$U(r) = E\psi_1^2 \frac{1}{2} \ln \left(\frac{C^2 a^2}{r^2} + 1 \right), \quad (3.1)$$

where C is a constant, which was found experimentally to be $C \simeq \sqrt{3}$, and

$$\psi_1^2 = \frac{2Z_1 Z_2 e^2}{Ed}. \quad (3.2)$$

Z_1, Z_2 are the atomic numbers of the recoiling and lattice nuclei respectively, d is the spacing between atoms in the row, a is the Thomas-Fermi screening distance, $a = 0.4685 \text{\AA} (Z_1^{1/2} + Z_2^{1/2})^{-2/3}$ [40, 33] and $E = Mv^2/2$ is the kinetic energy of the propagating ion. In our case, E is the recoil energy imparted to the ion after a collision with a WIMP,

$$E = \frac{|\vec{\mathbf{q}}|^2}{2M}, \quad (3.3)$$

where $\vec{\mathbf{q}}$ is the recoil momentum. The string of crystal atoms is at $r = 0$.

The transverse averaged continuum potential of a plane of atoms, relevant for planar channeling, given by Lindhard [23] as a function of the distance x perpendicular to the plane is

$$U_p(x) = E\psi_a^2 \left[\left(\frac{x^2}{a^2} + C^2 \right)^{\frac{1}{2}} - \frac{x}{a} \right], \quad (3.4)$$

where ψ_a is

$$\psi_a = \left(\frac{2\pi n Z_1 Z_2 e^2 a}{E} \right)^{\frac{1}{2}} \quad (3.5)$$

and $n = Nd_{\text{pch}}$ is the average number of atoms per unit area, where N is the atomic density and d_{pch} is the width of the planar channel, i.e. the interplanar spacing (thus the average

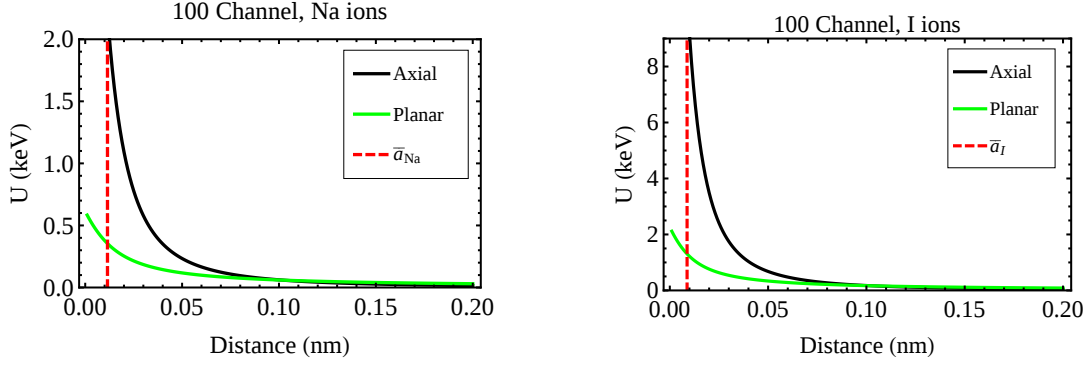


Figure 3.1: Continuum axial (black) and planar (green/gray) potentials for (a) Na and (b) I ions, propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of an NaI crystal. The screening radii shown as vertical lines are $\bar{a}_{\text{Na}} = 0.00878$ nm and $\bar{a}_{\text{I}} = 0.0115$ nm (see Appendix A.1).

distance of atoms within a plane is $d_p = 1/\sqrt{Nd_{\text{pch}}}$. The plane is at $x = 0$. Examples of axial and planar continuum potentials are shown in Fig. 3.1.

The continuum model does not imply that the potential energy of an ion moving near an atomic row is well approximated by the continuum potential U . The actual potential consists of sharp peaks near the atoms and deep valleys in between. The continuum model says that the net deflection due to the succession of impulses from the peaks is identical to the deflection due to a force $-U'$. This is only so if the ion never approaches any individual atom so closely that it suffers a large-angle collision. Lindhard proved that for a string of atoms this is so only if

$$U''(r) < \frac{8}{d^2} E, \quad (3.6)$$

where the double prime denotes the second derivative with respect to r . Replacing the inequality in Eq. 3.6 by an equality defines an energy dependent critical distance r_c such that $r > r_c$ for the continuum model to be valid. Morgan and Van Vliet [59] also derived a condition for axial channels, similar to Eq. 3.6 (but with the factor 8 replaced by 16).

The condition in Eq. 3.6 for the validity of the continuum model on the axial effective potential is equivalent (as shown initially by Lindhard and proven below) to insuring that

the minimum distance of approach to the string remains larger than $\simeq d \psi_1$ for large E (MeV and above) and $\simeq d \psi_2$ (with ψ_2 given in Eq. 3.18) for small E (below 100's of keV). Thus, the smaller the atomic interdistance d and the larger the ion velocity (i.e. the smaller ψ_1 or ψ_2) the more accurate the continuum model [36].

The appearance of the angle ψ_1 in this condition can be easily understood by considering the “Coulomb shadow” formed by individual atoms behind the direction of arrival of a parallel beam of positive ions. For an unscreened Coulomb potential and small angle deflections, the trajectories of the projectiles give rise to a shadow cone in which the projectiles do not enter. A distance z behind the deflecting nucleus in the direction of arrival of the projectiles, the shadow cone radius is $D(z) = \sqrt{2zd} \psi_1$ (here d enters through the definition of ψ_1). As the incident angle of the incoming ions with respect to the row of atoms decreases, there is a critical value of the incident angle at which the edge of the shadow of an atom passes through the adjacent atom. This critical angle is approximately $D(d)/d = \sqrt{2} \psi_1$. For angles of incidence larger than $\sim \psi_1$, the shadow cones of the atoms in a row are independent of each other. But for incident angles smaller than $\sim \psi_1$, the shadow cones interfere with each other, so that the atoms in a row are effectively shadowed and not exposed to the projectiles [65, 36]. In this case the incident ions do not approach the shadowed atoms closer than a distance $D(d) \simeq d \psi_1$, as mentioned above. For a more realistic screened Coulomb potential (as considered in this chapter) the shadow cone radius is smaller than for the unscreened potential and the difference between the two becomes smaller for higher ion energies.

The breakdown of the continuum theory for planar channeling is more involved than for axial channeling because the atoms in the plane contributing to the scattering of the propagating ion are usually displaced laterally within the plane. Thus the moving ion does not encounter atoms at a fixed separation or at fixed impact parameter as is the case for a row. Morgan and Van Vliet [59] reduced the problem of scattering from a plane of atoms to the scattering from an equivalent row of atoms contained in a strip centered on the projection of the ion path on the plane of atoms. They then applied Eq. 3.6 to the “fictitious string” defined in this way as the condition for planar channeling (more about this below).

3.1.2 The transverse energy

Lindhard proved that for channeled particles the longitudinal component $v \cos \phi$, i.e. the component along the direction of the row or plane of the velocity, may be treated as constant (if energy loss processes are neglected). Then, in the continuum model, the trajectory of the ions can be completely described in terms of the transverse direction, perpendicular to the row or plane considered. For small angle ϕ between the ion's trajectory and the atomic row (or plane) in the direction perpendicular to the row (or plane), the so called “transverse energy”

$$E_{\perp} = E \sin^2 \phi + U \simeq E \phi^2 + U \quad (3.7)$$

is conserved. In Eq. 3.7 relativistic corrections are neglected.

In each binary collision of the ion with the closest atom, $E_{\perp}$ changes abruptly, because the angle ϕ changes in a very short time (i.e. while the potential is practically constant). Then, between two collisions, the change is compensated because the potential component of $E_{\perp}$ changes continuously as the ion propagates while the angle ϕ is constant [36]. A good way to test to what extent this compensation takes place is to calculate the value of $E_{\perp}$ far away from the collision sites, namely half-way between successive collision sites.

The condition in Eq. 3.6 was derived by Lindhard (in Appendix A of Ref. [23]) for axial channels by defining $E_{\perp}$ at the planes half-way between string of atoms and asking for $E_{\perp}$ at contiguous half-way planes to be conserved to first order (this is the so called “half-way plane” model). Morgan and Van Vliet [59] derived a condition for axial channeling very similar to Eq. 3.6 by calculating the difference between the scattering angle due to a binary collision and the deflection angle in the continuum potential when the ion travels the distance between two contiguous halfway planes (the half-way planes considered by Lindhard).

Let r_i be the initial position at which the WIMP nucleus collision occurs, i.e. if $r_i > 0$ the recoiling nucleus was displaced with respect to its position of equilibrium in the string when it collided with a WIMP. We call ϕ the angle of the initial recoil momentum with respect to the row of atoms, and E the initial recoil energy of the propagating ion. Given these initial

parameters, the issue of where to define $E_{\perp}$ arises. Namely, we define

$$E_{\perp} = E \sin^2 \phi + U(r^*), \quad (3.8)$$

but there are different possible choices for r^* , the position at which to measure the potential U . In the “half-way plane model” used by Lindhard, U is measured after the recoiling ion propagates a distance $d/2$ along the string, when it is at a distance

$$r^* = r_{\text{HP}}^* \equiv r_i + (d/2) \tan \phi \quad (3.9)$$

perpendicular to the string at the halfway-plane. All angles we are dealing with are small enough that $\sin \phi \simeq \tan \phi \simeq \phi$. This choice was shown to work better in some respects [61] (such as the blocking angular distribution in axial channels) than the “continuum approximation.” In the latter, the transverse energy $E_{\perp}$ is considered to be conserved all along the string, not only at the halfway-planes, in which case r^* is chosen to be just

$$r^* = r_{\text{CA}}^* \equiv r_i. \quad (3.10)$$

The two choices $r^* = r_{\text{HP}}^*$ and $r^* = r_{\text{CA}}^*$ coincide only if $d \tan \phi / 2r_i \ll 1$, a condition that at energies below 100’s of keV is in general not fulfilled, in which case the “continuum approximation” is not a good approximation. In fact, assuming the “continuum approximation”, the angle at the first halfway plane must have a different value, ϕ' say, such that $\sin^2 \phi' - \sin^2 \phi = [U(r_i) - U(r_i + \frac{1}{2}d \tan \phi)]/E$. Fig. 3.1 shows that the potential U at a distance a or larger is in the 1-10 keV range. Thus the difference between both definitions of the transverse energy is very small at large enough values of the energy $E \gg 10$ keV, but for lower values of E , in the keV to the 10’s of keV range, the definitions $r^* = r_{\text{HP}}^*$ and $r^* = r_{\text{CA}}^*$ give different results unless ϕ is small enough. In Ref. [61] the predictions of both models for blocking of 400 keV protons in W and 7 MeV protons in Si were compared with the predictions of the binary-collision model. The “half-way plane model” results were found to be in agreement with those of the binary-collision model, even when those of the “continuum approximation” were not.

In all these cases, even when considering blocking, the propagating ion was always different than a lattice ion. In our case, the recoiling ion leaves an empty lattice site, thus it

moves away from an empty lattice site in the potential generated by its neighboring lattice atoms. So the potential that the recoiling ion moves through at the moment of collision is very small, and the recoiling ion conserves its momentum and direction of motion until it gets very near the nearest neighbor, a distance d away along the string. At this moment, it is at a distance

$$r^* = r_{\text{rec}}^* \equiv r_i + d \tan \phi_i \quad (3.11)$$

from its nearest neighbor. Therefore, we will make the approximation of defining the potential entering into Eq. 3.8 at $r^* = r_{\text{rec}}^*$.

3.1.3 Minimum distance of approach and critical channeling angle

The conservation of the transverse energy provides a definition of the minimum distance of approach to the string, r_{min} (or to the plane of atoms x_{min}), at which the trajectory of the ion makes a zero angle with the string (or plane), and also of the angle ψ at which the ion exits from the string (or plane), i.e. far away from it where $U \simeq 0$. In reality the furthest position from a string or plane of atoms is the middle of the channel, whose width we call d_{ach} for an axial channel or d_{pch} for a planar channel, thus

$$E_{\perp} = U(r_{\text{min}}) = E\psi^2 + U(d_{\text{ach}}/2). \quad (3.12)$$

We define the axial channel width d_{ach} in terms of the interatomic distance d as $d_{\text{ach}} = 1/\sqrt{Nd}$, where N is the atomic density.

For axial channeling Lindhard equates the condition for channeling with the condition in Eq. 3.6 for the validity of the continuum model. For Lindhard's axial potential, this condition reads

$$E > \frac{E_1 d^2}{8} \frac{1 + 3(\frac{r_{\text{min}}}{Ca})^2}{r_{\text{min}}^2 (1 + (\frac{r_{\text{min}}}{Ca})^2)^2}, \quad (3.13)$$

where $E_1 = E\psi_1^2$ (and ψ_1 was defined in Eq. 3.2). Since the right-hand side of this inequality is a monotonically decreasing function of r_{min} , one just needs to solve the equation obtained by replacing the inequality with an equality. Solving a cubic equation, the condition in Eq. 3.13 can be inverted to find $r_c(E)$, the minimum value of r_{min} . We find the following

decreasing function of E

$$r_c(E) = Ca \sqrt{\frac{2}{3} \left[\sqrt{1+z} \cos\left(\frac{1}{3} \arccos \frac{(1-3z/2)}{(1+z)^{3/2}}\right) - 1 \right]}, \quad (3.14)$$

where to simplify the expression we defined

$$z = \frac{9E_1 d^2}{8EC^2 a^2}. \quad (3.15)$$

This expression gives the smallest possible minimum distance of approach of the propagating ion with the row for a given energy E , i.e. $r_{\min} > r_c(E)$ and, since the potential $U(r)$ decreases monotonically with increasing r ,

$$U(r_{\min}) < U(r_c(E)). \quad (3.16)$$

Using Eq. 3.12, this can be further translated into an upper bound on $E_{\perp}$ and on ψ , the angle the ion makes with the string far away from it,

$$\psi < \psi_c(E) = \sqrt{\frac{U(r_c(E)) - U(d_{\text{ach}}/2)}{E}}. \quad (3.17)$$

$\psi_c(E)$ is the maximum angle the ion can make with the string far away from it (i.e. in the middle of the channel) if the ion is channeled. When $U(d_{\text{ach}}/2)$ can be neglected, i.e. when $r_c(E) < d_{\text{ach}}/2$, the limiting values of $\psi_c(E)$ (as already proven by Lindhard [23]) are $\psi_c(E) \simeq \psi_1$ (see Eq. 3.2) for large E ($z \ll 1$, typically close to MeV and larger) and $\psi_c(E) \simeq \psi_2$ at low E ($z \gg 1$, typically smaller than a few 100 keV), where

$$\psi_2 = \sqrt{\frac{Ca\psi_1}{d\sqrt{2}}}. \quad (3.18)$$

One can easily see that the critical distance r_c becomes $r_c \simeq d \psi_1 / 2\sqrt{2}$ for large E and $r_c \simeq d \psi_2$ for small E .

The critical distance $r_c(E)$ increases as E decreases. At low enough E , $r_c(E)$ becomes close to $d_{\text{ach}}/2$, and the critical angle $\psi_c(E)$, the maximum angle for channeling in the middle of the channel, goes to zero. This means that there is a minimum energy below which channeling cannot happen, even for ions moving initially in the middle of the channel.

This is a reflection of the fact that the range of the interaction between ion and lattice atoms increases with decreasing energy and at some point there is no position in the crystal where the ion would not be deflected at large angles. The existence of a minimum energy for channeling was found by Rozhkov and Dyuldy [66] in 1984 and later by Hobler [7, 49] in 1996. It is clear that to compute $r_c(E)$ when it is not small with respect to $d_{\text{ach}}/2$, and thus to compute the actual minimum energy for channeling, we would need to consider the effect of more than one row or plane (as done in Refs. [7, 49, 66]), thus our results are approximate in this case.

For planar channeling we will follow the definition of fictitious row in Morgan and Van Vliet [59, 7]. They reduced the problem of scattering from a plane of atoms to the scattering of an equivalent row of atoms contained in a strip of width $2R$ (R is defined below) centered on the projection of the ion path on the plane of atoms, and took the average area per atom in the plane to be $2R$ times the characteristic distance $\bar{d}$ between atoms along this fictitious row,

$$\bar{d} = 1/(Nd_{\text{pch}}2R). \quad (3.19)$$

Once the width $2R$ of the fictitious row is specified, one uses the channeling condition for the continuum string model, Eq. 3.6, with an average atomic composition of the plane. For R , Morgan and Van Vliet used the impact parameter in an ion-atom collision corresponding to a deflection of the order of the break-through angle $\sqrt{U_p(0)/E}$. This is the deflection necessary for an ion of energy E approaching the plane from far away (so that the initial potential can be neglected) to overcome the potential barrier at the center of the plane at $x = 0$ (namely so that $E_{\perp} = U_p(0)$). Using the Moliere approximation for the screened potential (which we do not use in this chapter), Morgan and Van Vliet found for $\bar{d}$

$$\bar{d}^{\text{MV}} = \left[A a N d_{\text{pch}} \ln \left(B Z_1 Z_2 e^2 / a \sqrt{E U_p(0)} \right) \right]^{-1}, \quad (3.20)$$

with coefficients $A = 1.2$ and $B = 4$. However, Morgan and Van Vliet [59] found discrepancies with this theoretical formula in simulations of binary collisions of 20 keV protons in a copper crystal and adjusted the coefficients to $A = 3.6$ and $B = 2.5$. Hobler [7] used both sets of coefficients and compared them with simulations and data of B and P in Si for energies of

about 1 keV and above. Hobler concluded that the original theoretical formula was better in his case. In any case, Hobler proposed yet another empirical relation to define $\bar{d}$.

In the absence of simulations for NaI, we are going to use an upper bound on R , given by the average interdistance of atoms in the plane, $2R < d_p = 1/\sqrt{Nd_{\text{pch}}}$, so that replacing the maximum value of R in Eq. 3.19 we find that the minimum value of $\bar{d}$ is the average interdistance of atoms in the plane, d_p

$$\bar{d}_{\text{min}} = d_p. \quad (3.21)$$

Thus, for planar channeling, we use the condition in Eq. 3.6 for a fictitious string, replacing the distance d by the distance d_p and replacing the composition of the string for the average composition of the plane. Let us call $\bar{r}_c(E)$ the critical distance obtained from Eq. 3.14 for this fictitious string, then the minimum distance of approach for planar channeling is

$$x_c(E) \equiv \bar{r}_c(E). \quad (3.22)$$

The use of $\bar{d} = d_p$ yields a lower bound on x_c , as shown in Fig. 3.2 (and thus an upper bound on the fraction of channeled recoils as explained later). Fig. 3.2 shows the planar critical distances of approach x_c (Eq. 3.22) using the theoretical (with coefficients $A = 1.2$ and $B = 4$) and adjusted (with coefficients $A = 3.6$ and $B = 2.5$) Morgan-Van Vliet expressions for $\bar{d}$ in Eq. 3.20. Our choice of x_c , with $\bar{d}$ in Eq. 3.21 is also plotted in Fig. 3.2. We can see that it is lower than the others.

Writing equations equivalent to Eq. 3.12 and 3.16 for planar channels, namely

$$E_{\perp} = U(x_{\text{min}}) = E(\psi^p)^2 + U_p(d_{\text{pch}}/2), \quad (3.23)$$

and

$$U_p(x_{\text{min}}) < U_p(x_c(E)), \quad (3.24)$$

we obtain an equation similar to Eq. 3.17 but for the maximum planar channeling angle,

$$\psi_c^p(E) = \sqrt{\frac{U_p(x_c(E)) - U_p(d_{\text{pch}}/2)}{E}}. \quad (3.25)$$

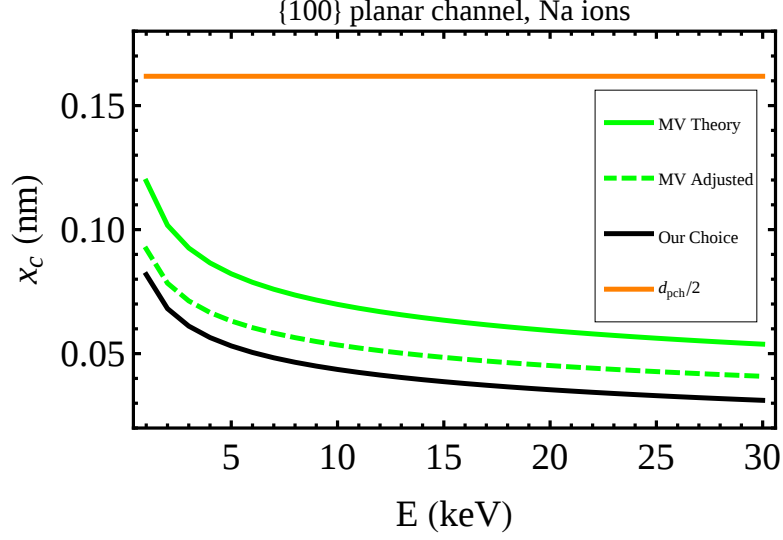


Figure 3.2: Comparison of planar critical distances of approach as given by the theoretical (solid line) and adjusted (dashed line) Morgan-Van Vliet (label MV, green/gray) expressions for $\bar{d}$ and our choice (black) of x_c , which we take as a lower bound, as function of the energy for Na ions travelling in $\{100\}$ planar channels. Also shown is the radius of the channel $d_{\text{pch}}/2$.

For very small energies, for which $x_c(E) \geq d_{\text{pch}}/2$ no channeling is possible (the maximum distance to any plane cannot be larger than half the width of the channel separating them). When $x_c(E)$ approaches the middle of the channel the effect of other planes should be considered, so our approximation of using the potential of only one plane is not correct in this regime.

The static lattice critical distances are presented in left panel of Figs. 3.4 and 3.5 for the 100 and 111 axial and planar channels.

There is an alternative way of treating planar channels presented by Matyukhin [67] in 2008, but we have doubts about the validity of this method, for which we have not found any comparison with either simulations or data. For completeness we present it in Appendix C. It predicts larger channeling fractions.

3.1.4 Temperature dependent critical distances and angles

So far we have been considering static strings and planes, but the atoms in a crystal are actually vibrating. We use the Debye model in this dissertation to take into account the zero point energy and thermal vibrations of the atoms in a crystal. The one dimensional rms vibration amplitude u_1 of the atoms in a crystal in this model is [33, 64]

$$u_1(T) = 12.1 \text{ \AA} \left[\left(\frac{\Phi(\Theta/T)}{\Theta/T} + \frac{1}{4} \right) (M\Theta)^{-1} \right]^{1/2}, \quad (3.26)$$

where the $1/4$ term accounts for the zero point energy, M is the atomic mass in amu, Θ and T are the Debye temperature and the temperature of the crystal in K, respectively, and $\Phi(x)$ is the Debye function,

$$\Phi(x) = \frac{1}{x} \int_0^x \frac{t dt}{e^t - 1}. \quad (3.27)$$

Eq. 3.26 was derived for monoatomic cubic crystals for which M is clearly specified. In the case of crystals composed of more than one kind of atom, experiments have shown that the difference of vibration amplitudes of both types is very small for $T > \Theta$ [68, 69], even when the difference of atomic weights of the various kinds of atoms is large, as is the case for NaI. Using as M the average mass

$$M = (M_{\text{Na}} + M_{\text{I}})/2 \quad (3.28)$$

produces an error of less than 10% in the actual vibration amplitudes at $T > \Theta$ [68, 69]. For NaI, we take the Debye temperature to be $\Theta = 165$ K [33, 70] (although it changes with T between 169 K at a few K and 155 K at 300 K [71]). The crystals in the DAMA experiment are at 20 °C, i.e. $T = 293.15$ K; $M_{\text{Na}} = 22.9$ amu and $M_{\text{I}} = 126.9$ amu, thus $M = 74.9$ amu. The vibration amplitude u_1 we get using this value of M is plotted in Fig. 3.3 as a function of the temperature T . At room temperature (20 °C) it is $u_1 = 0.0146$ nm which is similar to the measured value of $\sqrt{\langle u_1^2 \rangle} = 0.0145$ nm [72], while measured separate values of $\sqrt{\langle u_1^2 \rangle}$ for Na and I (always at room temperature) are 0.018 nm and 0.015 nm [73] respectively. (To use the data in Ref. [73] we must take into account that the Debye-Waller factor B is $B = 8\pi^2 \langle u_1^2 \rangle$).

At low temperatures ($T \ll \Theta$) the individual vibration amplitudes become progressively

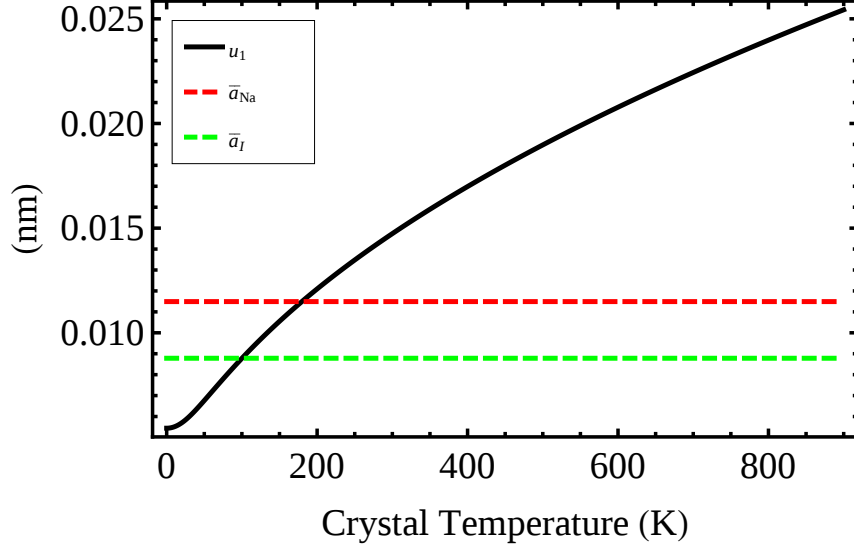


Figure 3.3: Plot of $u_1(T)$ for NaI (Eq. 3.26 with $M = (M_{\text{Na}} + M_I)/2$).

different [74, 75]. We are not taking this difference into account in our approach. However, at these temperatures the channeling fractions become so small (as we show below) that a better calculation is not important.

In principle there are modifications to the continuum potentials due to thermal effects, but we are going to take into account thermal effects in the crystal through a modification of the critical distances which was found originally by Morgan and Van Vliet [59] and later by Hobler [7] to provide good agreement with simulations and data. For axial channels it consists of taking the temperature corrected critical distance $r_c(T)$ to be,

$$r_c(T) = \sqrt{r_c^2(E) + [c_1 u_1(T)]^2}, \quad (3.29)$$

where the dimensionless factor c_1 in different references is a number between 1 and 2 (see e.g. Eq. 2.32 of Ref. [60] and Eq. 4.13 of Ref. [59]).

For planar channels the situation is more complicated, because some references give a linear and other a quadratic relation between $x_c(T)$ and u_1 . Following Hobler [7] we use an equation similar to that for axial channels,

$$x_c(T) = \sqrt{x_c^2(E) + [c_2 u_1(T)]^2}, \quad (3.30)$$

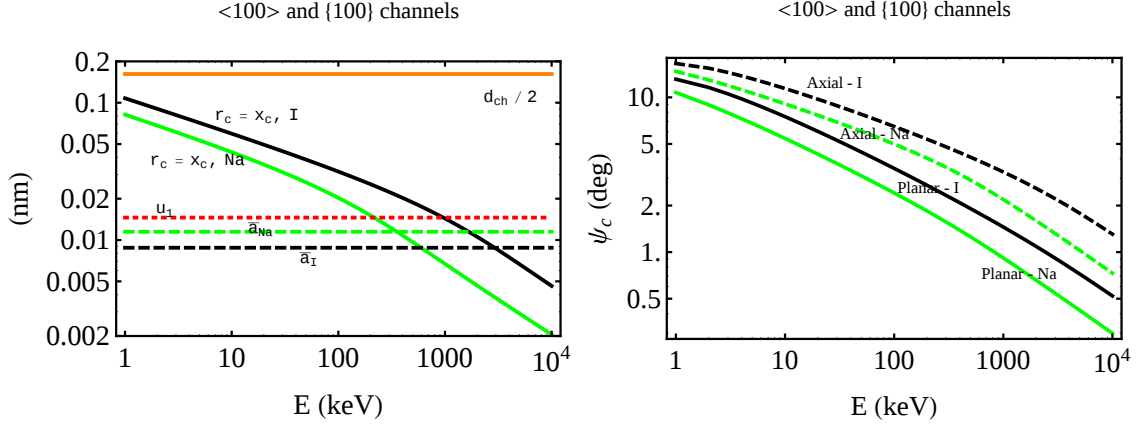


Figure 3.4: (a) Static critical distances of approach and u_1 at 20 °C and (b) critical channeling angles at 20 °C with $c_1 = c_2 = 1$ as a function of the energy of propagating Na (green/gray) and I (black) ions in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels. Here $d_{ach} = d_{pch}$.

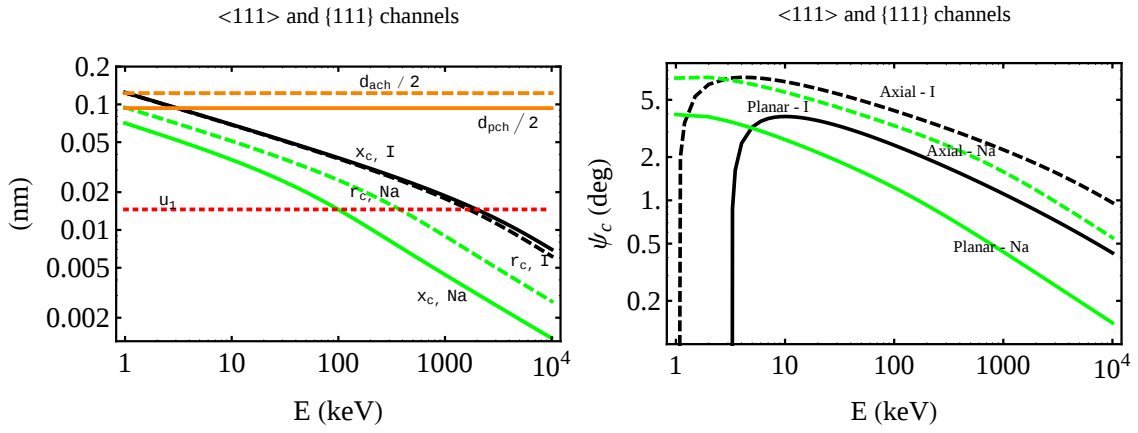


Figure 3.5: Same as Fig. 3.4 but for the $\langle 111 \rangle$ axial and $\{111\}$ planar channels. Here $d_{ach} \neq d_{pch}$.

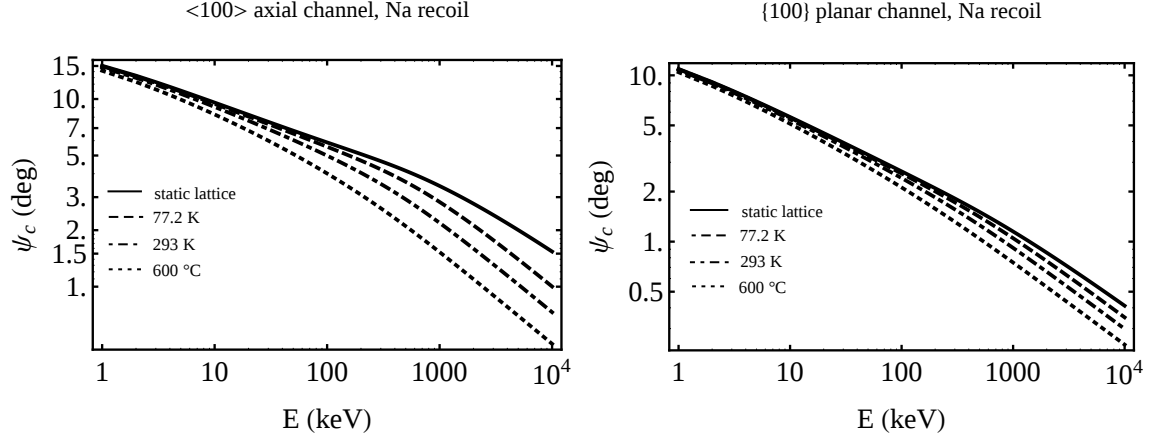


Figure 3.6: Static and T corrected critical angles as a function of energy of Na recoil for $T=77.2$ K, $T=20$ °C, and $T=600$ °C for (a) $\langle 100 \rangle$ axial and (b) $\{100\}$ planar channels.

where again c_2 is a number between 1 and 2 (for example Barret [40] finds $c_2 = 1.6$ at high energies, and Hobler [7] uses $c_2 = 2$). We will mostly use $c_1 = c_2 = 1$ in the following, to try to produce upper bounds on the channeling fractions.

Using the T -corrected critical distances $r_c(T)$ and $x_c(T)$ instead of the static lattice critical distances r_c and x_c in Eqs. 3.14 and 3.22, we obtain the T -corrected critical axial and planar angles.

The static axial and planar critical distances are presented in Figs. 3.4.a and 3.5.a for the 100 and 111 channels, respectively, together with the amplitude of thermal vibrations u_1 at 20 °C. Figs. 3.4.b. and 3.5.b show the temperature corrected axial and planar critical angles at 20 °C (with $c_1 = c_2 = 1$) for the same channels as functions of energy of the traveling Na and I ions. We can clearly see in Fig. 3.5 that the critical angles become zero at low enough energies (for which the critical distance of approach should be larger than the radius of the channel) indicating the range of energies for which no channeling is possible. Figs. 3.6.a and 3.6.b show the static and T -corrected critical angles at several temperatures for traveling Na ions in the 100 axial and planar channels respectively.

In Appendix E it is shown that the variation of the lattice size with temperature, characterized by the variation of the lattice constant a_{lat} with temperature, has a negligible effect

on the channeling fractions. This is why we ignore this effect (not only in this chapter but also in the other chapters).

3.2 Channeling of incident particles

The channeling of ions in a crystal depends not only on the angle their initial trajectory makes with strings or planes in the crystal, but also on their initial position. Ions which start their motion close to the center of a channel, far from a string or plane, where they make an angle ψ or ψ^p respectively, defined in Eqs. 3.12 and 3.23, are channeled if the angle is smaller than a critical angle (as explain earlier) and are not channeled otherwise. Particles which start their motion in the middle of a channel (as opposed to a lattice site) must be incident upon the crystal (thus the title of this section).

Here we show that to a good approximation we can use analytic calculations and reproduce the channeling fraction in NaI presented in Ref. [5]. It must be noticed, however, that in Ref. [5] the channeling fraction is computed as if the Na or I ions started their motion already within a channel (in fact close to the middle of the channel, where they assume the potential to be negligible), instead of starting from crystal lattice sites, as is the case in direct dark matter detection. Thus these calculations do not apply to direct dark matter detection experiments.

Ref. [5] considers only a static lattice (i.e. no temperature effects taken into account) and the condition for axial channeling they use is $\psi < \psi_2$ [23], where ψ_2 is defined in Eq. 3.18. The equivalent condition for planar channeling used in Ref. [5] is

$$\psi^p < \theta_{pl} = a\sqrt{Nd_p} (Z_1 Z_2 e^2 / Ea)^{1/3}. \quad (3.31)$$

For an incident angle ψ with respect to each of the channels and an ion energy E , the fraction $\chi_{\text{inc}}(E, \psi)$ of channeled incident ions for axial and planar channels is $\chi_{\text{inc}} = 1$ if ψ is smaller than the critical angle for the corresponding channel and zero otherwise. The NaI structure and all the different channels are explained in Appendix A.1.

To find the total fraction P_{inc} of channeled incident nuclei, we average χ_{inc} over the

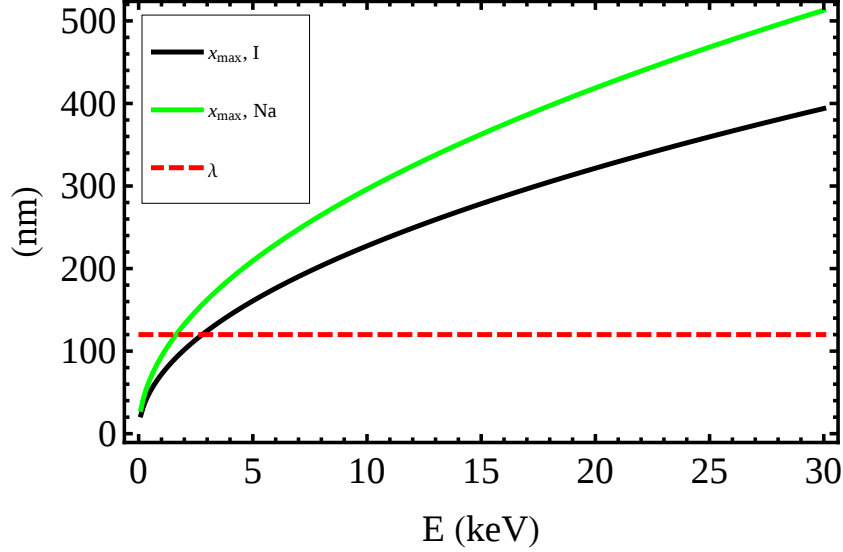


Figure 3.7: Maximum distance $x_{\max}(E)$ traveled by channeled Na (green/gray) or I (black) ions in mixed channels of a NaI crystal ($\langle 100 \rangle$ and $\langle 111 \rangle$ axial and $\{100\}$ and $\{110\}$ planar channels).

incident direction $\hat{\mathbf{q}}$,

$$P_{\text{inc}}(E) = \frac{1}{4\pi} \int \chi_{\text{inc}}(E, \hat{\mathbf{q}}) d\Omega_q. \quad (3.32)$$

This integral cannot be solved analytically, so we integrated numerically by performing a Riemann sum once the sphere of directions has been divided using a Hierarchical Equal Area iso-Latitude Pixelization (HEALPix) [76] (see Appendix B).

A channeled ion can be pushed out of a channel by an interaction with an impurity such as the atoms of Tl in NaI (Tl). The probability density for an ion to find an impurity after propagating a distance x within the crystal is

$$p(x) = \frac{1}{\lambda} \exp\left(-\frac{x}{\lambda}\right), \quad (3.33)$$

where λ is the average distance between the Tl atoms. We take for λ the value used by the DAMA collaboration, i.e. $\lambda = 120$ nm [5], which according to Ref. [38] corresponds to a molar concentration of 0.0013 Tl atoms for every Na atom.

Here we will simply assume that if a channeled ion interacts with a Tl atom it becomes dechanneled and thus it does not contribute to the fully channeled fraction any longer. We

thus neglect the possibility that after the interaction the ion may reenter into a channel, either the same or another, as we also neglect the possibility that initially non-channeled ions may be scattered into a channel. Both effects would increase somewhat the amount of channeled ions, but we do not have an analytic method of including them in our calculation. Thus the channeled fraction is simply reduced by the probability that the ion does not interact with a Tl atom,

$$P^{ch}(E) = \exp\left(-\frac{x_{\max}(E)}{\lambda}\right) P_{\text{inc}}(E). \quad (3.34)$$

Here $x_{\max}(E)$ is the range of the propagating ion, i.e. the maximum distance a channeled ion with initial energy E can propagate along the channel. Within the channel the ion loses energy into electrons. We use the Lindhard-Scharff [77, 63] model of electronic energy loss, valid for energies $E < (M_1/2)Z_1^{4/3}v_0^2$, where $v_0 = e^2/\hbar = 2.2 \times 10^8$ cm/sec is the Bohr's velocity [23]. M_1 and Z_1 are the mass and charge of the propagating ion. This model is valid for $E < 14.3$ MeV for Na and $E < 646.4$ MeV for I in NaI. In this model the energy $E(x)$ as a function of the propagated distance x and the initial energy E is the solution of the following energy loss equation [63]

$$-\frac{dE}{dx} = Kv, \quad (3.35)$$

where $v = \sqrt{2E/M_1}$ is the ion velocity and K is the function

$$K = \frac{\xi_e 8\pi e^2 N a_0 Z_1 Z_2}{\left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{\frac{3}{2}} v_0}. \quad (3.36)$$

Here ξ_e is a dimensionless constant of the order of $Z_1^{\frac{1}{6}}$ [63], N is the number of atomic centers per unit volume and $a_0 \simeq 0.53$ Å is the Bohr radius of the hydrogen atom. Explicitly, an ion with initial energy E at $x = 0$ has energy

$$E(x) = E \left(1 - \frac{x}{x_{\max}}\right)^2 \quad (3.37)$$

after traveling a distance x . The range of the propagating ion is

$$x_{\max}(E) = \frac{\sqrt{2M_1 E_R}}{K}. \quad (3.38)$$

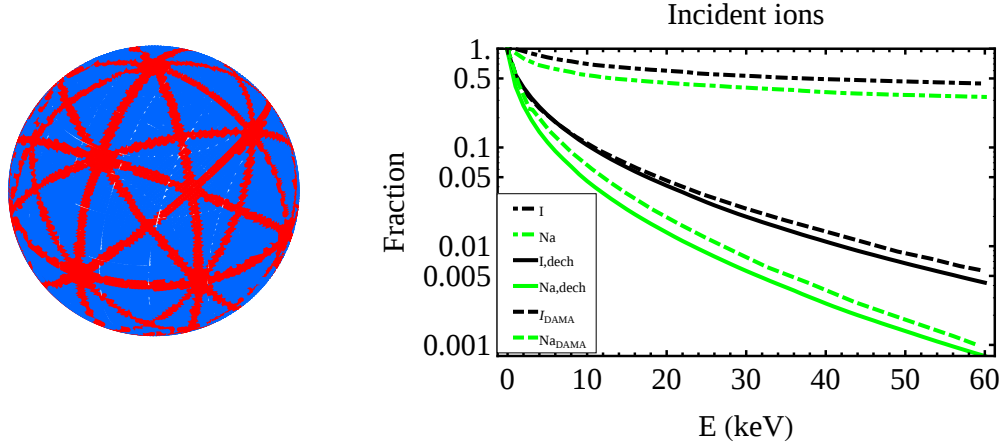


Figure 3.8: (a) Channeling fraction for a 50 keV Na ion in different directions plotted on a sphere using the HEALPix pixelization: probability equal to one in red, and probability equal to zero in blue. (b) Fraction of channeled incident I (black) and Na (green/gray) ions as a function of their incident energy E with the static lattice without (dot dashed lines) and with (solid lines) dechanneling due to interactions with Tl impurities. The results of DAMA are also included (dashed lines).

Fig. 3.7 shows the maximum distance $x_{\max}$ traveled by channeled Na or I ions in mixed channels of an NaI crystal ($\langle 100 \rangle$ and $\langle 111 \rangle$ axial and $\{100\}$ and $\{110\}$ planar channels). The average distance λ between Tl atoms is also shown.

Fig. 3.8.a shows the axial and planar channels of the NaI crystal in the HEALPix pixelization of the sphere for incoming Na ions with an energy of 50 keV: red points indicate a channeling probability of 1 (when the incident angle is smaller than the critical angle with respect to any axial or planar channel) and blue points indicate a channeling probability of zero (when the incident angle is larger than the critical angle). We include here only the channels with lower crystallographic indices, i.e. 100, 110 and 111, which provide the dominant contribution to the channeling fraction, as is also done in Ref. [5]. Fig. 3.8.b shows the fraction of incident I (black lines) or Na (green/gray lines) ions as a function of their incident energy E using the static lattice (solid lines). For comparison, Fig. 3.8.b also shows the channeling fraction obtained by DAMA (dashed lines). Good agreement with the chan-

neling fractions of DAMA is achieved only when dechanneling due to the interaction with Tl impurities is included.

3.3 Channeling of recoiling lattice nuclei

The recoiling nuclei start initially from lattice sites (or very close to them), thus blocking effects are important. In fact, as argued originally by Lindhard [23], in a perfect lattice and in the absence of energy-loss processes the probability that a particle starting from a lattice site is channeled would be zero. The argument uses statistical mechanics in which the probability of particle paths related by time-reversal is the same. For example, in optics if a source of radiation and a point of observation are interchanged, the intensity of the light measured at the new place of observation is the same as the old. Thus the probability of an incoming ion to have a particular path within the crystal is the same as the probability of the same ion to move backwards along the same path [33]. This is what Lindhard called the “Rule of Reversibility.”

Using this rule, since the probability of an incoming channeled ion to get very close to a lattice site is zero (otherwise it would suffer a large angle scattering and it would not be channeled), the probability of the same ion to move in the time-reversed path, starting at a nuclear site and ending inside a channel, is zero too. However, any departure of the actual lattice from a perfect lattice, for example due to vibrations of the atoms in the lattice, would violate the conditions of this argument and allow for some of the recoiling lattice nuclei to be channeled.

The channeling of particles emitted at lattice sites due to lattice vibrations, such as protons scattered at large angles, was measured and already understood in the 70’s. Komaki *et al.* [78] in a 1971 paper titled “Channeling Effects in the Blocking Phenomena” observed channeling of protons scattered at large angles within thin Si and Ge crystals and explained it as due to the fact that the scattering or emitting lattice atom is not exactly at the lattice site because of thermal vibrations.” They fit their data using the model presented by Komaki and Fujimoto [62] one year earlier.

We now estimate the channeling fractions in NaI (Tl) using the formalism presented so far.

3.3.1 Channeling fraction for each channel

We need to know how probable it is for the recoiling nucleus to be at a particular distance r from its equilibrium position in a crystal row when it collides with a WIMP. The probability distribution function $g(r)$ of the perpendicular distance to the row of the colliding atom due to thermal vibrations can be represented by a two-dimensional Gaussian (as done by Lindhard and many others [33], the relevant vibrations being in the plane orthogonal to the row),

$$g(r) = \frac{r}{u_1^2} \exp(-r^2/2u_1^2). \quad (3.39)$$

The one dimensional vibration amplitude u_1 is given in Eq. 3.26.

The channeled fraction $\chi_{\text{axial}}(E, \hat{\mathbf{q}})$ of nuclei with recoil energy E moving initially in the direction $\hat{\mathbf{q}}$ making an angle ϕ with respect to the axis is given by the fraction of nuclei which can be found at a distance r larger than a minimum distance $r_{i,\min}$ from the row at the moment of collision, determined by the critical distance of approach as shown in the next subsection,

$$\chi_{\text{axial}}(E, \phi) = \int_{r_{i,\min}}^{\infty} dr g(r) = \exp(-r_{i,\min}^2/2u_1^2). \quad (3.40)$$

Note that here we are approximating the upper limit of the integral of $g(r)$ with ∞ , instead of the radius of the axial channel $d_{\text{ach}}/2$. This is a good approximation because $d_{\text{ach}}/2 \simeq 10a$ or more and the integral is dominated by the values of $g(r)$ close to $u_1 \ll 2a$.

If $\phi > \psi_c$ no channeling can occur and $\chi_{\text{axial}}(E, \phi) = 0$. This can easily be seen from Eqs. 3.8, 3.11, 3.12 and 3.16, taking into account that $U(r_i + d \tan \phi) \geq U(r_c)$.

For a planar channel, the Gaussian thermal distribution for the planar potential is one-dimensional (the relevant vibrations occurring perpendicularly to the plane),

$$g(x) = (2\pi u_1^2)^{-1/2} \exp(-x^2/2u_1^2). \quad (3.41)$$

This is normalized to 1 for $-\infty < x < +\infty$. In our calculations we only consider positive

values of x for each plane, thus we multiply $g(x)$ by a factor of 2 to find the fraction of channeled nuclei for a planar channel,

$$\chi_{\text{planar}}(E, \phi) = \int_{x_{i,\min}}^{\infty} 2g(x)dx = \frac{2}{\sqrt{\pi}} \int_{x_{i,\min}}^{\infty} \frac{e^{(-x^2/2u_1^2)}}{\sqrt{2}u_1} dx = \text{erfc}\left(\frac{x_{i,\min}}{\sqrt{2}u_1}\right). \quad (3.42)$$

Here ϕ is the angle $\hat{\mathbf{q}}$ makes with the plane, defined as the complementary angle to the angle between $\hat{\mathbf{q}}$ and the normal to the plane, or as the smallest angle between $\hat{\mathbf{q}}$ and vectors lying on the plane. Similar to the axial case, we approximate the upper limit of the integral of $g(x)$ with ∞ , instead of the radius of the planar channel $d_{\text{pch}}/2$. This is a good approximation because $d_{\text{pch}}/2 \simeq 10u_1$ or more, and $\text{erfc}[d_{\text{pch}}/(2\sqrt{2}u_1)]$ is negligible. Also in this case, $\chi_{\text{planar}}(E, \phi) = 0$ if ϕ is larger than the critical channeling angle of the particular channel, i.e. if $\phi > \psi_c^p$.

We conclude this subsection by noticing an important point. In Eq. 3.40, $r_{i,\min}$, which is a function of $r_c(T)$, enters exponentially. Thus any uncertainty in our modeling of $r_c(T)$ becomes exponentially enhanced in the channeling fraction. The same happens with the dependence of the channeling fraction in Eq. 3.42 on $x_{i,\min}$, which depends on $x_c(T)$. This is the major difficulty of the analytical approach we are following.

3.3.2 Minimum initial distance of the recoiling lattice nucleus

For axial channels, using Eqs. 3.8, 3.11, 3.12 and 3.16, we can write the condition for channeling as

$$E \sin^2 \phi + U(r_i + d \tan \phi) = U(r_{\min}) < U(r_c(E)). \quad (3.43)$$

Therefore, the minimum initial distance $r_{i,\min}$ is the solution of the equation

$$U(r_{i,\min} + d \tan \phi) = U(r_c(E)) - E \sin^2 \phi. \quad (3.44)$$

Inverting the function $U(r)$ we obtain

$$r_{i,\min}(E, \phi) + d \tan \phi = U^{-1}[U(r_c(E)) - E \sin^2 \phi]. \quad (3.45)$$

The inverse of Lindhard's potential function $U(r)$ is

$$U^{-1}(r) = \frac{Ca}{\sqrt{e^{2r/E_1} - 1}}, \quad (3.46)$$

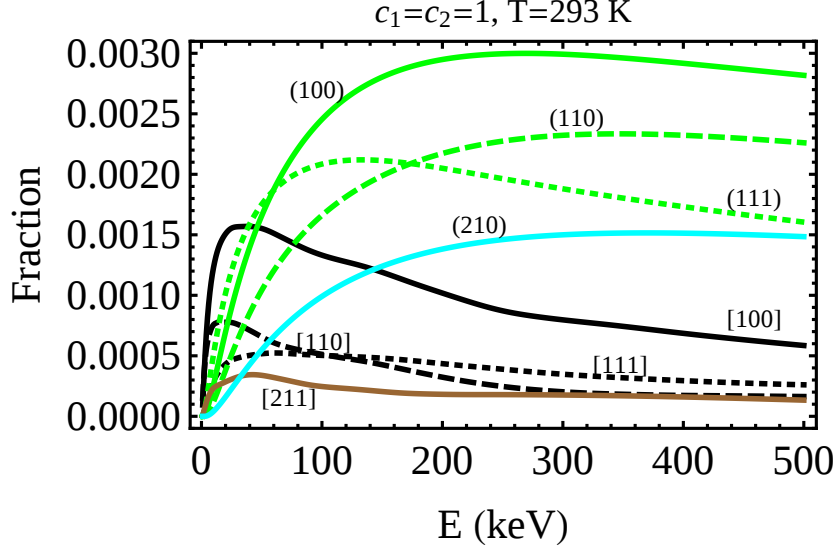


Figure 3.9: Upper bounds to the channeling fractions of Na recoils for single planar (green/gray lines) and axial (black lines) channels, as function of the recoil energy E , for $T=293$ K and $c_1 = c_2 = 1$, without including dechanneling. Two additional channels not included in the total channeling fractions are also shown: axial $[211]$ (brown line) and planar (210) (cyan line).

which together with the expression for $r_c(E)$ in Eq. 3.14 yields a fully analytic expression for $r_{i,\min}(E, \phi)$,

$$r_{i,\min}(E, \phi) = \frac{Ca}{\sqrt{\left(1 + \frac{C^2 a^2}{r_c^2}\right) \exp(-2 \sin^2 \phi / \psi_1^2) - 1}} - d \tan \phi. \quad (3.47)$$

Applying the same arguments to planar channels, we have

$$U(x_{i,\min} + d_p \tan \phi) = U(x_c(E)) - E \sin^2 \phi. \quad (3.48)$$

For Lindhard's potential, the minimum initial distance is given by

$$x_{i,\min}(E, \phi) = \frac{a}{2} \frac{C^2 - \left[\sqrt{\frac{x_c^2}{a^2} + C^2} - \frac{x_c}{a} - \sin^2 \phi / \psi_a^2 \right]^2}{\left[\sqrt{\frac{x_c^2}{a^2} + C^2} - \frac{x_c}{a} - \sin^2 \phi / \psi_a^2 \right]} - d_p \tan \phi. \quad (3.49)$$

Here, $x_c(E)$ is found in Eq. 3.22.

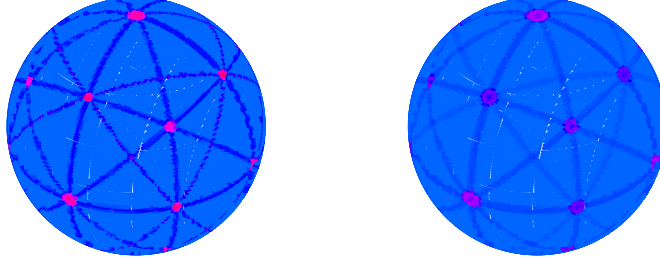


Figure 3.10: Channeling probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ (Eq. 3.51) for a 200 keV recoil of (a) an Na ion and (b) an I ion at 20 °C with $c_1 = c_2 = 1$ and neglecting dechanneling. The probability is computed for each direction and plotted on a sphere using the HEALPix pixelization. The red, pink, dark blue and light blue colors indicate a channeling probability of 1, 0.625, 0.25 and zero, respectively.

Fig. 3.9 shows upper bounds to the channeling fractions of Na recoils for individual channels with $c_1 = c_2 = 1$ and $T = 293$ K, without including dechanneling. The black and green (or gray) lines correspond to single axial and planar channels respectively. Two additional channels not included in the total channeling fractions are also shown for comparison: the axial [211] (brown line) and the planar (210) (cyan line) channels. The upper bounds of channeling fractions for planar channels are more generous than those of axial channels because of our choice of x_c in Eq. 3.22. This does not mean that planar channels are dominant in the actual channeling fractions.

3.3.3 Total geometric channeling fraction

The geometric channeling fraction is the fraction of recoiling ions that propagate in the 1st, or 2nd, or ... or 26th channel. Here “geometric” refers to assuming that the distribution of recoil directions is isotropic. In reality, in a dark matter direct detection experiment, the distribution of recoil directions is expected to be peaked in the direction of the average

WIMP flow. For comparison with previous work of others, here we examine this geometric channeling fractions.

We include only the channels with lowest crystallographic indices, i.e. 100, 110 and 111, which are in total 26 axial and planar channels, as explained in Appendix A.1. We have also checked other axial and planar channels, such as the [211] and (210) channels shown in Fig. 3.9, and found that their contribution to the channeling fractions is negligible (additional planar channels are always less important than the planar channels we keep and the same happens for axial channels).

The probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ that an ion with initial energy E is channeled in a given direction $\hat{\mathbf{q}}$ is the probability that the recoiling ion enters any of the available channels. We compute it using a recursion of the addition rule in probability theory over all axial and planar channels:

$$\begin{aligned} P(A_1 \text{ or } A_2) &= P(A_1) + P(A_2) - P(A_1)P(A_2). \\ P(A_1 \text{ or } A_2 \text{ or } A_3) &= P(A_1 \text{ or } A_2) + P(A_3) - P(A_1 \text{ or } A_2)P(A_3). \end{aligned} \quad (3.50)$$

We continue this recursive computation until we find the probability with which the recoiling ion goes into any of the 26 channels

$$\chi_{\text{rec}}(E, \hat{\mathbf{q}}) = P(A_1 \text{ or } A_2 \text{ or } \dots \text{ or } A_{26}). \quad (3.51)$$

For each channel A_k ($k = 1, \dots, 26$), $P(A_k) = \chi_{\text{axial}-k}(E, \phi_k)$ or $P(A_k) = \chi_{\text{planar}-k}(E, \phi_k)$ for an axial or planar channel, respectively. Notice that $P(A_k) \neq 0$ only for the channels for which $\phi_k < (\psi_c)_k$, i.e. for which the angle that $\hat{\mathbf{q}}$ makes with the axis or plane of the channel, respectively, is smaller than the critical angle for the channel.

Here we are treating channeling along different channels as independent events, so that the conditional probabilities coincide with the non-conditional probabilities, e.g. $P(A_1|A_2) = P(A_1)$. This is correct for different axial channels, which never overlap, and a good approximation for different planar channels. However, axial channels happen at the crossing of two or more planar channels, thus channeling into axial and planar channels may not be entirely

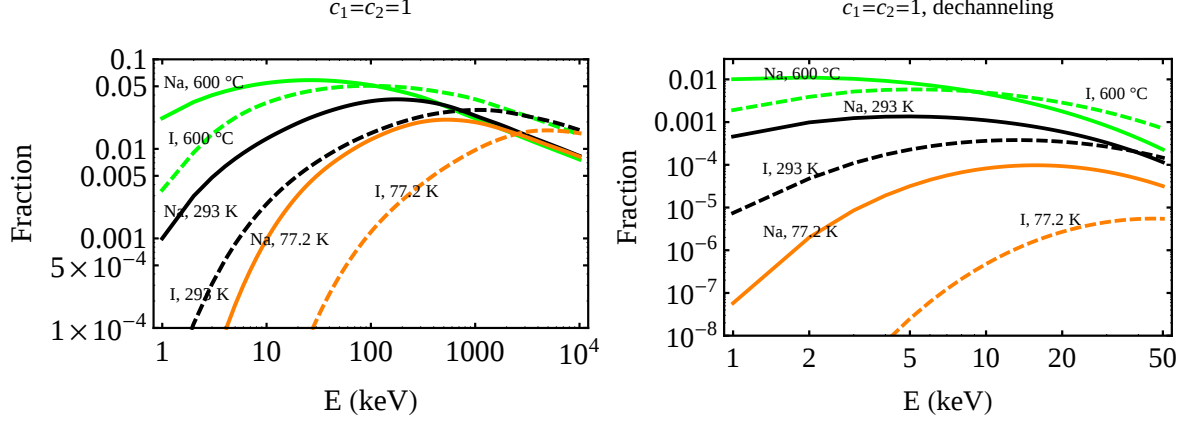


Figure 3.11: Upper bounds to the channeling fraction of Na and I recoils as a function of the recoil energy E for $T=600$ °C (green/light gray), 293 K (black), and 77.2 K (orange/dark gray) in the approximation of $c_1 = c_2 = 1$, (a) without and (b) with dechanneling as in Eq. 3.34.

independent. We prove in Appendix D that considering them as independent is, however, a good approximation.

Fig. 3.10 shows the channeling probability for an $E = 200$ keV recoil of Na (left panel) or I (right panel) at 20 °C with $c_1 = c_2 = 1$ and neglecting dechanneling, computed for each direction $\hat{\mathbf{q}}$ and plotted on a sphere using the HEALPix pixelization. The red, pink, dark blue and light blue colors indicate a channeling probability of 1, 0.625, 0.25 and zero, respectively.

To obtain the geometrical channeling fraction, we average the channeling probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ over the directions $\hat{\mathbf{q}}$, assuming an isotropic distribution of the initial recoiling directions $\hat{\mathbf{q}}$,

$$P_{\text{rec}}(E) = \frac{1}{4\pi} \int \chi_{\text{rec}}(E, \hat{\mathbf{q}}) d\Omega_{\hat{\mathbf{q}}}. \quad (3.52)$$

This integral is computed using HEALPix [76] (see Appendix B).

The channeling fraction as a function of recoil energy is shown in Figs. 3.11 and 3.12 with $c_1 = c_2 = 1$ and $c_1 = c_2 = 2$, respectively. These curves include thermal effects in the lattice at various crystal temperatures, and are shown without (left panels) and with (right panels)

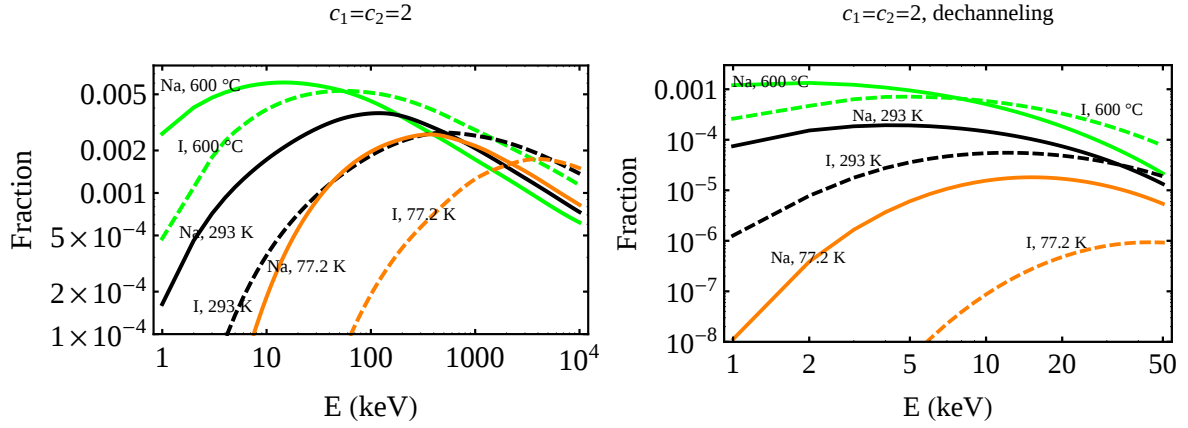


Figure 3.12: Same as Fig. 3.11 but for $c_1 = c_2 = 2$.

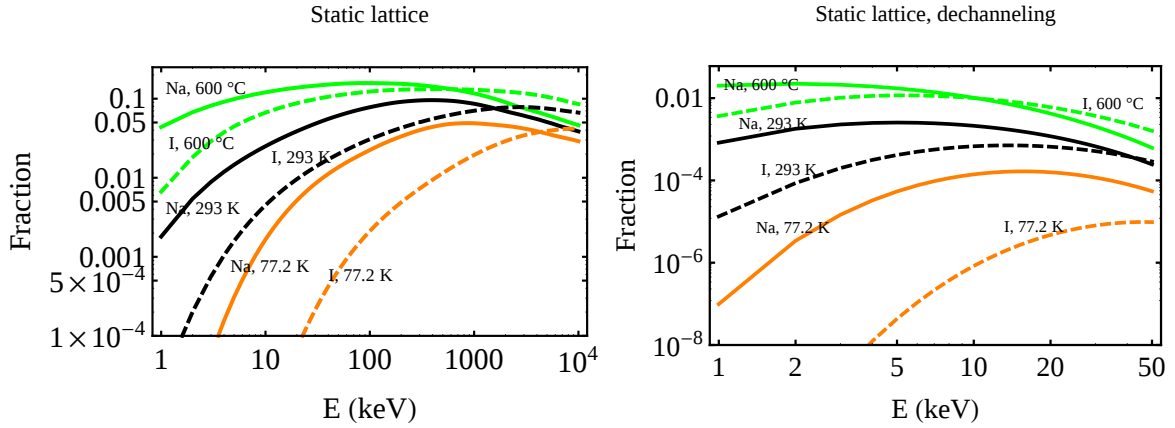


Figure 3.13: Same as Fig. 3.11 but for $c_1 = c_2 = 0$ (static lattice), provided as an upper bound with respect to any non-zero values of c_1 and c_2 .

dechanneling according to Eq. 3.34. Note that the dechanneling as included here is possibly too extreme, since it does not allow for the possibility of an ion reentering a channel (the original or another one) after a collision with a Tl impurity.

Notice that while the effect of increasing temperatures on the initial position of the recoiling nucleus makes the channeling fractions larger (the recoiling nucleus can be initially further out from the string, i.e. u_1 in Eqs. 3.40 and 3.42 increases), the effect of increasing temperatures on the other lattice atoms is to increase the critical distances, which makes the channeling fractions smaller ($r_{i,\min}$ and $x_{i,\min}$ in Eqs. 3.40 and 3.42 increase). Figs. 3.11 and 3.12 show that in our calculations for NaI (Tl) the first effect is almost always dominant, except that for $c_1 = c_2 = 2$ at some energies the temperature effects in the lattice are larger (see the left panel of Fig. 3.12, where some fractions are smaller at higher temperatures). Neglecting the temperature effects in the lattice, by setting $c_1 = c_2 = 0$, but including the thermal vibrations of the nucleus that is going to recoil, we obtain the largest estimates for the channeling fractions. Although it is physically inconsistent to take only the temperature effects on the initial position of the recoiling nuclei but not on the lattice, this was done by Lindhard [23] and Andersen [57] early on, and we do it here because it provides the most generous upper bound on the channeling fraction (any non-zero value of c_1 or c_2 would lead to smaller fractions).

Fig. 3.14.a shows what we consider to be our main predictions for the range expected as an upper limit to the channeling fraction in NaI (Tl), if dechanneling is ignored. Fig. 3.14.b shows the channeling fraction reduced by dechanneling. As we see in Fig. 3.14.a, neglecting interactions with Tl atoms, the channeling fraction is never larger than 5% and the maximum happens at 100's of keV. This maximum occurs because the critical distances decrease with the ion energy E , making channeling more probable, and the critical angles also decrease with E , making channeling less probable. With dechanneling, the probability that the channeled ion does not interact with a Tl atom decreases with energy (since more energetic ions propagate further within channels). Thus, interactions with Tl atoms decrease the channeling fraction at high energies. The simple extreme model of dechanneling we use predicts much smaller fractions, at most in the 0.1% level, with the maximum shifted to

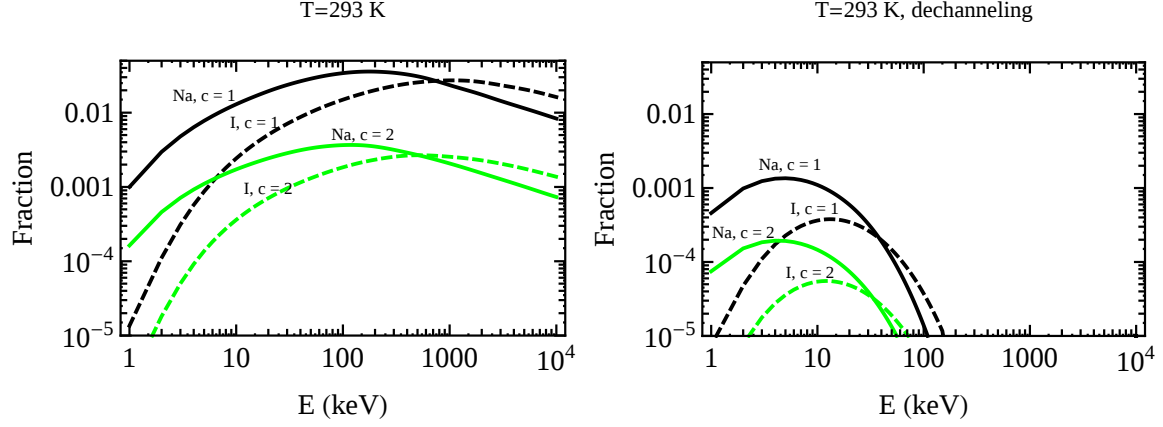


Figure 3.14: Channeling fractions at $T=293$ K for Na (solid lines) and I (dashed lines) ions for $c = c_1 = c_2 = 1$ (black) and $c = c_1 = c_2 = 2$ (green/gray) cases (a) without and (b) with dechanneling included as in Eq. 3.34.

small energies, less than 10 keV (see Fig. 3.14.b). This reduction may eventually prove to be too extreme and at present we do not have a better formalism to model dechanneling.

CHAPTER 4

Channeling fraction in Si and Ge crystals

Si and Ge crystals are used in several direct dark matter detection experiments, such as CDMS [16], CoGeNT [2, 17], EDELWEISS [18], TEXONO [79], EURECA [80], HDMS [81] and IGEX [82]. In Chapter 3 we introduced the general ideas and analytic models [23, 63, 33, 57, 58, 59, 60, 61, 62, 64, 7] that we use to describe these phenomena in the context of dark matter detection, and applied them to NaI (Tl). Besides the different crystal structure (see Appendix A.2) for Si and Ge, in this chapter we use a different expression for the continuum potentials (see Eqs. 4.1 to 4.4), which leads to a different expression for the critical channeling distance for axial channels (see Eq. 4.8). We also use a different way of deriving the critical distance for planar channels (see Eqs. 4.10 to 4.13).

4.1 Models of Channeling

4.1.1 Continuum potentials

Except when said otherwise, in this chapter we use Molière’s approximation for the screened potential, following the work of Hobler [7] and Morgan and Van Vliet [58, 59, 60]. Molière’s approximations of the continuum potentials are more complicated and also somewhat better than Lindhard’s expressions, which we used in Chapter 3 devoted to NaI. Lindhard’s expressions are easier to manipulate algebraically to obtain different quantities of interest. Still in this chapter we use some expressions derived from Lindhard’s form of the potentials.

In Molière’s approximation [33] the axial continuum potential, as a function of the trans-

verse distance r to the string, is

$$U_{\text{Mol}}(r) = (2Z_1Z_2e^2/d) f(r/a) = E\psi_1^2 f(r/a), \quad (4.1)$$

where E is the energy of the propagating particle and ψ_1 is a dimensionless parameter defined in Eq. 3.2. Molière's screening function [33] for the continuum potential is

$$f(\xi) = \sum_{i=1}^3 \alpha_i K_0(\beta_i \xi). \quad (4.2)$$

Here K_0 is the zero-order modified Bessel function of the second kind, and the dimensionless coefficients α_i and β_i are $\alpha_i = \{0.1, 0.55, 0.35\}$ and $\beta_i = \{6.0, 1.2, 0.3\}$ [83], for $i = 1, 2, 3$. The string of crystal atoms is at $r = 0$.

The continuum planar potential in Molière's approximation [33], as a function of the distance x perpendicular to the plane, is

$$U_{\text{Mol},p}(x) = (2\pi nZ_1Z_2e^2a) f_p(x/a) = E\psi_a^2 f_p(x/a). \quad (4.3)$$

The subscript p denotes “planar”. The dimensionless parameter ψ_a is defined in Eq. 3.5, and

$$f_p(\xi) = \sum_{i=1}^3 (\alpha_i/\beta_i) \exp(-\beta_i \xi), \quad (4.4)$$

where the coefficients α_i and β_i are the same as above. The plane is at $x = 0$.

Examples of axial and planar continuum potentials for a Si ion propagating in a Si crystal and a Ge ion propagating in a Ge crystal are shown in Fig. 4.1.

4.1.2 Minimum distances of approach and critical channeling angles

As explained in Section 3.1.3, we can define the minimum distance of approach to the string, $r_{\min}$ (or to the plane of atoms $x_{\min}$), and the angle ψ at which the ion exits from the string (or plane), i.e. far away from it where $U \simeq 0$ using the conservation of the transverse energy. Thus, for an axial channel

$$E_{\perp} = U_{\text{Mol}}(r_{\min}) = E\psi^2 + U_{\text{Mol}}(d_{\text{ach}}/2). \quad (4.5)$$

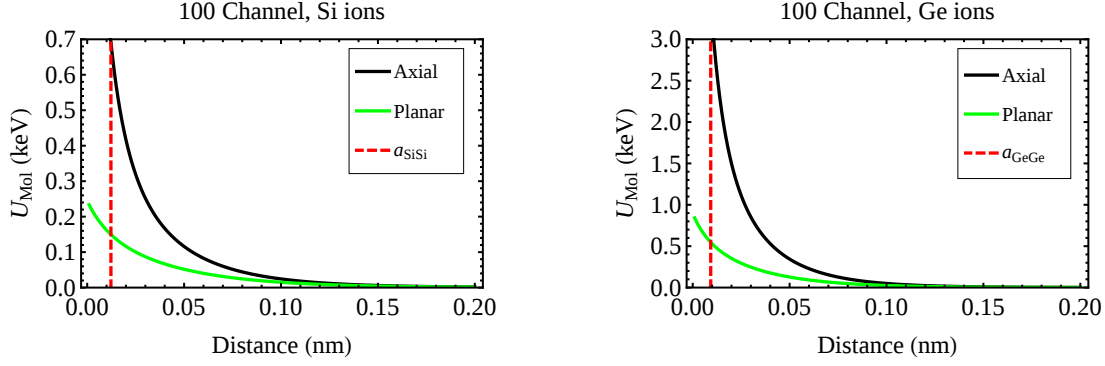


Figure 4.1: Continuum axial (black) and planar (green/gray) potentials for (a) Si and (b) Ge ions, propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a Si or Ge crystal respectively. The screening radii shown as vertical lines are $a_{\text{SiSi}} = 0.01225$ nm and $a_{\text{GeGe}} = 0.009296$ nm (see Appendix A.2).

We proceeded in two ways to define the axial channel radius ($d_{\text{ach}}/2$) for the axial channels we included in our calculation. We used the contour plots of the axial continuum potentials plotted in a plane perpendicular to the channels shown in Fig. 3 of the paper of Hobler [7] to read off the channel radius $d_{\text{ach}}/2$ of the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ axial channels in terms of the lattice constant a_{lat} . They are $0.25 a_{\text{lat}}$, $0.375 a_{\text{lat}}$, and $\sqrt{0.2^2 + 0.12^2} a_{\text{lat}} = 0.233 a_{\text{lat}}$, respectively. For the other axial channels we considered, $\langle 211 \rangle$ and $\langle 311 \rangle$, we define the channel width d_{ach} in terms of the interatomic distance d in the corresponding row as $d_{\text{ach}} = 1/\sqrt{Nd}$. For a planar channel we replace the axial potential at the middle of the axial channel $U_{\text{Mol}}(d_{\text{ach}}/2)$ in Eq. 4.5 by the planar potential at the middle of the planar channel $U_{\text{Mol},p}(d_{\text{pch}}/2)$ (the channel width d_{pch} was defined after Eq. 3.5).

For axial channeling Lindhard equates the condition for channeling with the condition in Eq. 3.6 for the validity of the continuum model. Replacing the inequality in Eq. 3.6 by an equality defines an energy dependent critical distance r_c , so that channeling can happen only if the propagating ion always keeps a distance $r > r_c$. Morgan and Van Vliet [59] use 5 instead of 8 in Eq. 3.6, because this agrees better with their simulations of channeling in copper crystals. Following Hobler [7], we use here Morgan and Van Vliet's equation to define

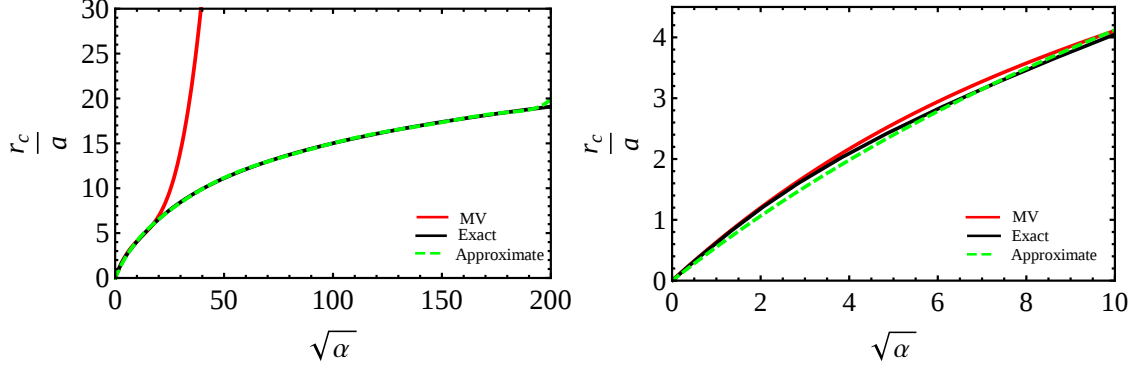


Figure 4.2: Comparison of the exact numerical solution (solid black) of Eq. 4.6 for the critical distance of approach $r_c(E)$ and the approximate analytic expression in Eq. 4.8 (dashed green) as a function of $\sqrt{\alpha} = \sqrt{Z_1 Z_2 e^2 d / a^2 E}$ for (a) the high $\sqrt{\alpha}$ (low energy) range, and (b) the low $\sqrt{\alpha}$ (high energy) range. The Morgan and Van Vliet approximation to $r_c(E)$ in Eq. 4.7 is also shown (solid red- labeled MV).

r_c , i.e.

$$U''_{\text{Mol}}(r_c) = \frac{5}{d^2} E. \quad (4.6)$$

With Molière's form of the potential it is not possible to solve analytically for r_c . Morgan and Van Vliet [59] gave the following approximate analytical solution for the axial channeling minimum distance of approach,

$$r_c^{\text{MV}} = (2/3)a\sqrt{\alpha} [1 - (\sqrt{\alpha}/19) + (\alpha/700)] \quad (4.7)$$

with $\alpha = (Z_1 Z_2 e^2 d / a^2 E)$. This solution is not correct at low energies (high values of α). As can be seen in Fig. 4.2 (and also in Figs. 8 and 13 of the paper of Hobler [7]) the steep increase in the approximate Morgan and Van Vliet solution at low energies (see the curve labeled “MV” in Fig. 4.2.a) is not present in the numerical solution (see the curve labeled “Exact” in Fig. 4.2.a) of r_c . Instead of Eq. 4.7 we use here a better approximate analytic

solution obtained by fitting a degree nine polynomial to the exact solution of Eq. 4.6,

$$\begin{aligned}
r_c^{\text{Mol}} = a [& 0.57305\sqrt{\alpha} - 0.0220301(\sqrt{\alpha})^2 + 0.000728889(\sqrt{\alpha})^3 \\
& - 0.0000155189(\sqrt{\alpha})^4 + 2.04162 \times 10^{-7}(\sqrt{\alpha})^5 - 1.65057 \times 10^{-9}(\sqrt{\alpha})^6 \\
& + 7.9749 \times 10^{-12}(\sqrt{\alpha})^7 - 2.11041 \times 10^{-14}(\sqrt{\alpha})^8 \\
& + 2.35121 \times 10^{-17}(\sqrt{\alpha})^9].
\end{aligned} \tag{4.8}$$

Eq. 4.8 is valid from E of 1 keV to 29 TeV (which corresponds to values of $\sqrt{\alpha}$ between 180 and 0.000158). Fig. 4.2 shows a comparison of the exact numerical solution $r_c(E)$ of Eq. 4.6 and the approximate analytic solution Eq. 4.8 as a function of $\sqrt{\alpha}$ (divided by the screening distance a). The high and low $\sqrt{\alpha}$ range in Figs. 4.2.a and 4.2.b respectively corresponds to low and high energies. The maximum percentage error between the exact solution and the analytic approximation we use is 11.5 %.

Fig. 4.3 shows the critical distance of approach $r_c^{\text{Mol}}(E)$ in Eq. 4.8 as a function of energy of the propagating ion for several axial channels, for Si ions propagating in a Si crystal and Ge ions propagating in a Ge crystal.

As explained in Section 3.1.3 and using Eqs. 4.5 and 4.8, we can find the critical channeling angle $\psi_c^{\text{Mol}}(E)$ for the particular axial channel,

$$\psi < \psi_c^{\text{Mol}}(E) = \sqrt{\frac{U_{\text{Mol}}(r_c^{\text{Mol}}(E)) - U_{\text{Mol}}(d_{\text{ach}}/2)}{E}}. \tag{4.9}$$

The critical distance $r_c^{\text{Mol}}(E)$ increases as E decreases (see Figs. 4.3, 4.5 and 4.7 to 4.13). At low enough E , $r_c^{\text{Mol}}(E)$ becomes close to the radius of the channel $d_{\text{ach}}/2$, and the critical angle $\psi_c^{\text{Mol}}(E)$ goes to zero (see Figs. 4.7 to 4.10 and 4.14, 4.15).

For planar channeling we will follow the procedure of defining a fictitious row introduced by Morgan and Van Vliet [59, 7] as explained in Section 3.1.3. The characteristic distance between atoms along the fictitious row is $\bar{d} = 1/(Nd_{\text{pch}}2R)$ (Eq. 3.19), where $2R$ is the width of a strip containing the equivalent row of atoms. For R , Morgan and Van Vliet used the impact parameter in an ion-atom collision corresponding to a deflection angle of the order of the break-through angle. For small scattering angles, the deflection angle δ is related to

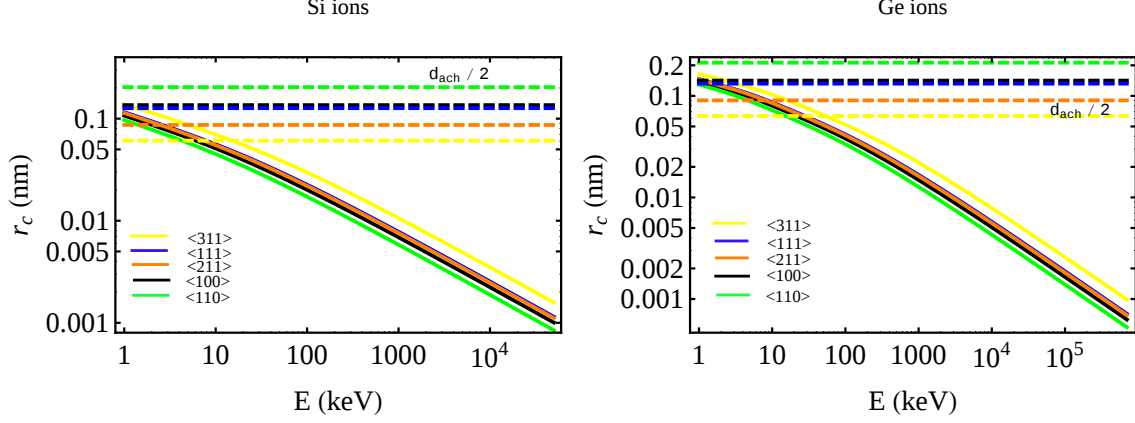


Figure 4.3: Critical channeling distance of approach $r_c^{\text{Mol}}(E) = r_c$ in Eq. 4.8 as a function of energy of the propagating ion for several axial channels, for (a) Si ions propagating in a Si crystal and (b) Ge ions propagating in a Ge crystal.

the impact parameter, in this case R , as (see e.g. Eq. 2.1' of Lindhard [23])

$$2E\delta = -d U'_{\text{Mol}}(R), \quad (4.10)$$

where U'_{Mol} is the derivative of the axial continuum potential, and Morgan and Van Vliet define R by taking $\delta = \sqrt{U_{\text{Mol},p}(0)/E}$. Using the Molière's approximation for the potentials, Morgan and Van Vliet found the following expressions for R

$$R^{\text{MV}} = a \left(\frac{A}{2} \right) \ln \left(B Z_1 Z_2 e^2 / a \sqrt{E U_{\text{Mol},p}(0)} \right), \quad (4.11)$$

with coefficients $A = 1.2$ and $B = 4$. This leads to the $\bar{d}^{\text{MV}}$ value given in Eq. 3.20.

While Eq. 4.10 seems to provide a good condition for R , there is a channel dependent energy upper limit of applicability of its approximate analytical solution in Eq. 3.20, because the logarithm in $\bar{d}^{\text{MV}}$ approaches zero as E approaches $(4Z_1 Z_2 e^2 / a)^2 / U_{\text{Mol},p}(0)$. Close to this value of E there is an unphysical fast increase in $\bar{d}^{\text{MV}}$ (and consequently in $x_c(E)$) that indicates the break-down of the approximate solution $\bar{d}^{\text{MV}}$ in Eq. 3.20 (and, as shown in Fig. 13 of Hobler [7], is not found in other expressions of x_c).

We decided to keep the Morgan and Van Vliet definition for R in Eq. 4.10 and use the following approximate analytical solution obtained by fitting a degree five polynomial in $\ln y$

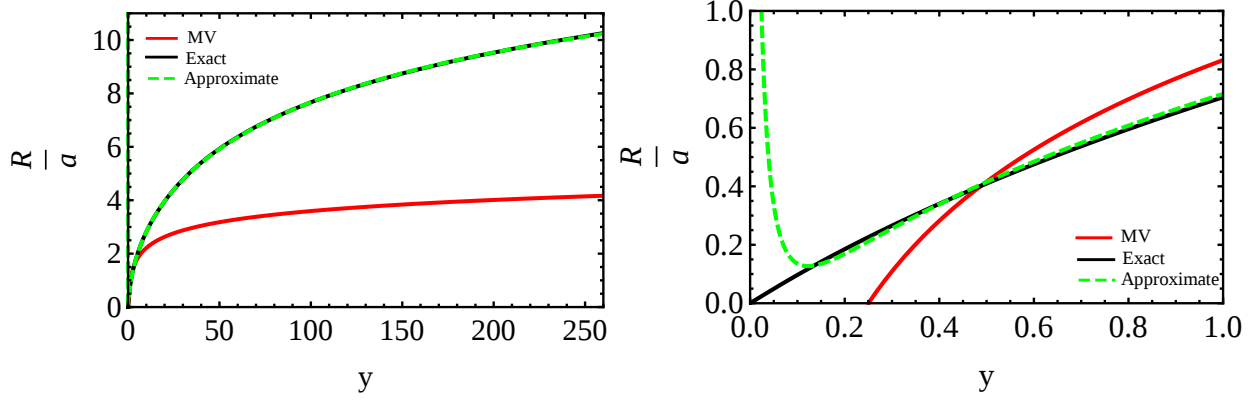


Figure 4.4: Comparison of the exact solution (solid black) of Eq. 4.10 for R/a and its analytical approximation in Eq. 4.12 (dashed green) as a function of $y = Z_1 Z_2 e^2 / a \sqrt{E U_{\text{Mol},p}(0)}$ for the (a) high y (low E) range and the (b) low y (high E) range. Also the Morgan and Van Vliet approximation to R/a in Eq. 4.11 is shown (solid red- labeled MV).

to the exact numerical solution of Eq. 4.10

$$R^{\text{Mol}} = a \left(0.716014 + 0.510922 \ln y + 0.12047 (\ln y)^2 + 0.0180492 (\ln y)^3 + 0.00442459 (\ln y)^4 - 0.000824744 (\ln y)^5 \right), \quad (4.12)$$

where $y = Z_1 Z_2 e^2 / a \sqrt{E U_{\text{Mol},p}(0)}$.

Fig. 4.4 shows a comparison of the exact numerical solution of Eq. 4.10 for R and its analytical approximation in Eq. 4.12 (divided by a) as a function of y . Also the approximate expression of Morgan and Van Vliet in Eq. 3.20 is shown in Fig. 4.4 (labeled MV). The high and low y ranges in Fig. 4.4.a and 4.4.b respectively corresponds to low and high energies. The approximate solution is not valid at $y < 0.15$ which corresponds to $E > 50$ MeV for Si, and $E > 700$ MeV for Ge. Within its range of validity, the percentage error of the analytic approximation in Eq. 4.12 is less than 9%.

Let us call $\bar{r}_c^{\text{Mol}}(E)$ the critical distance obtained from Eq. 4.8 for the fictitious row, whose interatomic distance is $\bar{d} = 1/(N d_{\text{pch}} 2 R^{\text{Mol}})$ in which the distance R^{Mol} is given in Eq. 4.12. Then, the minimum distance of approach for planar channeling is

$$x_c^{\text{Mol}}(E) \equiv \bar{r}_c^{\text{Mol}}(E). \quad (4.13)$$

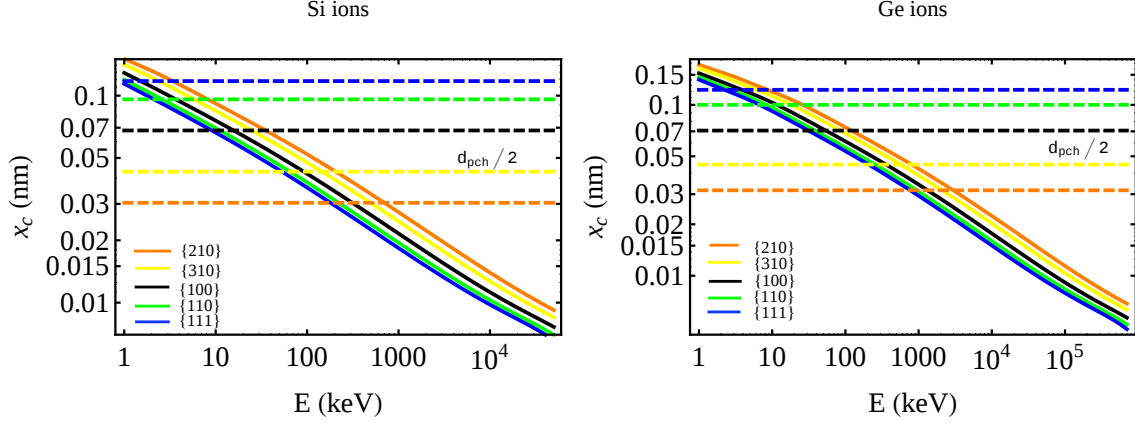


Figure 4.5: Critical channeling distances $x_c^{\text{Mol}}(E) = x_c$ in Eq. 4.13 as a function of the energy of the propagating ion for different planar channels, for (a) Si ions propagating in a Si crystal and (b) Ge ions in Ge.

Fig. 4.5 shows the plot of $x_c^{\text{Mol}}(E)$ (obtained from using Eq. 4.12 for the fictitious string) as a function of energy for the most important planar channels, i.e. $\{100\}$, $\{110\}$, $\{111\}$, $\{210\}$ and $\{310\}$. Fig. 4.5 shows that we can safely extend our approximation to 50 MeV for Si ions in a Si crystal and to 700 MeV for Ge ions in Ge crystals.

We can obtain an equation similar to Eq. 4.9 but for the critical planar channeling angle,

$$\psi_c^{\text{Mol},p}(E) = \sqrt{\frac{U_{\text{Mol},p}(x_c^{\text{Mol}}(E)) - U_{\text{Mol},p}(d_{\text{pch}}/2)}{E}}. \quad (4.14)$$

For very small energies, for which $x_c^{\text{Mol}}(E) \geq d_{\text{pch}}/2$ no channeling is possible and $\psi_c^{\text{Mol},p} = 0$ (see Figs. 4.5, 4.7 to 4.10 and 4.14.b, 4.15.b).

The static lattice critical distances presented in Figs 4.3 and 4.5 (also in the left panels of Figs. 4.7, 4.8, 4.9 and 4.10) do not include thermal effects. These are important and must be taken into account. They increase the critical channeling distances and consequently decrease the critical channeling angles as the temperature increases (as clearly shown in Fig. 4.12 and 4.13).

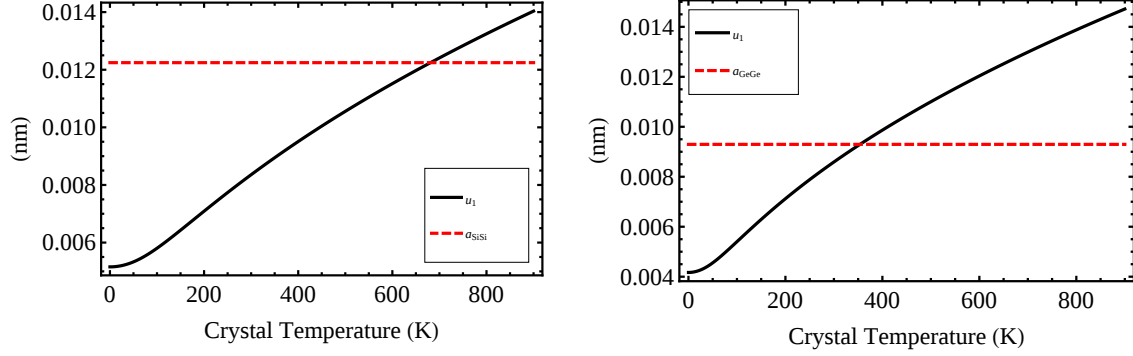


Figure 4.6: Temperature dependent Debye model one dimensional rms vibration amplitude $u_1(T)$ (Eq. 3.26) of the atoms in (a) a Si crystal and (b) a Ge crystal. For comparison the Thomas-Fermi screening distances for two Si atoms and two Ge atoms, a_{SiSi} and a_{GeGe} respectively are also indicated (see Appendix A.2).

4.1.3 Temperature dependent critical distances and angles

As done in Section 3.1.4, we use the Debye model (see Eqs. 3.26 and 3.27) to take into account the zero point energy and thermal vibrations of the atoms in a crystal. The Debye temperatures of Ge and Si are respectively $\Theta = 290$ °K and $\Theta = 490$ °K [33, 7]. The vibration amplitude u_1 as a function of the temperature T is plotted in Fig. 4.6 for Si and Ge crystals. At room temperature (20 °C), $u_1 = 0.00849$ nm for Ge and $u_1 = 0.00827$ nm for Si.

We take into account thermal effects in the crystal through a modification of the critical distances (as explained in Section 3.1.4). The temperature corrected critical distances of approach are

$$\begin{aligned} r_c^{\text{Mol}}(T) &= \sqrt{[r_c^{\text{Mol}}(E)]^2 + [c_1 u_1(T)]^2}, \\ x_c^{\text{Mol}}(T) &= \sqrt{[x_c^{\text{Mol}}(E)]^2 + [c_2 u_1(T)]^2}. \end{aligned} \quad (4.15)$$

Using $r_c^{\text{Mol}}(T)$ and $x_c^{\text{Mol}}(T)$ (Eq. 4.15) instead of the static lattice critical distances r_c^{Mol} and x_c^{Mol} (Eqs. 4.8 and 4.13), in the definition of critical angles, Eqs. 4.9 and 4.14, we obtain the temperature corrected critical axial and planar angles, examples of which are shown in

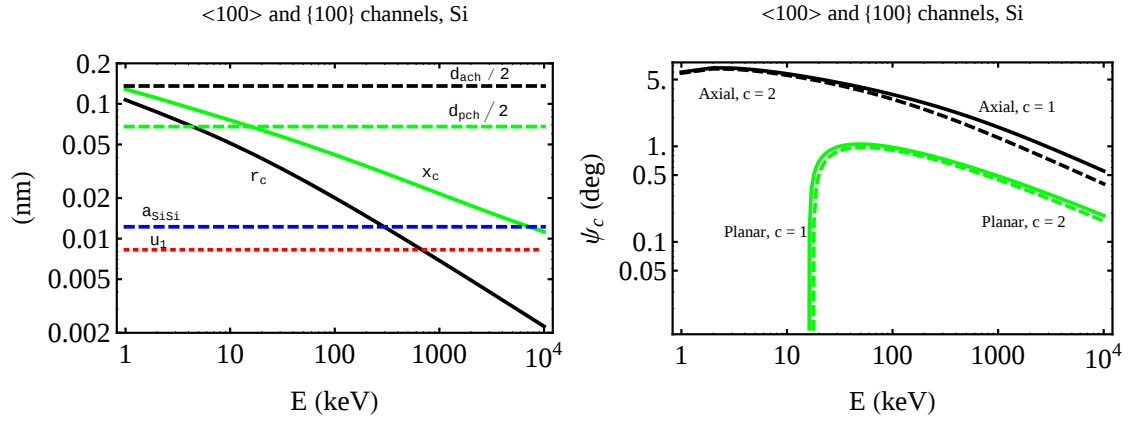


Figure 4.7: (a) Static critical distances of approach ($r_c^{\text{Mol}} = r_c$ and $x_c^{\text{Mol}} = x_c$) and Debye one dimensional rms vibration amplitude u_1 of the atoms in the crystal at 20 °C and (b) critical channeling angles ($\psi_c^{\text{Mol}} = \psi_c$) at 20 °C with temperature effects computed assuming $c_1 = c_2 = c$ and $c = 1$ or $c = 2$ as indicated, as a function of the energy of propagating Si ions in the <100> axial (black) and {100} planar (green/light gray) channels of a Si crystal.

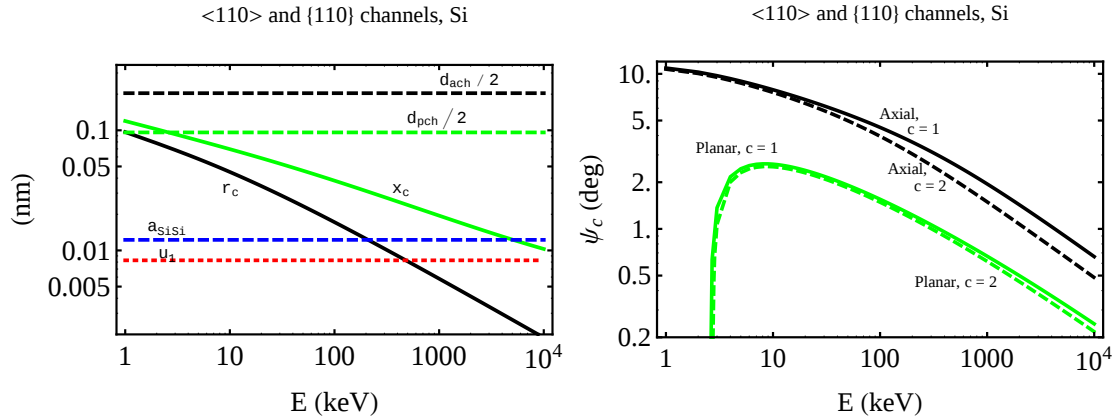


Figure 4.8: Same as in Fig. 4.7 but for the <110> axial and {110} planar channels of a Si crystal.

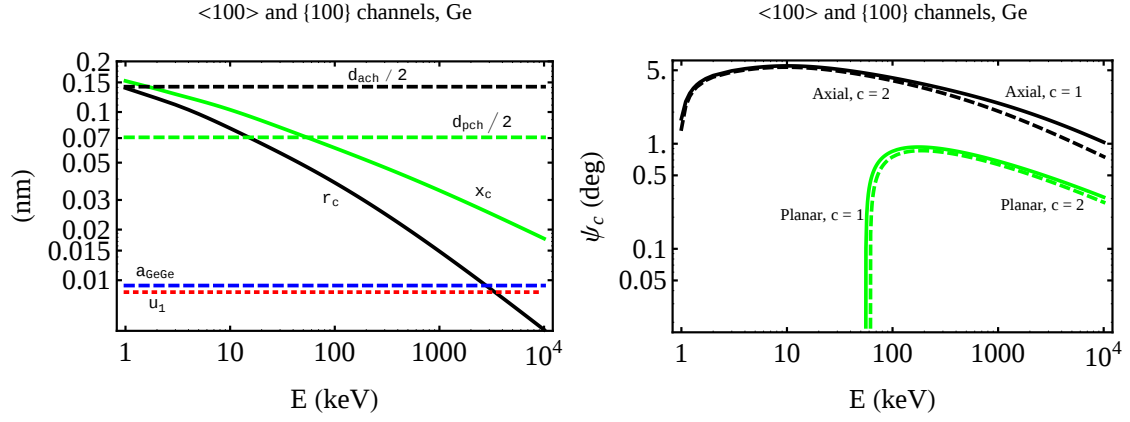


Figure 4.9: Same as in Fig. 4.7 but for Ge ions propagating in the $\langle 100 \rangle$ axial (black) and $\{100\}$ planar (green/light gray) channels of a Ge crystal.

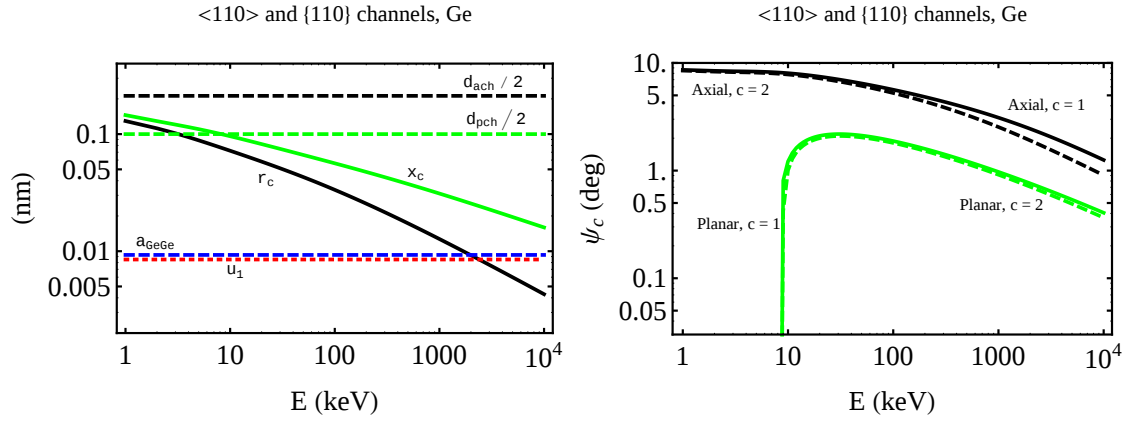


Figure 4.10: Same as in Fig. 4.9 but for the $\langle 110 \rangle$ axial and $\{110\}$ planar channels.

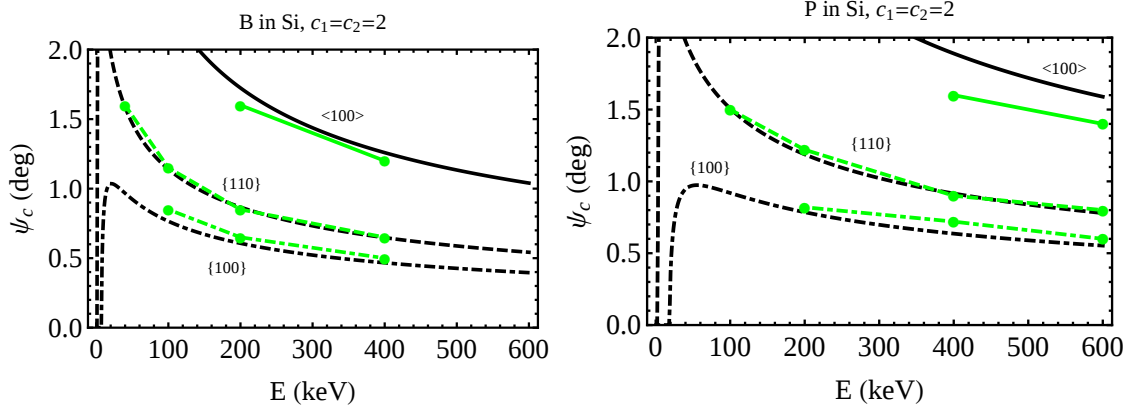


Figure 4.11: Comparison of theoretical (black lines) temperature corrected critical angles $\psi_c^{\text{Mol}} = \psi_c$ (with $c_1 = c_2 = 2$) and measured critical angles at room temperature extracted from thermal wave measurements [7] (green dots joined by straight lines to guide the eye) as a function of the energy of (a) B ions and (b) P ions propagating in a Si crystal at $T=20^\circ\text{C}$, for the indicated axial and planar channels.

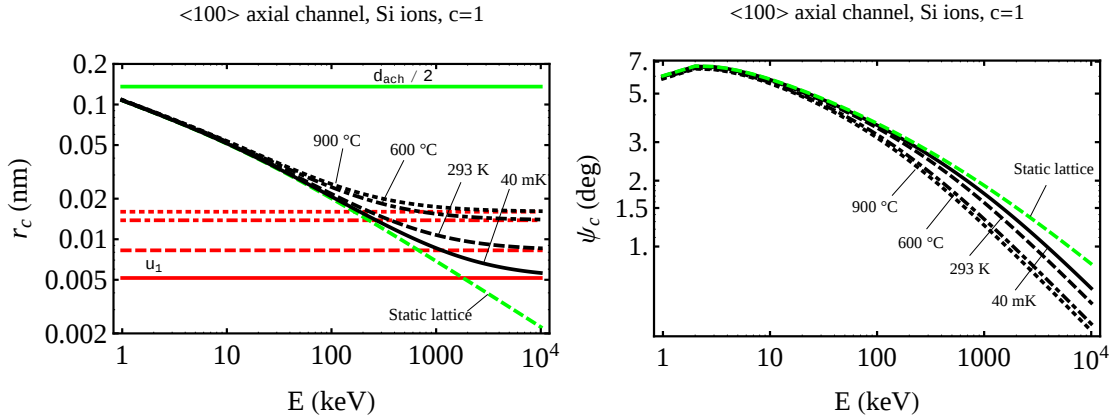


Figure 4.12: Static (green) and temperature corrected with $c_1 = c_2 = c = 1$ (black) (a) critical distances of approach $r_c^{\text{Mol}} = r_c$ (and $u_1(T)$ in red) and (b) the corresponding critical channeling angles $\psi_c^{\text{Mol}} = \psi_c$ as a function of the energy of propagating Si ions in $\langle 100 \rangle$ axial channels of a Si crystal.

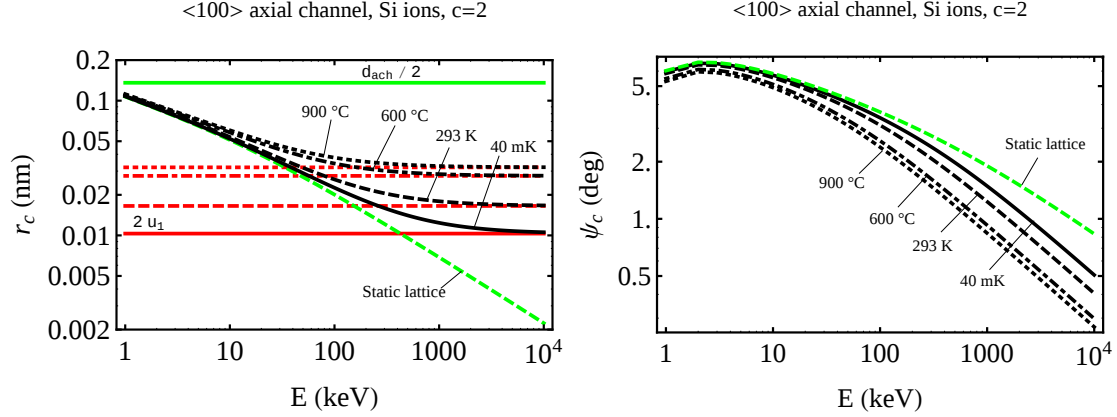


Figure 4.13: Same as Fig. 4.12 but using $c_1 = c_2 = c = 2$ in the temperature corrected critical distances of approach.

the right panels of Figs. 4.7 to 4.10 ($c_1 = c_2 = c$ and $c = 1$ or $c = 2$ at room temperature).

As shown in Fig. 4.11, with this formalism and using $c_1 = c_2 = 2$ we fit relatively well the critical angles measured at room temperature for B and P ions in a Si crystal (shown in green) in several channels, for energies between 20 keV and 600 keV that Hobler [7] extracted from thermal wave measurements.

Figs. 4.12 and 4.13 show clearly the temperature effects in the critical distances and angles for a specific channel, the $\langle 100 \rangle$ axial channel of a Si crystal and for a propagating Si ion. At small energies the static critical distance of approach is much larger than the vibration amplitude, so temperature corrections are not important. For small enough energies the critical distance becomes larger than the radius of the channel indicating that nowhere in the channel an ion can be far enough from the row of lattice atoms for channeling to take place (thus the critical channeling angle is zero). The exact calculation of the energy at which this happens would require considering the effect of more than a single row of atoms (which we do not do here) thus our results at these low energies are only approximate. As the energy increases, the static critical distance of approach decreases and when it becomes small with respect to the vibration amplitude u_1 , the temperature corrected critical distance becomes equal to $(c_1 u_1)$ which is larger for larger values of c_1 . When $u_1(T)$ becomes important in determining the critical distance, this becomes larger, and therefore the critical channeling

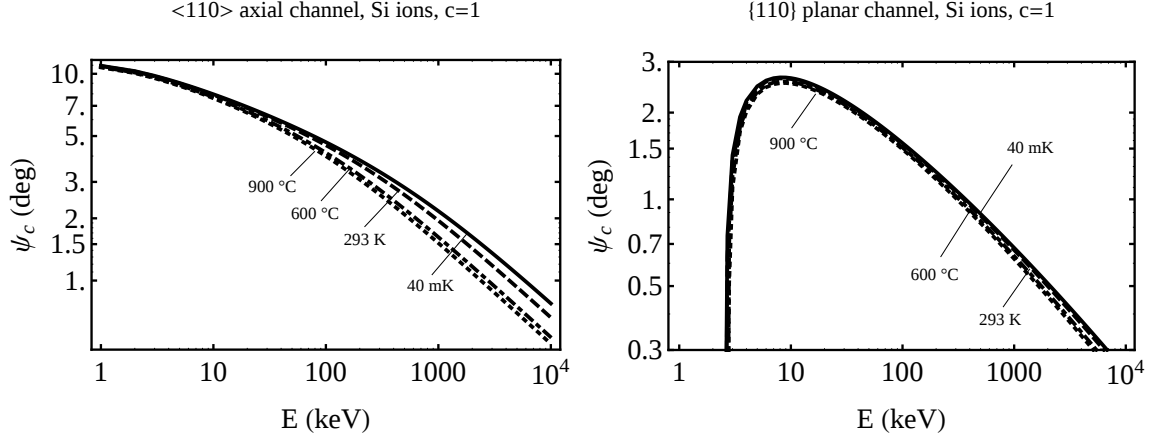


Figure 4.14: Temperature corrected critical channeling angles $\psi_c^{\text{Mol}} = \psi_c$ for $T=40$ mK, $T=20$ °C, $T=600$ °C, and $T=900$ °C as a function of the energy of a Si ion propagating in the (a) $\langle 110 \rangle$ axial channels and (b) $\{110\}$ planar channels of Si crystal.

angle become smaller, for higher temperatures.

Figs. 4.14 and 4.15 show how the critical channeling angles change with temperature for four particular channels, the $\langle 110 \rangle$ and $\langle 100 \rangle$ axial and the $\{110\}$ and $\{100\}$ planar channels, for Si ions in Si and Ge ions in Ge, respectively. In both cases the axial channeling angles are larger than the planar critical angles. The $\langle 110 \rangle$ and $\{111\}$ critical channeling angles are the largest among the axial and planar channels respectively. For example, at $E = 200$ keV for Si ions in Si, the channels with the largest channeling angles are (in order of decreasing channeling angles): $\langle 110 \rangle$, $\langle 100 \rangle$, $\langle 211 \rangle$, $\langle 111 \rangle$, $\{111\}$, $\langle 311 \rangle$, $\{110\}$, $\{100\}$, $\{310\}$, and $\{210\}$. We can clearly see that the critical angles become zero at low enough energies indicating the range of energies for which no channeling is possible.

4.2 Penetration length of channeled ions

Fig. 4.16 shows the maximum distance, $x_{\text{max}}(E)$ a channeled ion with initial energy E propagates in a crystal channel, according to the Lindhard-Scharff [77, 63] model of electronic energy loss, for a Si ion channeled in a Si crystal and a Ge ion in a Ge crystal. As explained

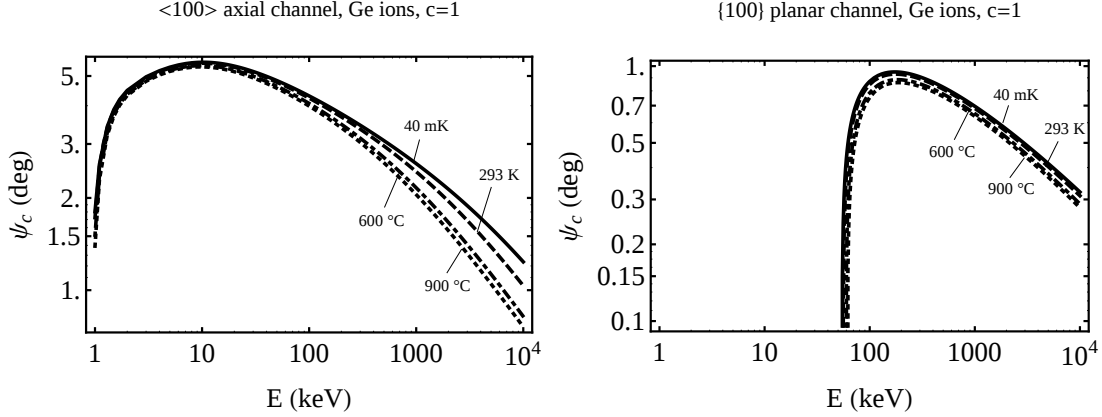


Figure 4.15: Same as Fig. 4.14 but for a Ge ion propagating in the (a) $\langle 100 \rangle$ axial channels and (b) $\{100\}$ planar channels of a Ge crystal.

in Section 3.2, this model is valid for small enough energies, $E < (M_1/2)Z_1^{4/3}v_0^2$ which is $E < 24.3$ MeV for a Si ion propagating in a Si crystal and $E < 188.7$ MeV for a Ge ion propagating in a Ge crystal. The range of the propagating ion, $x_{\max}(E)$ is given in Eq. 3.38.

Fig. 4.16 shows that even at energies of a few keV a channeled ion interacts with hundreds of lattice atoms. The characteristic interdistance of atoms along the channels is the lattice constant, i.e. approximately 0.5 nm for Si and Ge crystals (see Appendix A.2).

4.3 Channeling fractions

We use Eqs. 3.39 to 3.49 in Chapter 3 to compute the channeling fraction for each channel in Si and Ge. In Section 3.3.2 we derived the analytic expressions for the minimum distances $r_{i,\min}$ and $x_{i,\min}$ (given in Eq. 3.47, and 3.49, respectively) from Lindhard's approximation to the potential. In this Chapter we also use Eqs. 3.47 and 3.49 because it is not possible to find similar analytic expressions using Molière's approximation to the potentials (although following Hobler we use Molière's approximation to obtain the critical distances and angles).

We include in our calculation only the most important channels, the same considered by Hobler [7]. These are the $\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$, $\langle 211 \rangle$ and $\langle 311 \rangle$ axial channels and

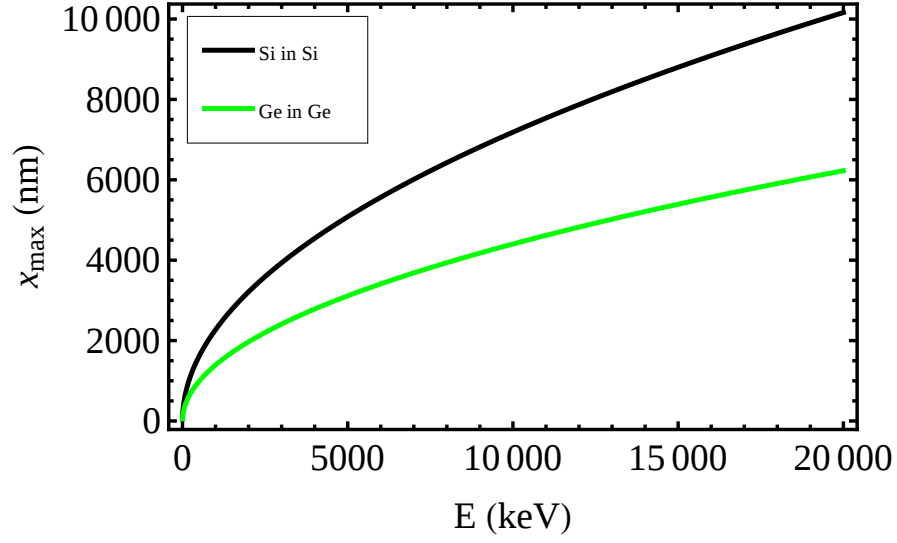


Figure 4.16: Maximum distance $x_{\max}(E)$ traveled by channeled Si ions in Si (black) or Ge ions in Ge (green/gray).

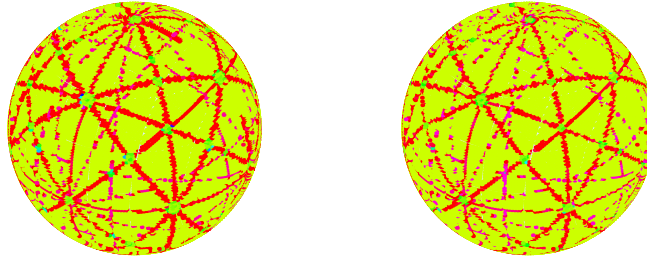


Figure 4.17: Geometric channeling fraction $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ including 74 channels (Eq. 4.16) for each direction $\hat{\mathbf{q}}$ plotted using the HEALPix pixelization of a sphere, for (a) a 200 keV Si ion recoil in a Si crystal, and (b) a 1 MeV Ge ion recoil in a Ge crystal, at 20 °C. Temperature effects in the lattice were included with $c_1 = c_2 = 1$. The light green, light blue, dark blue, pink, red, and yellow colors indicate a channeling fraction of 0.5, 0.013, 7.5×10^{-4} , 4×10^{-5} , 10^{-5} and zero, respectively.

the $\{100\}$, $\{110\}$, $\{111\}$, $\{210\}$ and $\{310\}$ planar channels. These constitute a total of 74 channels, as explained in Appendix A.2.

The probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ that an ion with initial energy E is channeled in a given direction $\hat{\mathbf{q}}$ is the probability that the recoiling ion enters any of the available channels, i.e.

$$\chi_{\text{rec}}(E, \hat{\mathbf{q}}) = P(A_1 \text{ or } A_2 \text{ or } \dots \text{ or } A_{74}). \quad (4.16)$$

We compute this probability in the same way we did in Section 3.3.3, using a recursion of the addition rule in probability theory and treating channeling along different channels as independent (see in Appendix D that this is a good approximation).

Fig. 4.17 shows the channeling probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ for a 200 keV recoiling Si ion in a Si crystal and a 1 MeV Ge ion recoil in a Ge crystal, at 20 °C. Temperature effects were included with $c_1 = c_2 = 1$. The probability is computed for each direction and plotted using the HEALPix pixelization of a sphere. The light green, light blue, dark blue, pink, red, and yellow colors indicate a channeling probability of 0.5, 0.013, 7.5×10^{-4} , 4×10^{-5} , 10^{-5} and zero, respectively.

To obtain the geometric total channeling fraction, we use Eq. 3.52 in which the channeling probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ is averaged over the directions $\hat{\mathbf{q}}$, assuming an isotropic distribution of the initial recoiling directions $\hat{\mathbf{q}}$.

Our results for the geometric total channeling fraction for Si ions in a Si crystal and Ge ions in a Ge crystal are shown in Figs. 4.18, 4.19 and 4.20 for three different assumptions for the effect of thermal vibrations in the lattice, which depend on the values of the parameters c_1 and c_2 used in the temperature corrected critical distances of approach $r_c^{\text{Mol}}(T)$ and $x_c^{\text{Mol}}(T)$ in Eq. 4.15.

We show the $c_1 = c_2 = 1$ choice in Fig. 4.19 and the $c_1 = c_2 = 2$ in Fig. 4.20. As the values of c_1 and c_2 increase, also the minimal distances from row or planes at which propagating ions must be to be channeled increase, thus the critical channeling angles decrease, which makes the channeling fractions smaller. If the values of c_1 and c_2 found by Hobler [7] and by us (see Fig. 4.11) to fit measured channeling angles for B and P ions propagating in Si apply also to the propagation of Si ions in Si, then the case of $c_1 = c_2 = 2$ in Fig. 4.20 should be

chosen and the channeling fractions would never be larger than 0.3%. With $c_1 = c_2 = 1$ the channeling fractions reach about 1% and they increase with temperature. The unrealistic case of $c_1 = c_2 = 0$ is shown in Fig 4.18 for different temperatures because it provides an upper limit to the channeling fractions. In this case the channeling fractions reach a few % and they increase with temperature.

As explained in Chapter 3, the channeling fraction χ_{axial} , Eq. 3.40, or χ_{planar} , Eq. 3.42 for axial and planar channels respectively, increases as $u_1(T)$ increases. This is the effect that dominates the temperature dependence in Figs. 4.18 and 4.19, in which the geometric channeling fractions in Si and Ge increase with increasing temperature. However, $r_{i,\text{min}}$, Eq. 3.47 or $x_{i,\text{min}}$, Eq. 3.49, increase with increasing critical distances and this decreases the channeling fraction. The increase of the critical distances with temperature is more accentuated for large values of c_1 and c_2 . This can be seen in Fig. 4.20, in which $c_1 = c_2 = 2$ and some channeling fractions are larger at lower temperatures.

Please note that we have not considered the possibility of dechanneling of initially channeled ions due to imperfections in the crystal. Any mechanism of dechanneling will decrease the fractions obtained here.

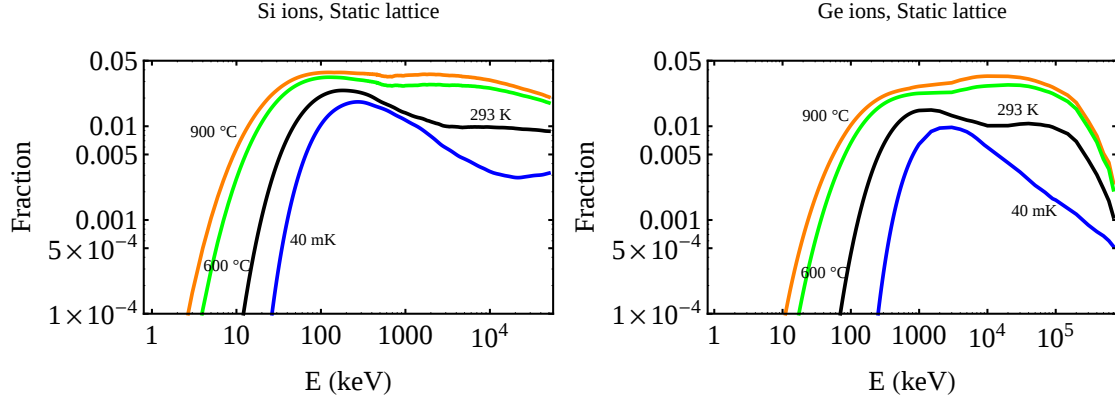


Figure 4.18: Channeling fractions of (a) Si and (b) Ge recoils in a Si and a Ge crystal respectively, as a function of the ion energy for temperatures $T=900$ °C (orange or medium gray), 600 °C (green or light gray), 293 K (black), and 44 mK (blue or dark gray) in the approximation of $c_1 = c_2 = 0$ (“static lattice”). This is an upper bound with respect to any non-zero values of c_1 and c_2 . Temperature effect are included in the vibrations of the colliding atom.

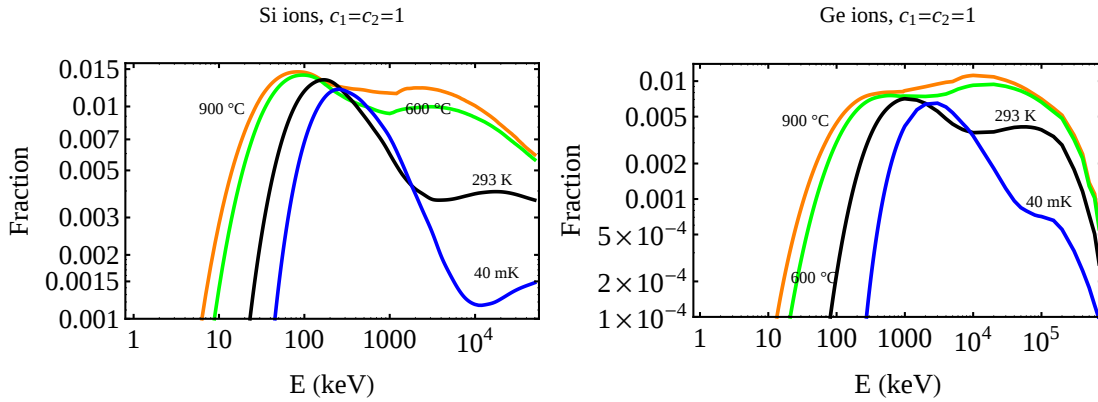


Figure 4.19: Same as Fig. 4.18 but with $c_1 = c_2 = 1$.

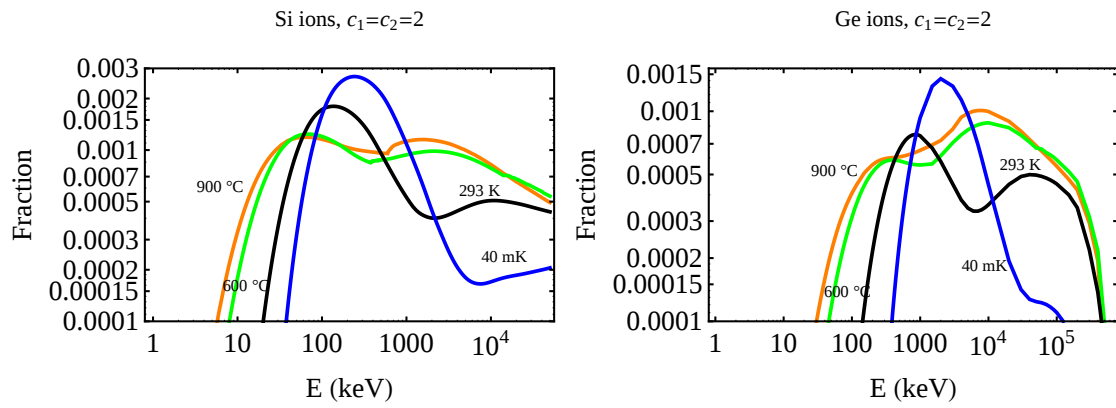


Figure 4.20: Same as Fig. 4.18 but with $c_1 = c_2 = 2$.

CHAPTER 5

Channeling fraction in CsI crystals

In dark matter searches, CsI (Tl) crystals are used by the KIMS collaboration [84, 85]. In this chapter we give upper bounds to the geometric channeling fraction of recoiling ions in CsI crystals. We proceed in a similar manner as we did for NaI, a very similar crystal, in Chapter 3. We use Lindhard's expression for the transverse continuum string and plane potentials, $U(r)$ (given in Eq. 3.1) and $U_p(x)$ (given in Eq. 3.4) respectively, because it is the simplest and allows to find analytical expressions for the quantities we need.

Examples of axial and planar continuum potentials for Cs ions propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a CsI crystal are shown in Fig. 5.1. The potentials for Cs and I ions are practically identical, because $Z_{\text{Cs}} \simeq Z_{\text{I}}$ (see Appendix A.3).

For a static lattice, the critical distances of approach r_c and x_c are given in the Eqs. 3.14 and 3.22, expressions that were derived in Chapter 3. For planar channeling, the characteristic distance $\bar{d}$ between atoms along the fictitious row needs to be estimated using data or simulations which are not available for a CsI crystal. As explained in Section 3.1.3, the choice of $\bar{d}$ equal to the average interdistance of atoms in the plane d_p , i.e. $\bar{d} = d_p$, yields a lower bound on x_c , which translates into an upper bound on the fraction of channeled recoils into planar channels.

We use the temperature corrected critical distances of approach $r_c(T)$ and $x_c(T)$ (Eqs. 3.29 and 3.30) instead of the static lattice critical distances r_c and x_c . In the one dimensional rms vibration amplitude u_1 (Eq. 3.26 and 3.27), M for a compound is the average atomic mass (in amu), i.e. for CsI, $M = (M_{\text{Cs}} + M_{\text{I}})/2$. With $M_{\text{Cs}} = 132.9$ amu and $M_{\text{I}} = 126.9$ amu, then $M = 129.9$ amu. We take the Debye temperature of CsI to be $\Theta = 125$ K [33, 70]. Fig. 5.2 shows the plot of u_1 in CsI as a function of the temperature T . The crystals in the

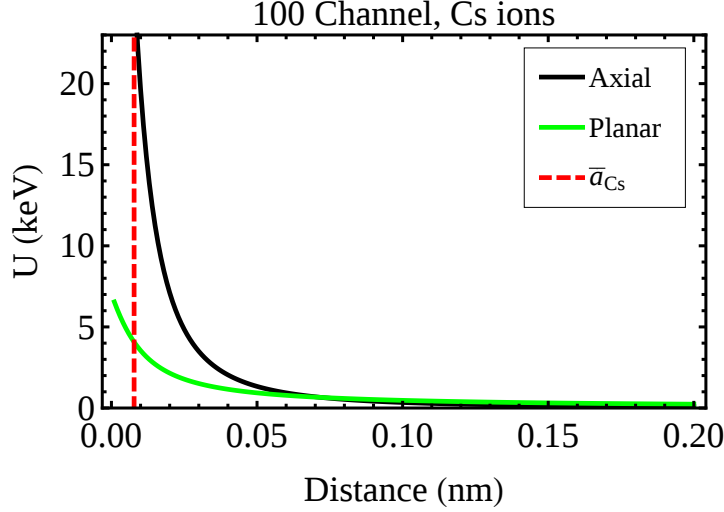


Figure 5.1: Continuum axial (black) and planar (green/gray) potentials for Cs ions, propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a CsI crystal. The screening radius shown as a vertical line is $\bar{a}_{\text{Cs}} = 0.007785$ nm (see Appendix A.3).

KIMS experiment were kept at 0 °C in 2007 [86]. Currently the operating temperature of the crystals is 20 °C [87]. The vibration amplitude is $u_1 = 0.0141$ nm at 0 °C, and $u_1 = 0.0146$ nm at 20 °C.

Using the temperature corrected critical distances of approach $r_c(T)$ and $x_c(T)$ (Eqs. 3.29 and 3.30) or the static lattice critical distances r_c and x_c (Eqs. 3.14 and 3.22), we obtain the corresponding critical axial and planar channeling angles ψ_c (see Chapter 3 for details). Examples are shown in Figs. 5.3 to 5.5, for $c_1 = c_2 = c$ and $c = 1$ or $c = 2$ as indicated.

Fig. 5.3 clearly shows how the critical distances and angles change with temperature for a Cs or I ion propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a CsI crystal, with temperature effects computed with $c_1 = c_2 = c = 1$. Notice that for the 100 channels, the widths of axial and planar channels are the same, $d_{\text{ach}} = d_{\text{pch}}$ and $r_c = x_c$.

Fig. 5.4 shows the same effects for the $\langle 111 \rangle$ axial channel. In this channel, the critical distance becomes larger than the radius of the channel at energies below a few keV, shown in the figures, and thus the critical channeling angle is zero. Notice that for the 111 channels,

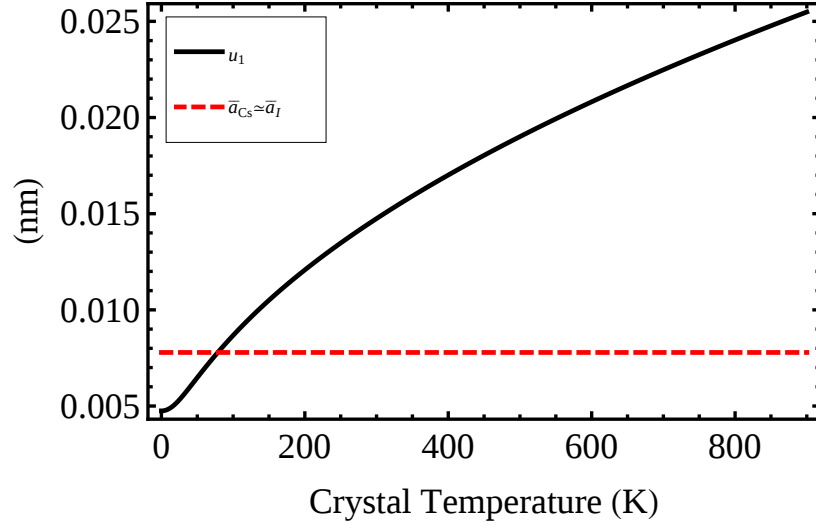


Figure 5.2: Plot of $u_1(T)$ for CsI (Eq. 3.26 with $M = (M_{Cs} + M_I)/2$).

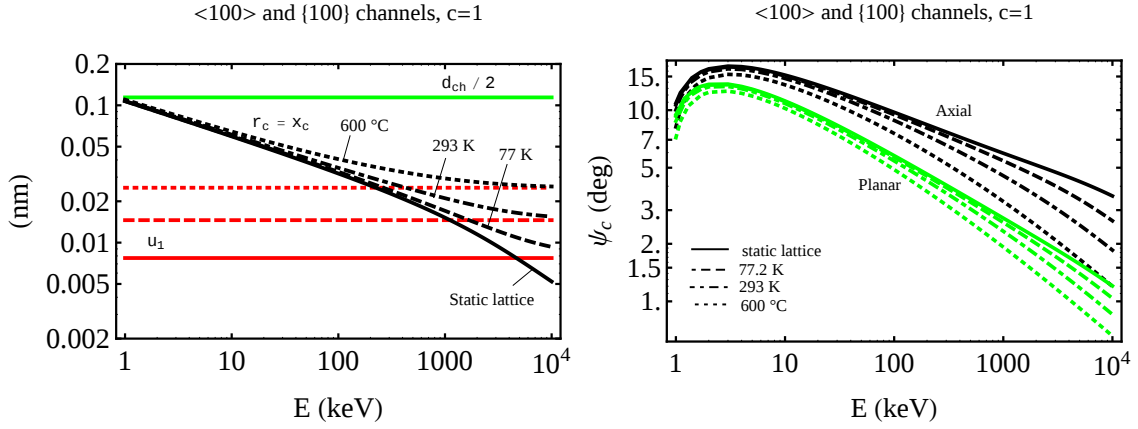


Figure 5.3: Static (green) and temperature corrected with $c_1 = c_2 = c = 1$ (black) (a) critical distances of approach (and $u_1(T)$ in red) and (b) the corresponding critical channeling angles, as a function of the energy of propagating Cs or I ions (they are practically the same for both) in the $\langle 100 \rangle$ axial (black) and $\{100\}$ planar (green) channels. Here $d_{ach} = d_{pch}$.

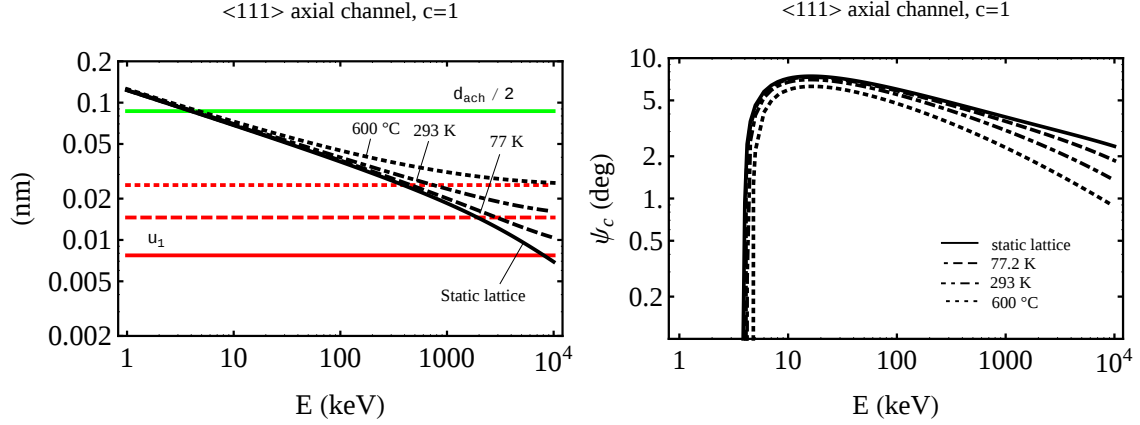


Figure 5.4: Same as Fig. 5.3 but for the $\langle 111 \rangle$ axial channel.

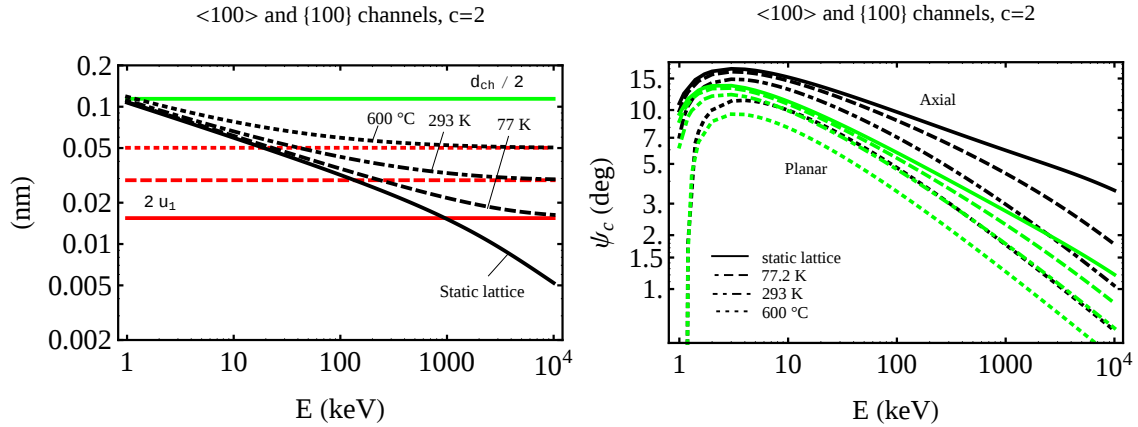


Figure 5.5: Same as Fig. 5.3 but with $c_1 = c_2 = c = 2$.

the $\langle 111 \rangle$ axial and $\{111\}$ planar channels do not have the same widths, $d_{\text{ach}} \neq d_{\text{pch}}$, and we only show the critical distance and angles for the axial channel.

Figs. 5.5.a and 5.5.b show the static and T -corrected critical distances and angles respectively at several temperatures for traveling Cs or I ions in the 100 axial and planar channels with $c_1 = c_2 = c = 2$.

We use Eqs. 3.39 to 3.49 obtained in Chapter 3 to compute the channeling fraction for each channel in CsI. In order to obtain the total geometric channeling fraction we need to sum over all the individual channels we consider. Taking only the channels with lowest crystallographic indices, 100, 110 and 111, we have a total of 26 axial and planar channels,

as explained in Appendix A.3 (CsI and NaI have the same crystal structure).

Fig. 5.6 shows upper bounds to the channeling probability computed for each initial recoil direction $\hat{\mathbf{q}}$ and plotted on a sphere using the HEALPix pixelization for (a) a $E = 200$ keV and (b) a 1 MeV Cs ion at 20 °C with $c_1 = c_2 = 1$ assumed for the temperature effects. The red, pink, dark blue and light blue colors indicate a channeling probability of 1, 0.625, 0.25 and zero, respectively. The results are practically identical for an I ion.

Fig. 5.7 shows upper bounds to the channeling fractions of Cs recoils for individual channels, for $T = 20^\circ\text{C}$ and assuming $c_1 = c_2 = 1$. The black and green (or gray) lines correspond to single axial and planar channels respectively. The upper bounds of the channeling fractions of planar channels are more generous than those of axial channels because of our choice of x_c in Eq. 3.22. This does not mean that planar channels are dominant in the actual channeling fractions.

Upper bounds to the geometric channeling fractions of Cs and I ions as function of the recoil energy are shown in Figs. 5.8 and 5.9 with thermal effects taken into account with $c_1 = c_2 = 1$ and $c_1 = c_2 = 2$, respectively.

Notice that we have not included here any dechanneling due to the presence of impurities in the crystal (such as Tl atoms), which would decrease the channeling fractions presented.

As shown in Fig. 5.8, the channeling fraction for CsI (Tl) is never larger than 5% at 293 K (with $c_1 = c_2 = 1$) and the maximum fraction happens at around 1 MeV. This is comparable to the channeling fraction of Na (Tl) which is also never larger than 5%, but in the case of Na (Tl) the maximum happens at 100's of keV (see Fig. 3.11.a). For Si and Ge (with $c_1 = c_2 = 1$) the channeling fractions reach about 1% and the maximum happens at 100's of keV for Si and at around 1 MeV for Ge (see Fig. 4.19). Fig. 5.9, shows that the maximum channeling fraction for Cs or I recoils at 293 K would be below 0.5% if $c_1 = c_2 = 2$ instead. However, since we do not know which are the correct values of the crucial parameters c_1 and c_2 for CsI, we could ask ourselves how the upper bounds on channeling fractions would change if the values of these parameters would be smaller than 1. The values of c_1 and c_2 cannot be smaller than zero, thus Fig. 5.10 shows our most generous upper bounds on the

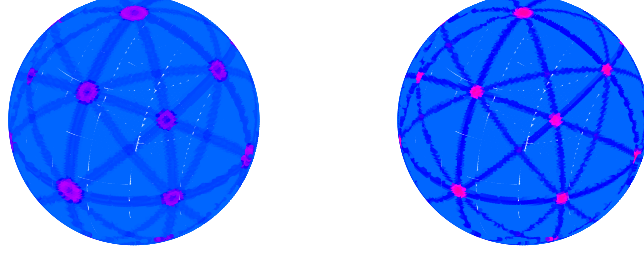


Figure 5.6: Upper bounds on the channeling probability of a Cs ion (for an I ion the figure would be practically identical) as function of the initial recoil direction for a (a) 200 keV and (b) 1 MeV recoil energy at 20 °C (with $c_1 = c_2 = 1$). The probability is computed for each direction and plotted on a sphere using the HEALPix pixelization. The red, pink, dark blue and light blue colors indicate a channeling probability of 1, 0.625, 0.25 and zero, respectively.

geometric channeling fraction, obtained by setting $c_1 = c_2 = 0$ (static lattice). Even in this physically inconsistent case, the channeling fractions at 293 K cannot be larger than 10%.

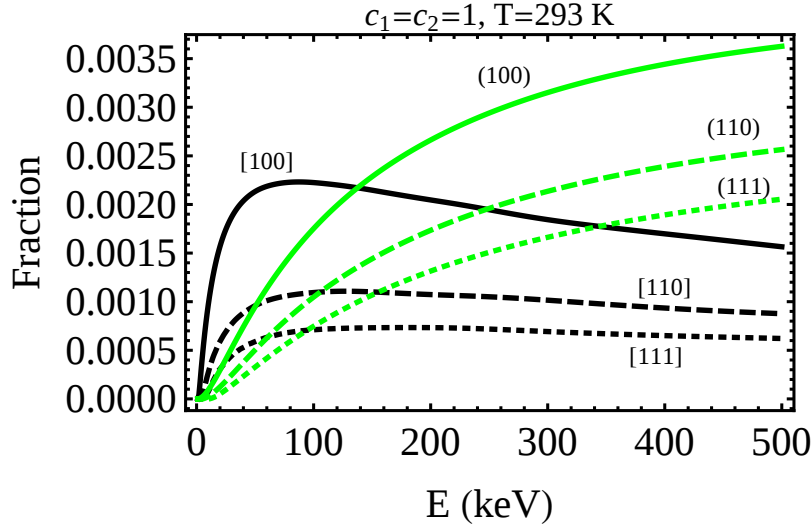


Figure 5.7: Upper bounds on the channeling fractions of Cs recoils as a function of the recoil energy E when only one channel is open, for $T = 293$ K with temperature corrections included in the critical distances with the coefficients $c_1 = c_2 = 1$. Black and green/gray lines correspond to axial and planar channels respectively. Solid, dashed, and dotted lines are for 100, 110, and 111 channels respectively. The corresponding figure for an I ion would be practically identical.

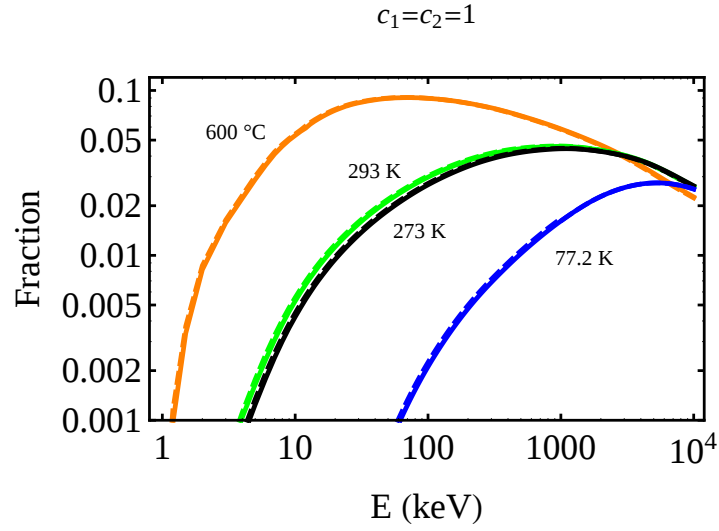


Figure 5.8: Upper bounds on the channeling fraction of Cs (solid lines) and I (dashed lines) recoils as a function of the recoil energy E for $T = 600\text{ }^{\circ}\text{C}$ (orange/medium gray), 293 K (green/light gray), 273 K (black), and 77.2 K (blue/dark gray) in the approximation of $c_1 = c_2 = 1$ without dechanneling.

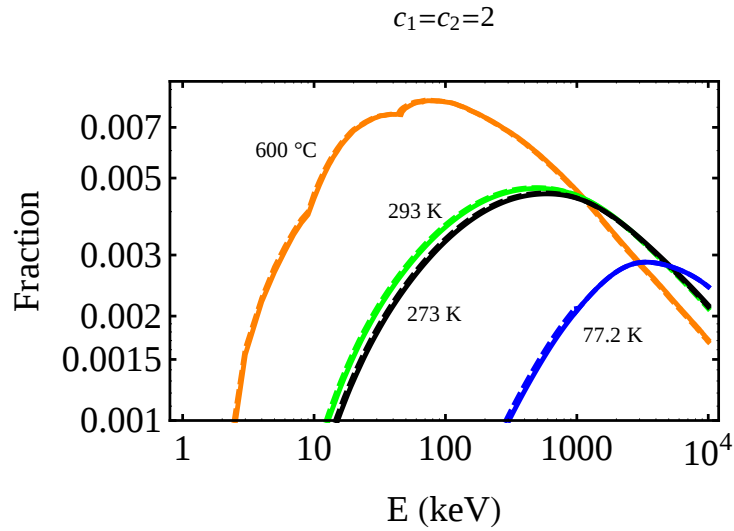


Figure 5.9: Same as Fig. 5.10 but for $c_1 = c_2 = 2$.

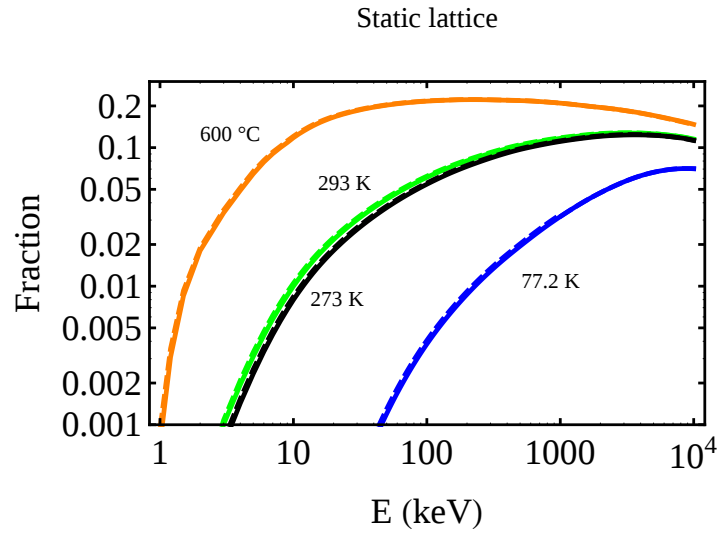


Figure 5.10: Same as Fig. 5.10 but for $c_1 = c_2 = 0$ (static lattice), which provides an extreme upper bound (any larger values of c_1 and c_2 , which can reasonably be as large as 2, yield smaller fractions).

CHAPTER 6

Channeling fraction in solid Xe, Ar and Ne crystals

The level of background in future experiments is a crucial element to determine if the daily modulation is observable and the advantage of using solidified noble gas detectors is the possibility of achieving a low background level for WIMP searches [88]. Xenon and Neon have no long life radioisotopes and thus contain no intrinsic background source of radiation. Argon has the drawback that it contains ^{39}Ar beta source which induces electron recoil signature in the detector. Solid or crystallized Xenon detector can be ideal for dark matter searches, whereas a crystallized Xenon detector would be necessary to have channeling. At present, solid Xe crystals are used by the Solid Xenon R&D Project [89].

In this chapter we compute the geometric channeling fractions of recoiling ions in solid Xe, Ar, and Ne crystals. At room temperature and pressure Xe, Ar and Ne are noble gases. At temperatures below 161.45 K, 83.80 K and 24.56 K respectively (at room pressure) they become solids. All of them form monatomic face-centered cubic (f.c.c.) crystals (see Appendix A.4).

We proceed in a similar manner as we did for Si and Ge in Chapter 4. As in Chapter 4, here we use Molière's approximation for the atomic potential, following the work of Hobler [7] and Morgan and Van Vliet [58, 59, 60]. The axial and planar continuum potentials in Molière's approximation, $U_{\text{Mol}}(r)$ and $U_{\text{Mol},p}(x)$ are given in Eqs. 4.1 and 4.3, respectively.

Examples of axial and planar continuum potentials, generically called U_{Mol} , for Xe, Ar, and Ne ions propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a Xe, Ar, and Ne crystal respectively are shown in Fig. 6.1.

As in Chapter 4, we use Morgan and Van Vliet's [59] equation to define the critical

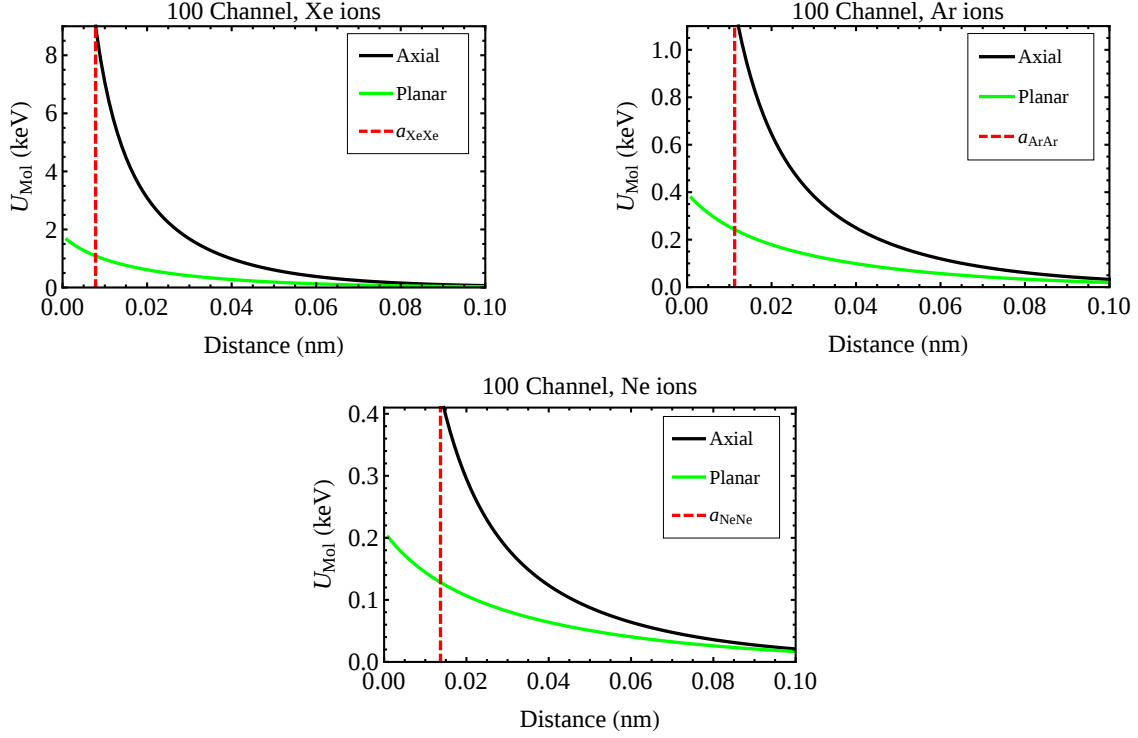


Figure 6.1: Continuum axial (black) and planar (green/gray) potentials as function of the distance from the row or plane of lattice atoms, respectively, for (a) Xe ions, (b) Ar ions, and (c) Ne ions, propagating in the $\langle 100 \rangle$ axial and $\{100\}$ planar channels of a Xe, Ar, and Ne crystal respectively. The screening radius shown as a vertical line is $a_{\text{XeXe}} = 0.007808$ nm for Xe, $a_{\text{ArAr}} = 0.01126$ nm for Ar and $a_{\text{NeNe}} = 0.01370$ nm for Ne (see Appendix A.4).

distance r_c , i.e. $U''_{\text{Mol}}(r_c) = 5E/d^2$. For a static lattice, we use an approximate analytic expression for r_c (which we call r_c^{Mol}) obtained by fitting a degree nine polynomial in the parameter $\sqrt{\alpha} = (Z_1 Z_2 e^2 d / a^2 E)^{1/2}$ to the exact solution of Eq. 4.6. The expression for r_c^{Mol} obtained in this way (Eq. 4.8) is valid for recoil energies $E > 3$ keV for Xe, and for $E > 1$ keV for Ar and Ne.

To find the static critical distance x_c of a planar channel, the characteristic distance between atoms along the fictitious row needs to be estimated using data or simulations which are not available for Xe, Ar and Ne crystals. As explained in Section 3.1.3, this characteristic distance depends on the width $2R$ of the strip considered. As described in

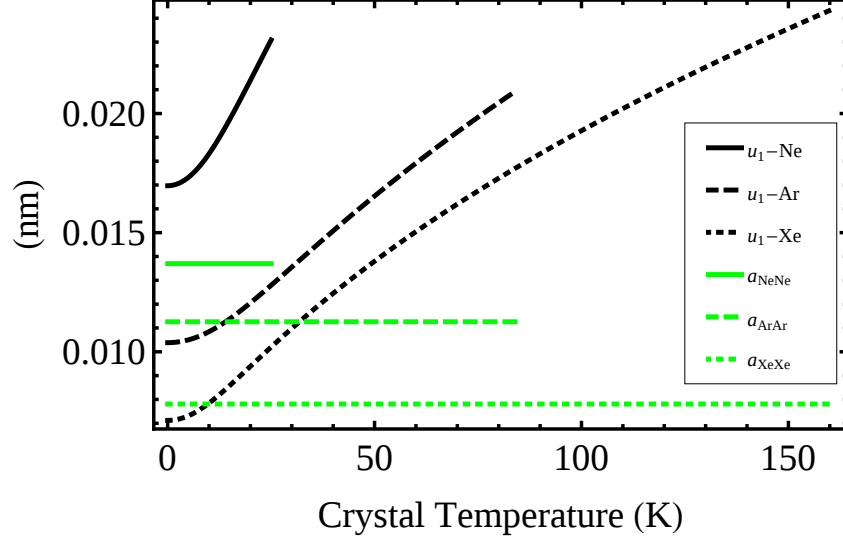


Figure 6.2: Plot of $u_1(T)$ for Ne (solid line), Ar (dashed line), and Xe (dotted line) as a function of the crystal temperature. The plots are cut at the respective melting temperatures.

Chapter 4, we decided to keep the Morgan and Van Vliet definition for R , because Hobler [7] found that it is in quite good agreement with the binary collision simulations and data of B and P ions propagating in Si for energies of about 1 keV and above. We used an approximate analytical solution for R (called R^{Mol} in Eq. 4.12) obtained by fitting a degree five polynomial in $(\ln y)$ where $y = Z_1 Z_2 e^2 / a \sqrt{E U_p(0)}$, to the exact numerical solution of Eq. 4.10. The planar critical distance x_c^{Mol} we obtained (Eq. 4.13) is valid for $E < 7$ GeV for Xe, $E < 160$ MeV for Ar, and $E < 20$ MeV for Ne. These conditions provide the energy ranges for which our channeling fraction estimates are valid. Within its range of validity, the percentage error of the analytic approximation we used for x_c^{Mol} is less than 9%.

The critical distances of approach in a non-static lattice depend on the temperature, through the vibration of the atoms in the lattice (thermal expansion effects are negligible, as shown in Appendix E). The one dimensional rms vibration amplitude u_1 of the atoms in a crystal in the Debye model (see Eqs. 3.26 and 3.27) is plotted in Fig. 6.2 for Xe, Ar, and Ne crystals as function of the temperature T up to their respective melting points. The crystals in the Solid Xenon R&D Project experiment will be operating at 77.2 K and higher [90].

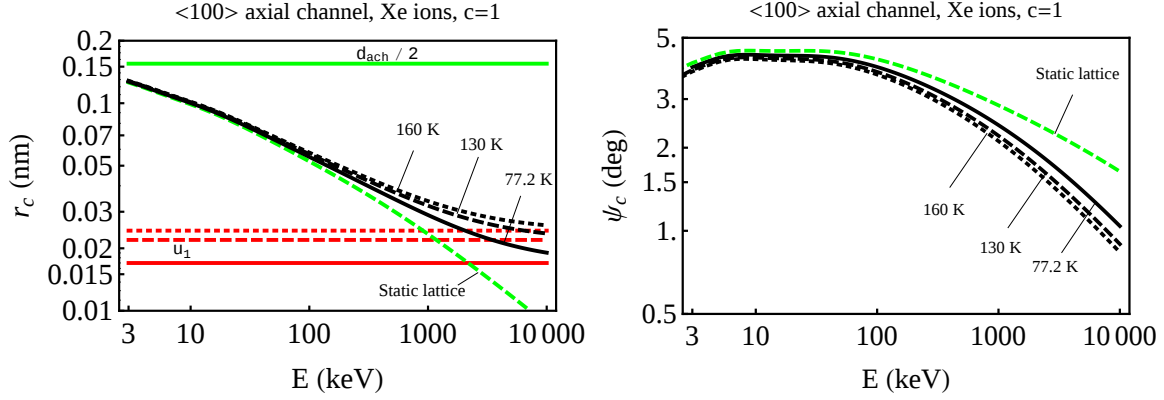


Figure 6.3: Static (green) and temperature corrected with $c_1 = c_2 = c = 1$ (black) (a) critical distances of approach $r_c^{\text{Mol}} = r_c$ (and $u_1(T)$ in red) and (b) the corresponding critical channeling angles $\psi_c^{\text{Mol}} = \psi_c$, for $T = 77.2$ K, $T = 130$ K, and $T = 160$ K as a function of the energy of propagating Xe ions in the $\langle 100 \rangle$ axial channel of a Xe crystal.

Using the temperature corrected critical distances of approach $r_c^{\text{Mol}}(T)$ and $x_c^{\text{Mol}}(T)$ (Eq. 4.15) or the static lattice critical distances r_c^{Mol} and x_c^{Mol} (Eqs. 4.8 and 4.13), we obtain the corresponding temperature corrected critical axial and planar channeling angles, ψ_c^{Mol} and $\psi_c^{\text{Mol},p}$ respectively. Examples of critical distances and angles are shown in Figs. 6.3 to 6.5, for $c_1 = c_2 = c$ and $c = 1$ or $c = 2$ as indicated.

Fig. 6.3 clearly shows how the critical distances and angles change with temperature for Xe ions propagating in the $\langle 100 \rangle$ axial channel of a Xe crystal, with temperature effects computed with $c_1 = c_2 = 1$. Fig. 6.4 shows the same as Fig. 6.3 but for $c_1 = c_2 = 2$. Figs. 6.5.a and 6.5.b show the critical distances at several temperatures for Xe ions propagating in the $\{100\}$ planar channel with $c_1 = c_2 = 1$ and $c_1 = c_2 = 2$ respectively.

We use Eqs. 3.39 to 3.49 obtained in Chapter 3 to compute the channeling fraction for each channel in solid Xe, Ar, and Ne. To obtain the total geometric channeling fraction we sum over only the channels with lowest crystallographic indices, 100, 110 and 111. We have a total of 26 axial and planar channels (see Appendix A.4). We treat channeling along different channels as independent events when computing the probability that an ion enters any of the available channels. We find that the method explained in Appendix D for obtaining an

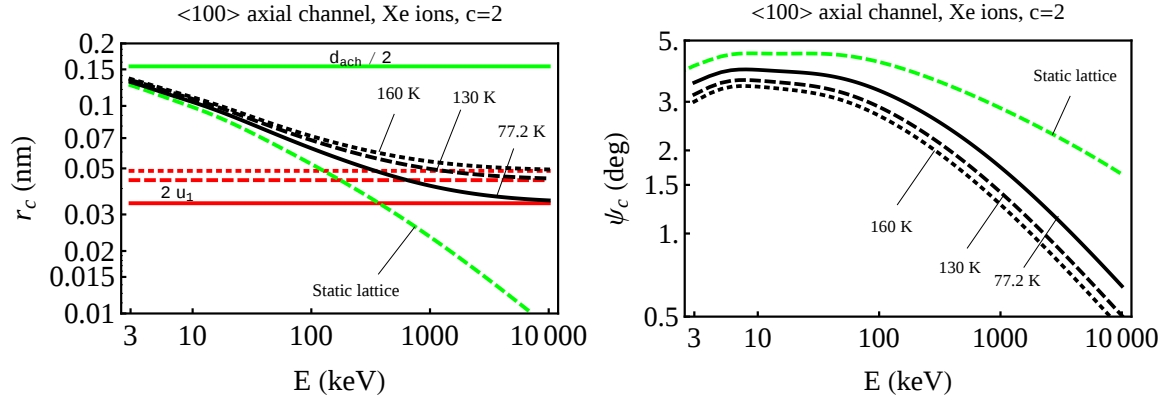


Figure 6.4: Same as Fig. 6.3 but with $c_1 = c_2 = c = 2$.

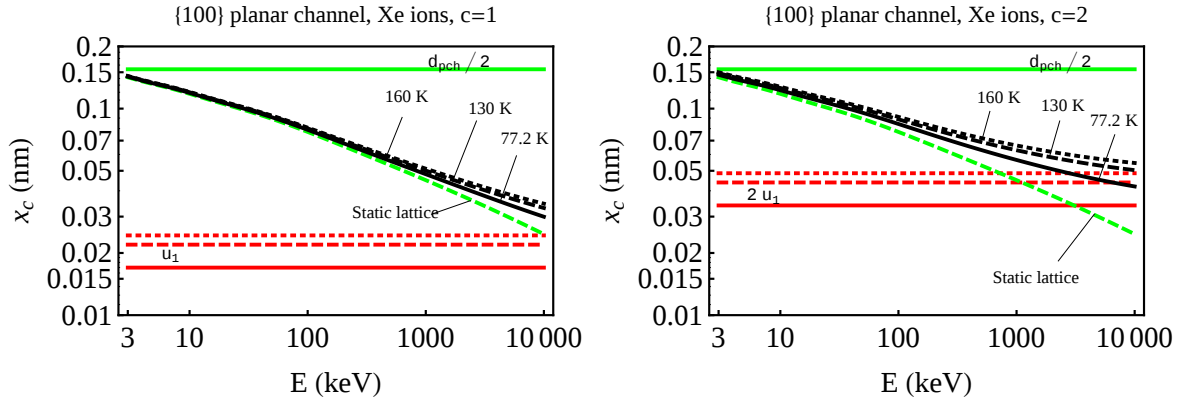


Figure 6.5: Static (green) and temperature corrected (black) with (a) $c_1 = c_2 = c = 1$ and (b) $c_1 = c_2 = c = 2$ critical distances of approach $x_c^{\text{Mol}} = x_c$ for $T = 77.2$ K, $T = 130$ K, and $T = 160$ K as a function of the energy of propagating Xe ions in the {100} planar channel of a Xe crystal.

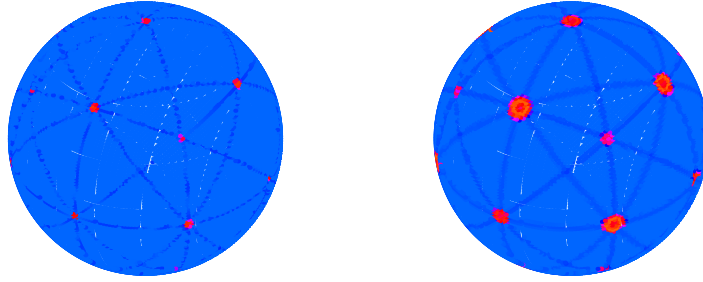


Figure 6.6: Geometric channeling probabilities as function of the initial recoil direction for (a) a 1 MeV Xe ion propagating in a Xe crystal at 160 K and (b) a 20 keV Ne ion propagating in a Ne crystal at 23 K (with $c_1 = c_2 = 1$). The probability is computed for each direction and plotted on a sphere using the HEALPix pixelization. The red, pink, dark blue and light blue colors indicate a channeling probability of 1, 0.625, 0.25 and zero, respectively.

upper limit to the channeling probability of overlapping channels gives results practically indistinguishable from those obtained assuming that channeling along different channels are independent events.

Fig. 6.6 shows the channeling probability computed for each initial recoil direction $\hat{\mathbf{q}}$ plotted on a sphere using the HEALPix pixelization for a 1 MeV Xe ion propagating in a Xe crystal at 160 K and a 20 keV Ne ion propagating in a Ne crystal at 23 K ($c_1 = c_2 = 1$ is assumed for the temperature effects). The red and blue indicate a channeling probability of 1 and zero, respectively (see the colors in the figure).

Fig. 6.7 shows the channeling fractions for several individual channels of Xe ions propagating in a Xe crystal at $T = 77.2$ K, Ar ions propagating in an Ar crystal at $T = 40$ mK, and Ne ions propagating in a Ne crystal at $T = 40$ mK (again with $c_1 = c_2 = 1$). The curves correspond to single axial or planar channels. Notice that at low energies channeling is dominated by axial channels, and at higher energies planar channels dominate.

The geometric total channeling fractions of Xe, Ar, and Ne ions as function of the recoil

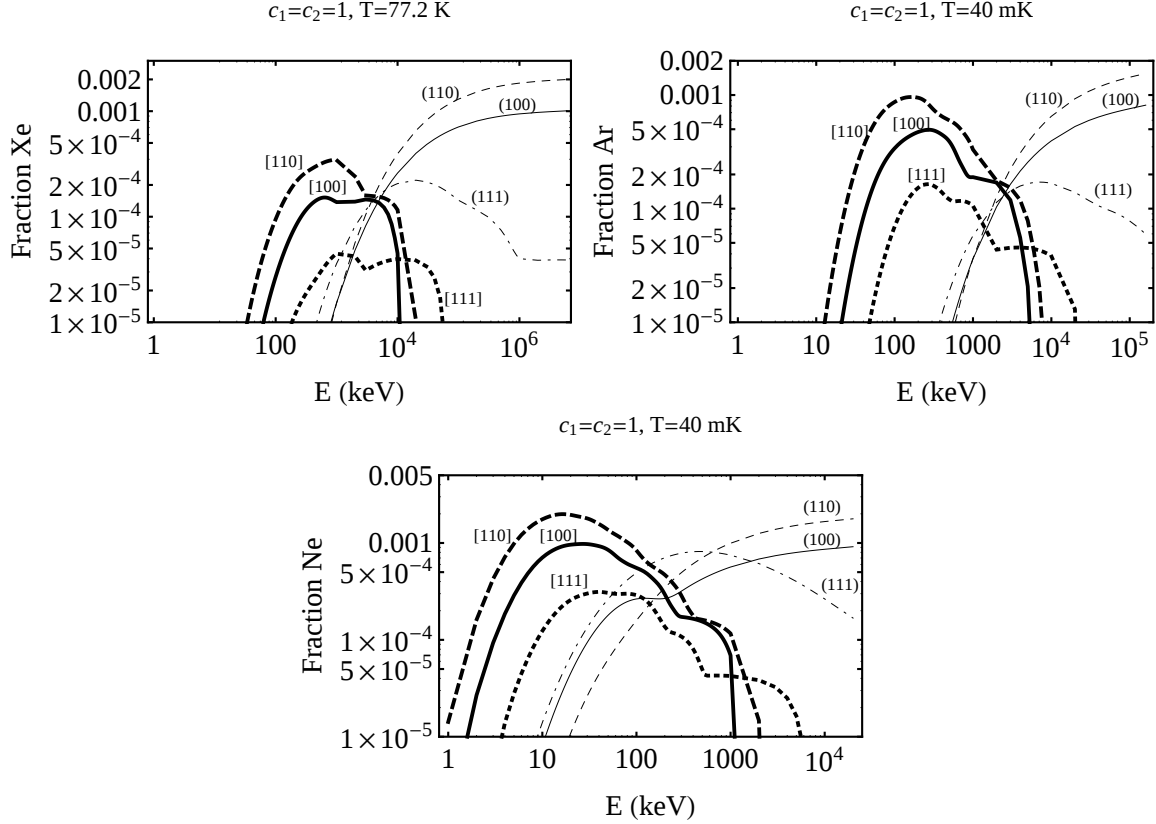


Figure 6.7: Channeling fraction of (a) Xe recoils at $T = 77.2$ K, (b) Ar recoils at $T = 40$ mK, and (c) Ne recoils at $T = 40$ mK for single planar and axial channels, as a function of the recoil energy E in the approximation of $c_1 = c_2 = 1$.

energy are shown in Figs. 6.8, 6.9, and 6.10 respectively. For each crystal, we include three possibilities for thermal effects: (a) $c_1 = c_2 = 1$, a reasonable middle ground, (b) maximum effects, i.e. $c_1 = c_2 = 2$, and (c) $c_1 = c_2 = 0$, which corresponds to the unrealistic case of not having thermal effects in the lattice.

Notice that we have not considered the possibility of dechanneling of initially channeled ions due to imperfections in the crystal. Any mechanism of dechanneling will decrease the fractions obtained here.

As we see in Fig. 6.8 to 6.10 the channeling fraction increases with energy, reaches a maximum at a certain energy, then has a dip and finally raises again. The maximum reflects the shape of the single channeling fractions, which all have maxima. At the maximum of the

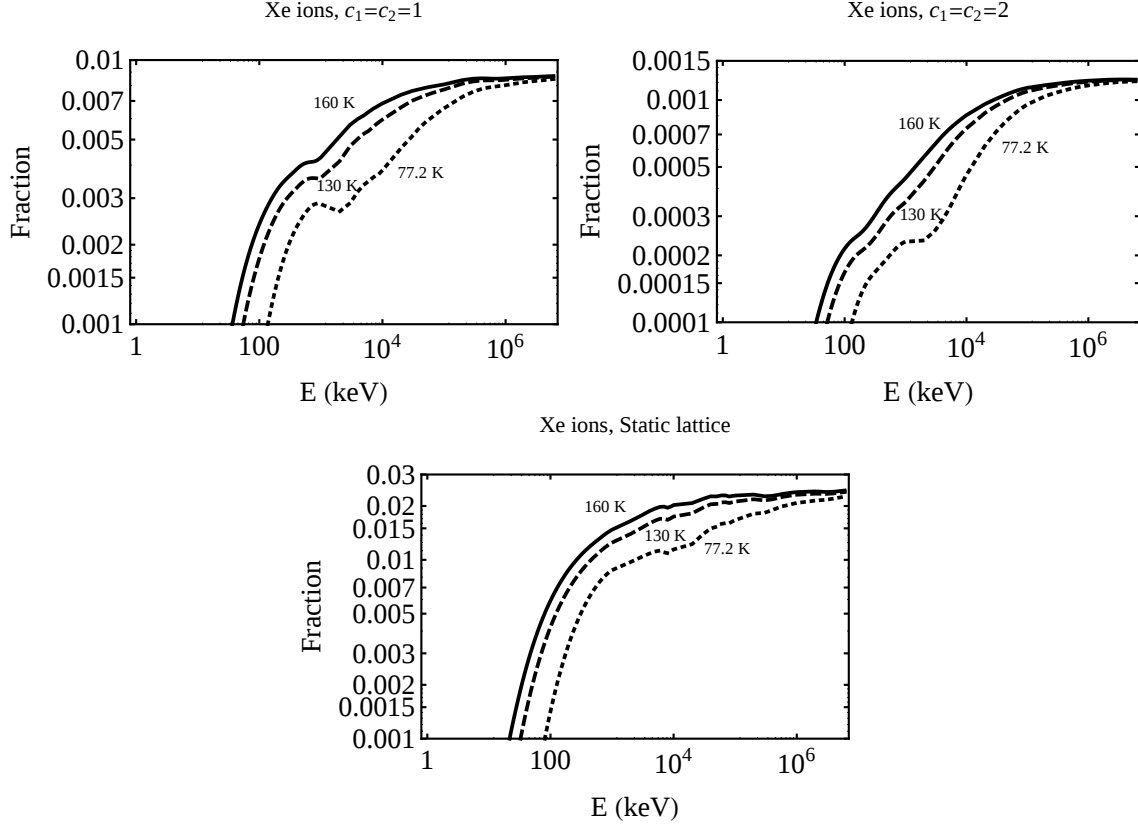


Figure 6.8: Channeling fraction of Xe recoils as a function of the recoil energy E for $T = 160$ K (solid line), 130 K (dashed line), and 77.2 K (dotted line) in the approximation of (a) $c_1 = c_2 = 1$, (b) $c_1 = c_2 = 2$ and (c) static lattice with $c_1 = c_2 = 0$.

channeling fraction the axial channels dominate, in particular the channels $[110]$ and $[100]$ (as seen in Fig 6.7). The dip and the raise result from having multiple axial and planar channels contributing to the channeling fraction. At lower E axial channels dominate and at higher E planar channels dominate. The dip happens at the cross-over between both types of channels, when as the energy increases the contribution of axial channels dies out and that of planar channels is increasing. This increase causes the subsequent raise in the channeling fraction as the energy increases further.

As shown in Figs. 6.8.a, 6.9.a, and 6.10.a, the channeling fractions are never larger than 1% for Xe and Ar and never larger than 2% for Ne (with $c_1 = c_2 = 1$). Figs. 6.8.b, 6.9.b, and 6.10.b show that with $c_1 = c_2 = 2$, the maximum channeling fraction for Xe ions at 160 K,

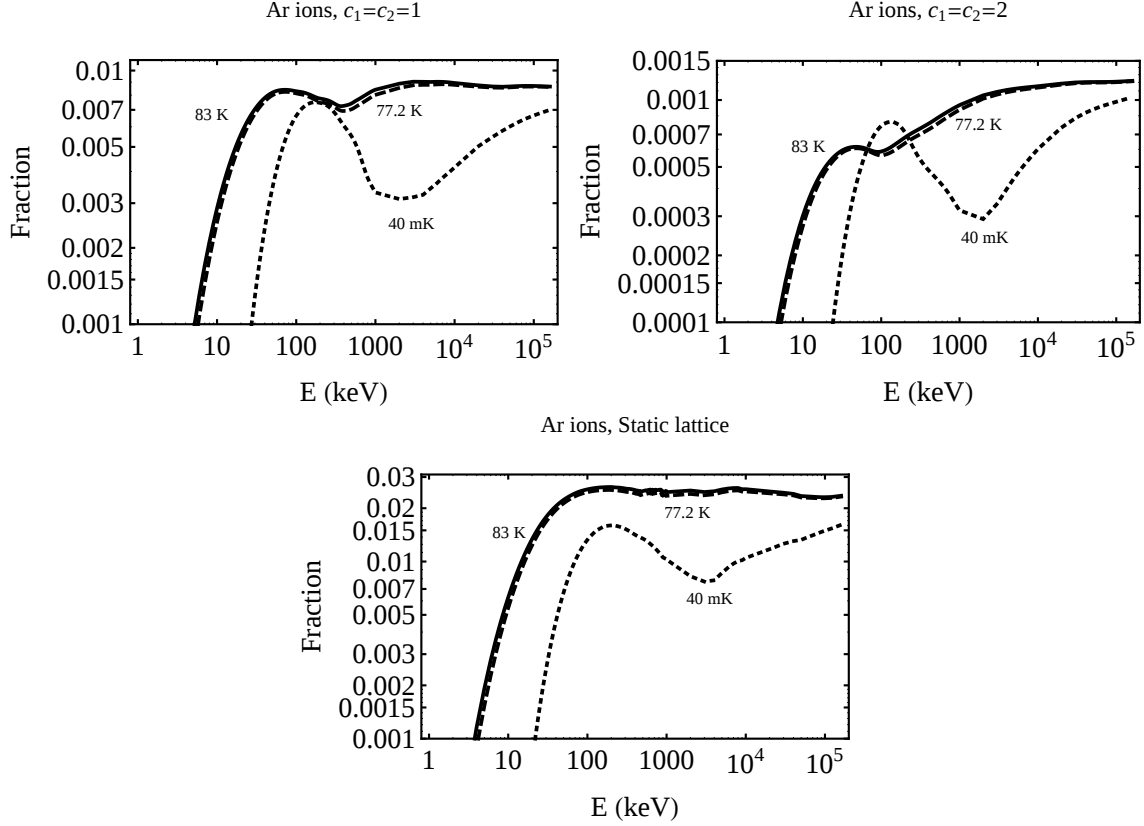


Figure 6.9: Channeling fraction of Ar recoils as a function of the recoil energy E for $T = 83$ K (solid line), 77.2 K (dashed line), and 40 mK (dotted line) in the approximation of (a) $c_1 = c_2 = 1$, (b) $c_1 = c_2 = 2$ and (c) static lattice with $c_1 = c_2 = 0$.

Ar ions at 83 K, and Ne ions at 23 K would be below 0.2%. Figs. 6.8.c, 6.9.c, and 6.10.c show the upper bounds on the geometric channeling fraction, obtained by setting $c_1 = c_2 = 0$ for a static lattice. Even in this physically inconsistent case, the channeling fractions cannot be larger than 5%.

Increasing the temperature of a crystal usually increases the fraction of channeled recoiling ions, but when the values of c_1 and c_2 are large (i.e. close to 2) so the critical distances increase rapidly with the temperature, the opposite may happen (see Fig. 6.9.b).

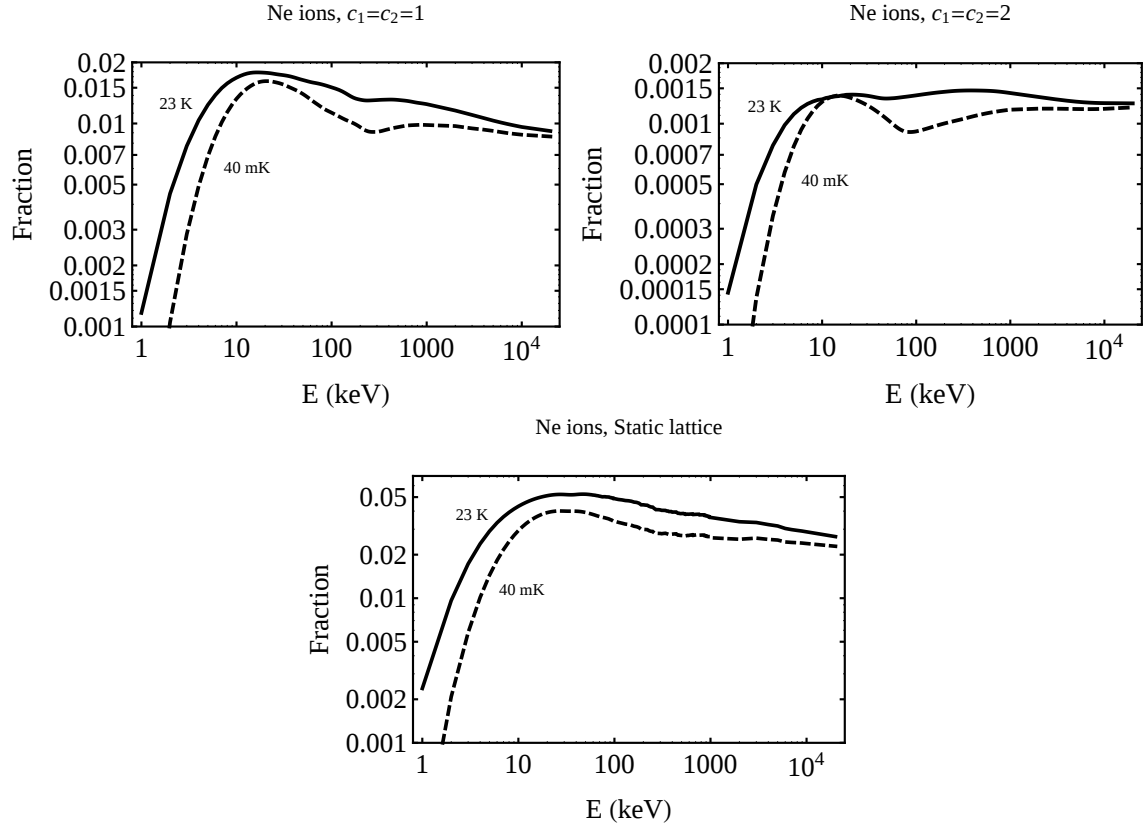


Figure 6.10: Channeling fraction of Ne recoils as a function of the recoil energy E for $T = 23$ K (solid line) and 40 mK (dashed line) in the approximation of (a) $c_1 = c_2 = 1$, (b) $c_1 = c_2 = 2$ and (c) static lattice with $c_1 = c_2 = 0$.

CHAPTER 7

Daily modulation due to channeling

In 2008, Avignone, Creswick, and Nussinov [21] suggested that a daily modulation due to channeling could occur in NaI crystals, which would be a background free dark matter signature. Such a modulation of the rate due to channeling is expected to occur at some level because the “WIMP wind” arrives to Earth on average from a particular direction fixed to the Galaxy. Assuming that the dark matter halo is on average at rest with respect to the Galaxy, this is the direction towards which the Earth moves with respect to the Galaxy. Earth’s daily rotation naturally changes the direction of the “WIMP wind” with respect to the crystal axes, thus changing the amount of recoiling ions that are channeled vs. non-channeled. This amounts to a daily modulation of the dark matter signal detectable via scintillation or ionization.

In the previous chapters, we computed channeling probabilities as function of the recoil energy E and initial direction $\hat{\mathbf{q}}$ of a recoiling ion in different materials. We also obtained the “geometric” channeling fraction $P_{\text{geometric}}(E)$ in the crystals we studied, by averaging the channeling probability $\chi(E, \hat{\mathbf{q}})$ over the initial recoil directions $\hat{\mathbf{q}}$ (assuming an isotropic distribution in $\hat{\mathbf{q}}$)

$$P_{\text{geometric}}(E) = \frac{1}{4\pi} \int \chi(E, \hat{\mathbf{q}}) d\Omega_q. \quad (7.1)$$

This integral was computed using HEALPix [76] of the recoil direction sphere. Here “geometric” refers to assuming that the distribution of recoil directions is isotropic. In reality, in a dark matter direct detection experiment, the distribution of recoil directions depends on the momentum distribution of the incoming WIMPs (see Section 7.1).

In this chapter, we use the (upper bounds to the) channeling probability $\chi(E, \hat{\mathbf{q}})$ and the actual differential recoil spectrum to compute the event rate, taking into account channeled

and non-channeled recoils (see Section 7.2, in particular Eqs. 7.17 and 7.18 and compare them with Eq. 7.1). We then use this rate to compute upper bounds to the amplitude of the daily modulation due to channeling expected in NaI crystals. In Section 7.3, we examine the possibility that such a daily modulation might be observable in the data accumulated by the DAMA collaboration.

7.1 Angular distribution of recoil directions due to WIMPs

Consider the WIMP-nucleus elastic collision for a WIMP of mass m and a nucleus of mass M . The 3-dimensional “Radon transform” of the WIMP velocity distribution can be used to define the differential recoil spectrum as function of the recoil momentum $\vec{q}$ [91]

$$\frac{dR}{dE d\Omega_q} = \frac{\rho\sigma_0 S(q)}{4\pi m\mu^2} \hat{f}_{\text{lab}}\left(\frac{q}{2\mu}, \hat{\mathbf{q}}\right), \quad (7.2)$$

where E is the recoil energy, $d\Omega_q = d\phi d\cos\theta$ denotes an infinitesimal solid angle around the recoil direction $\hat{\mathbf{q}} = \vec{q}/q$, $q = |\vec{q}|$ is the magnitude of the recoil momentum, $\mu = mM/(m+M)$ is the reduced WIMP-nucleus mass, $q/2\mu = v_q$ is the minimum velocity a WIMP must have to impart a recoil momentum q to the nucleus, or equivalently to deposit a recoil energy $E = q^2/2M$, ρ is the dark matter density in the solar neighborhood, σ_0 is the total scattering cross section of the WIMP with a (fictitious) point-like nucleus, and $S(q)$ is the nuclear form factor normalized to 1.

We concentrate here on WIMPs with spin-independent interactions, for which σ_0 is usually written in terms of the WIMP-proton cross section σ_p [92]

$$\sigma_0 = \frac{\mu^2}{\mu_p^2} A^2 \sigma_p, \quad (7.3)$$

where $\mu_p = mm_p/(m+m_p)$ is the WIMP-proton reduced mass and A is the atomic number of the nucleus. We use the Helm form factor [93]

$$S(q) = |F_{SI}(q)|^2 = \left(\frac{3j_1(qR_1)}{qR_1}\right)^2 e^{-q^2 s^2}, \quad (7.4)$$

where

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad (7.5)$$

is the first kind spherical Bessel function, R_1 is an effective nuclear radius, and s is the nuclear skin thickness. Following Duda, Kemper, and Gondolo [94] we set

$$R_1 = \sqrt{c^2 + \frac{7}{3}\pi^2 a^2 - 5s^2}, \quad (7.6)$$

and take $s \simeq 0.9$ fm, $a \simeq 0.52$ fm, and $c \simeq (1.23A^{1/3} - 0.6)$ fm. These parameters have been chosen to match the numerical integration of the Two-Parameter Fermi model of nuclear density [94].

The Maxwellian WIMP velocity distribution with respect to the Galaxy, with dispersion σ_v and truncated at the escape speed v_{esc} is given by [91]

$$f_{\text{WIMP}}(\mathbf{v}) = \frac{1}{N_{\text{esc}}(2\pi\sigma_v^2)^{3/2}} \exp\left[-\frac{(\mathbf{v} + \mathbf{V}_{\text{lab}})^2}{2\sigma_v^2}\right], \quad (7.7)$$

for $|\mathbf{v} + \mathbf{V}_{\text{lab}}| < v_{\text{esc}}$, and zero otherwise, where

$$N_{\text{esc}} = \text{erf}\left(\frac{v_{\text{esc}}}{\sqrt{2}\sigma_v}\right) - \sqrt{\frac{2}{\pi}} \frac{v_{\text{esc}}}{\sigma_v} \exp\left[-\frac{v_{\text{esc}}^2}{2\sigma_v^2}\right]. \quad (7.8)$$

Here we are assuming the detector has a velocity $\mathbf{V}_{\text{lab}}$ with respect to the Galaxy (thus $-\mathbf{V}_{\text{lab}}$ is the average velocity of the WIMPs with respect to the detector). $\mathbf{V}_{\text{lab}}$ is defined in terms of the galactic rotation velocity $\mathbf{V}_{\text{GalRot}}$ at the position of the Sun (or Local Standard of Rest (LSR) velocity), Sun's peculiar velocity $\mathbf{V}_{\text{Solar}}$ in the LSR, Earth's translational velocity $\mathbf{V}_{\text{EarthRev}}$ with respect to the Sun, and the velocity of Earth's rotation around itself $\mathbf{V}_{\text{EarthRot}}$ (see Appendix G),

$$\mathbf{V}_{\text{lab}} = \mathbf{V}_{\text{GalRot}} + \mathbf{V}_{\text{Solar}} + \mathbf{V}_{\text{EarthRev}} + \mathbf{V}_{\text{EarthRot}}. \quad (7.9)$$

We take V_{GalRot} either 220 km/s or 280 km/s, as reasonable low and high values (as done in Ref [95]), which correspond to V_{lab} either 228.4 km/s or 288.3 km/s, respectively (see Appendix G for details). Ref. [96] gives 100 km/s as the smallest estimate for the 1D velocity dispersion, which corresponds to a 3D dispersion $\sqrt{3}$ times larger, i.e. $\sigma_v = 173$ km/s. Thus here we take σ_v either 173 km/s or 300 km/s [91].

In order to visualize the arrival directions of WIMPs, we will plot $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$, the number of WIMPs per solid angle in the direction $\hat{\mathbf{v}}$ in several figures. If we limit ourselves

to the WIMPs with speed higher than v_q , then

$$f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q) = \int_{v_q}^{v_{\text{max}}(\hat{\mathbf{v}})} f_{\text{WIMP}}(\mathbf{v}) v^2 dv. \quad (7.10)$$

The upper limit of the integral in Eq. 7.10 is such that $|\mathbf{v} + \mathbf{V}_{\text{lab}}| = v_{\text{esc}}$ and depends on the direction $\hat{\mathbf{v}}$, since $(\mathbf{v} + \mathbf{V}_{\text{lab}})^2 = v^2 + 2v \hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + V_{\text{lab}}^2$,

$$v_{\text{max}}(\hat{\mathbf{v}}) = -\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + \sqrt{(\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}})^2 - V_{\text{lab}}^2 + v_{\text{esc}}^2}, \quad (7.11)$$

and

$$f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q) = \frac{\exp\left(-\frac{V_{\text{lab}}^2}{2\sigma_v^2}\right)}{N_{\text{esc}}(2\pi\sigma_v^2)^{3/2}} \int_{v_q}^{v_{\text{max}}(\hat{\mathbf{v}})} \exp\left(\frac{-v^2}{2\sigma_v^2}\right) \exp\left(\frac{-2v \hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}}}{2\sigma_v^2}\right) v^2 dv. \quad (7.12)$$

This integral can be solved analytically and the result is in terms of error functions,

$$\begin{aligned} f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q) = & \frac{\exp\left(-\frac{V_{\text{lab}}^2}{2\sigma_v^2}\right)}{N_{\text{esc}}(2\pi\sigma_v^2)^{3/2}} \left(\frac{\sigma_v}{2}\right) \left\{ \sqrt{2\pi} [(\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}})^2 + \sigma_v^2] \exp\left(\frac{(\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}})^2}{2\sigma_v^2}\right) \right. \\ & \left[\text{erf}\left(\frac{\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + v_{\text{max}}(\hat{\mathbf{v}})}{\sqrt{2}\sigma_v}\right) - \text{erf}\left(\frac{\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + v_q}{\sqrt{2}\sigma_v}\right) \right] \\ & + (2\sigma_v) \left[(\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} - v_{\text{max}}(\hat{\mathbf{v}})) \exp\left(-\frac{v_{\text{max}}(\hat{\mathbf{v}})(2\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + v_{\text{max}}(\hat{\mathbf{v}}))}{2\sigma_v^2}\right) \right. \\ & \left. \left. + (-\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + v_q) \exp\left(-\frac{v_q(2\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} + v_q)}{2\sigma_v^2}\right) \right] \right\}. \end{aligned} \quad (7.13)$$

The maximum of $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$ happens when $\hat{\mathbf{v}} \cdot \mathbf{V}_{\text{lab}} = -V_{\text{lab}}$, i.e. in the direction of the “WIMP wind” average velocity $-\mathbf{V}_{\text{lab}}$. Dividing $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$ by this maximum we obtain a re-scaled distribution, a dimensionless number between 0 and 1, which we plot in Fig. 7.1 (see the color scale in the figure) on the sphere of velocity directions $\hat{\mathbf{v}}$ using the HEALPix pixelization [76] (see also Appendix B) for all WIMPs, which amounts to taking $v_q = 0$. We took $V_{\text{lab}} = 288.3$ km/s, and $\sigma_v = 300$ km/s or $\sigma_v = 173$ km/s for Fig. 7.1.a or b respectively.

For a truncated Maxwellian WIMP velocity distribution with respect to the Galaxy, truncated at the escape speed v_{esc} , the Radon-transform is [91]

$$\hat{f}_{\text{lab}}\left(\frac{q}{2\mu}, \hat{\mathbf{q}}\right) = \frac{1}{N_{\text{esc}}(2\pi\sigma_v^2)^{1/2}} \left\{ \exp\left[-\frac{[(q/2\mu) + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}]^2}{2\sigma_v^2}\right] - \exp\left[\frac{-v_{\text{esc}}^2}{2\sigma_v^2}\right] \right\}, \quad (7.14)$$

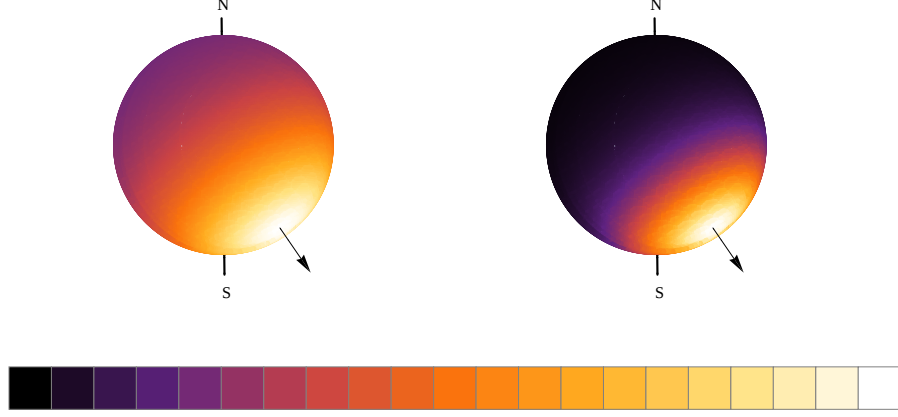


Figure 7.1: WIMPs number density per solid angle $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$ (in Eq. 7.13) for all WIMPs (namely $v_q = 0$) re-scaled to be a number between 0 (black) and 1 (white) plotted on the sphere of velocity directions $\hat{\mathbf{v}}$ using the HEALPix pixelization for $V_{\text{lab}} = 288.3$ km/s and (a) $\sigma_v = 300$ km/s and (b) $\sigma_v = 173$ km/s. The arrow shows the direction of the average velocity of the WIMP wind, $-\mathbf{V}_{\text{lab}}$. The North and South celestial poles are also indicated. The color scale shown in the horizontal bar between black and white corresponds to values between 0 and 1 in increments of 0.05.

if $(q/2\mu) + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}} < v_{\text{esc}}$, and zero otherwise.

The presence of $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}$ means that in order to compute the differential rate we need to orient the nuclear recoil direction $\hat{\mathbf{q}}$ with respect to $\mathbf{V}_{\text{lab}}$.

The maximum of $\hat{f}_{\text{lab}}(\frac{q}{2\mu}, \hat{\mathbf{q}})$ in Eq. 7.14 happens when $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}} = -q/2\mu$, if $v_q = q/2\mu < V_{\text{lab}}$ (or in the direction of $-\mathbf{V}_{\text{lab}}$ otherwise). Thus, we can re-scale $\hat{f}_{\text{lab}}$ to obtain a dimensionless number between 0 and 1,

$$\hat{f}_{\text{lab}}^{\text{re-scaled}} = \left\{ \exp \left[-\frac{[(q/2\mu) + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}]^2}{2\sigma_v^2} \right] - \exp \left[\frac{-v_{\text{esc}}^2}{2\sigma_v^2} \right] \right\} / \left(1 - \exp \left[\frac{-v_{\text{esc}}^2}{2\sigma_v^2} \right] \right). \quad (7.15)$$

In Figs. 7.2 and 7.3 we present side by side the WIMPs velocity distribution, for WIMPs which can generate a signal of a certain energy E , namely with speed above v_q (left panels) and the Radon transform (right panels) of the recoils of energy E that WIMP collisions produce.

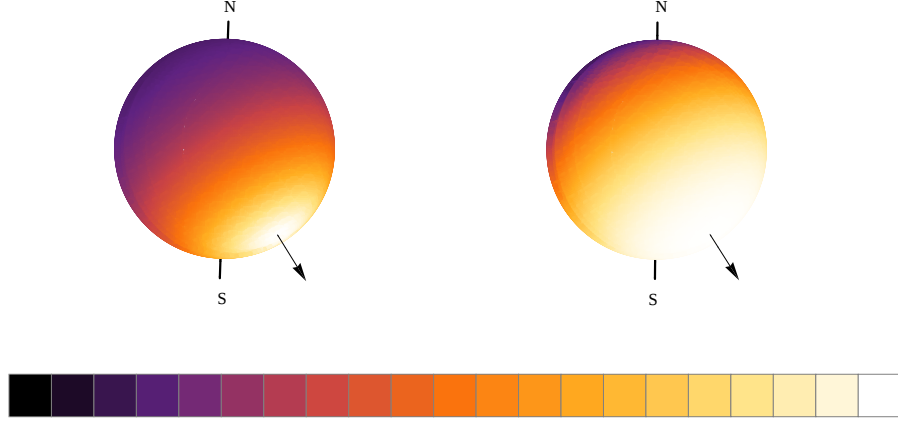


Figure 7.2: (a) $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$ (in Eq. 7.13) re-scaled to be between 0 and 1 plotted on the sphere of velocity directions $\hat{\mathbf{v}}$ and (b) $\hat{f}_{\text{lab}}$ (re-scaled as in Eq. 7.15) plotted on the sphere of recoil directions using the HEALPix pixelization for I recoils with $E = 10$ keV, $m = 30$ GeV (thus $v_q = 304.6$ km/s), $V_{\text{lab}} = 288.3$ km/s and $\sigma_v = 300$ km/s. The arrow shows the direction of the average velocity of the WIMP wind, $-\mathbf{V}_{\text{lab}}$. The North and South celestial poles are also indicated. The color scale shown in the horizontal bar corresponds to values between 0 (black) and 1 (white) in intervals of 0.05.

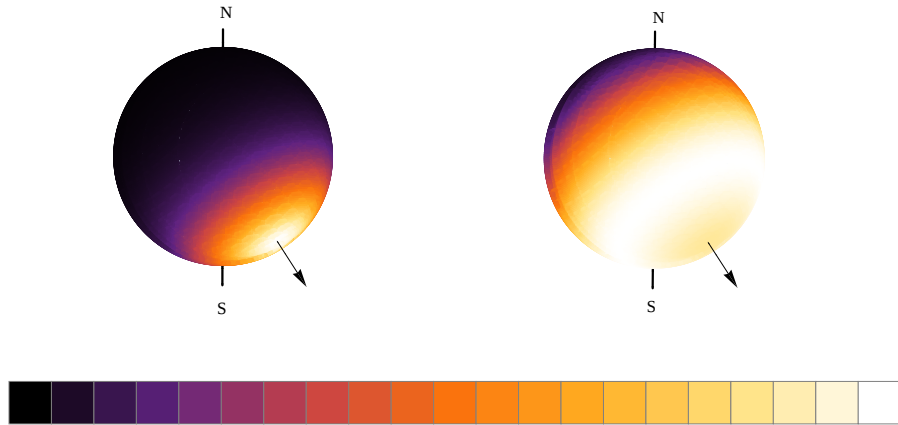


Figure 7.3: Same as Fig. 7.2 but for Na recoils and assuming $m = 60$ GeV (so $v_q = 196.7$ km/s) and $\sigma_v = 173$ km/s (and all other parameters the same).

In Fig. 7.2.a and b we respectively plot $f_{\text{WIMP}}(\hat{\mathbf{v}}, v_q)$ on the sphere of WIMP velocity directions $\hat{\mathbf{v}}$ and $\hat{f}_{\text{lab}}$ on the sphere of recoil directions (both re-scaled to be a number between 0 and 1) using the HEALPix pixelization [76] for I recoils assuming $V_{\text{lab}} = 288.3$ km/s, $E = 10$ keV, $\sigma_v = 300$ km/s and $m = 30$ GeV. Fig. 7.3.a and b show the same two distributions but for Na recoils and assuming $\sigma_v = 173$ km/s and $m = 60$ GeV (other parameters are the same). The color scale plotted on the spheres indicate different values of the rescaled distributions: between 0 (black) and 1 (white) in intervals of 0.05. In Fig. 7.2 the minimum WIMP speed required is $v_q = 304.6$ km/s (I recoils), and since $v_q > V_{\text{lab}}$, the maximum value of $\hat{f}_{\text{lab}}^{\text{re-scaled}}$, i.e. the maximum recoil rate, is in the direction of the “WIMP wind” average velocity, $-V_{\text{lab}}$, which is shown with an arrow. In Fig. 7.3 instead, $v_q = 196.7$ km/s (Na recoils) and the maximum value of $\hat{f}_{\text{lab}}^{\text{re-scaled}}$ occurs when $-\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}} = v_q$, i.e. when $\hat{\mathbf{q}}$ is at an angle of 47° of $-V_{\text{lab}}$.

7.2 Differential energy spectrum

Let $p(E_M, E, \hat{\mathbf{q}})dE_M$ be the probability that an energy E_M is measured when a nucleus recoils in the direction $\hat{\mathbf{q}}$ with initial energy E , normalized so that

$$\int p(E_M, E, \hat{\mathbf{q}})dE_M = 1. \quad (7.16)$$

With our analytic approach we cannot estimate the importance of dechanneling mechanisms, such as the presence of lattice imperfections, impurities or dopants. Thus we disregard dechanneling, and assume that a recoiling nucleus can only either be channeled, in which case the measured energy is the whole initial recoil energy $E_M = E$ (first term in the following equation) or not channeled, in which case the measured energy is $E_M = QE$ (second term),

$$p(E_M, E, \hat{\mathbf{q}}) = \chi(E, \hat{\mathbf{q}})\delta(E_M - E) + [1 - \chi(E, \hat{\mathbf{q}})]\delta(E_M - QE). \quad (7.17)$$

The first term accounts for the channeled (unquenched) events and the second term for the unchanneled (quenched) events, and Q is the quenching factor.

Using Eq. 7.17 the differential energy spectrum,

$$\frac{dR}{dE_M} = \int \frac{dR}{dE d\Omega_q} p(E_M, E, \hat{\mathbf{q}}) d\Omega_q dE, \quad (7.18)$$

can be written as

$$\begin{aligned} \frac{dR}{dE_M} &= \int \left(\chi(E_M, \hat{\mathbf{q}}) \frac{dR}{dE d\Omega_q} \Big|_{E=E_M} + [1 - \chi(E_M/Q, \hat{\mathbf{q}})] \frac{1}{Q} \frac{dR}{dE d\Omega_q} \Big|_{E=E_M/Q} \right) d\Omega_q \\ &= \frac{dR}{dE_M} \Big|_{\text{U}} + \int \chi(E_M, \hat{\mathbf{q}}) \frac{dR}{dE d\Omega_q} \Big|_{E=E_M} d\Omega_q \\ &\quad - \int \chi(E_M/Q, \hat{\mathbf{q}}) \frac{1}{Q} \frac{dR}{dE d\Omega_q} \Big|_{E=E_M/Q} d\Omega_q, \end{aligned} \quad (7.19)$$

where the differential recoil spectrum with subindex “U”, which stands for “Usual” (i.e. when channeling is not taken into account) is

$$\frac{dR}{dE_M} \Big|_{\text{U}} = \int \frac{1}{Q} \frac{dR}{dE d\Omega_q} \Big|_{E=E_M/Q} d\Omega_q = \frac{1}{Q} \frac{dR}{dE} \Big|_{E=E_M/Q}. \quad (7.20)$$

Defining $\tilde{q} \equiv \sqrt{2E_M M}$ and using Eq. 7.2, the measured differential rate becomes,

$$\begin{aligned} \frac{dR}{dE_M} &= \frac{dR}{dE_M} \Big|_{\text{U}} + \frac{\rho \sigma_0}{4\pi m \mu^2} \left[S(\tilde{q}) \int \chi(E_M, \hat{\mathbf{q}}) \hat{f}_{\text{lab}} \left(\frac{\tilde{q}}{2\mu}, \hat{\mathbf{q}} \right) d\Omega_q \right. \\ &\quad \left. - \frac{S(\tilde{q}/\sqrt{Q})}{Q} \int \chi(E_M/Q, \hat{\mathbf{q}}) \hat{f}_{\text{lab}} \left(\frac{\tilde{q}}{2\mu\sqrt{Q}}, \hat{\mathbf{q}} \right) d\Omega_q \right]. \end{aligned} \quad (7.21)$$

Inserting σ_0 from Eq. 7.3 in the above equation with the usual value for the mean local halo density $\rho = 0.3 \text{ GeV/cm}^3$, we can write the spin-independent detection rate of WIMPs in general for a crystal that may contain more than one element

$$\begin{aligned} \frac{dR}{dE_M} &= \frac{dR}{dE_M} \Big|_{\text{U}} + 1.306 \times 10^{-3} \frac{\text{events}}{\text{kg-day-keV}} \times \frac{\sigma_{44}}{4\pi m \mu_p^2} \\ &\quad \sum_n C_n A_n^2 \left[S(\tilde{q}) \int \chi_n(E_M, \hat{\mathbf{q}}) \hat{f}_{\text{lab}} \left(\frac{\tilde{q}}{2\mu_n}, \hat{\mathbf{q}} \right) d\Omega_q \right. \\ &\quad \left. - \frac{S(\tilde{q}/\sqrt{Q_n})}{Q_n} \int \chi_n(E_M/Q_n, \hat{\mathbf{q}}) \hat{f}_{\text{lab}} \left(\frac{\tilde{q}}{2\mu_n\sqrt{Q_n}}, \hat{\mathbf{q}} \right) d\Omega_q \right], \end{aligned} \quad (7.22)$$

where σ_{44} is the WIMP-proton cross section in units of 10^{-44} cm^2 , μ_p and m are in GeV and $\int \hat{f}_{\text{lab}} d\Omega_q$ is in $(\text{km/s})^{-1}$. The sum is over the nuclear species n in a crystal, and C_n , χ_n , Q_n and μ_n are the mass fraction, the channeling probability, the quenching factor and the

reduced WIMP-nucleus mass for the element n , respectively. For example, for NaI crystals, as used in the DAMA experiment, we have $C_{\text{Na}} = M_{\text{Na}}/(M_{\text{Na}} + M_{\text{I}})$ and $C_{\text{I}} = M_{\text{I}}/(M_{\text{Na}} + M_{\text{I}})$, where M_{Na} and M_{I} are the atomic masses of Sodium and Iodine respectively.

The integrals in Eq. 7.22 cannot be computed analytically. We integrate numerically by performing a Riemann sum once the sphere of directions has been divided using HEALPix [76] (see also Appendix B).

With the same notation, the usual rate is

$$\left. \frac{dR}{dE_M} \right|_{\text{U}} = 1.306 \times 10^{-3} \frac{\text{events}}{\text{kg-day-keV}} \times \frac{\sigma_{44}}{4\pi m\mu_p^2} \sum_n C_n A_n^2 \left[\frac{S(\tilde{q}/\sqrt{Q_n})}{Q_n} \int \hat{f}_{\text{lab}} \left(\frac{\tilde{q}}{2\mu_n \sqrt{Q_n}}, \hat{\mathbf{q}} \right) d\Omega_q \right]. \quad (7.23)$$

7.3 Daily Modulation in NaI Crystals

We present here the daily modulation amplitude due to channeling expected in NaI crystals for several WIMP masses and Na or I recoil energies. We assume that WIMPs have a truncated Maxwellian velocity distribution as in Eq. 7.7 with $v_{\text{esc}} = 650$ km/s. We use the upper bounds to channeling fractions for single channels $\chi_i(E, \hat{\mathbf{q}})$ given in Chapter 3. We take $T = 293$ K, the temperature of the DAMA experiment.

The spin-independent detection rate of WIMPs given in Eq. 7.22 has a time dependence through the Radon transform $\hat{f}_{\text{lab}}$. Notice that $\hat{f}_{\text{lab}}$ (see Eq. 7.14) changes during a day through the $(\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}})$ factor appearing in the exponent and the dependence of $\mathbf{V}_{\text{lab}}$ on $\mathbf{V}_{\text{EarthRot}}$ (see Eq. 7.9). The expression showing the time dependence of $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}$ is given in Eq. G.13 (in Appendix G). During a day, $\mathbf{V}_{\text{EarthRev}}$ which is responsible for the annual modulation changes too. Thus the rate does not return to exactly the same value after one day. For the cases we present in this chapter, this difference is less than 10% of the total modulation amplitude in a day, and we did not correct for this effect.

7.3.1 Relative Modulation Amplitudes

Here we show the signal rate as function of time during a particular arbitrary Solar day (September 25, 2010). We define the relative signal modulation amplitude A_s (taking into account the signal only) in terms of the maximum and minimum daily signal rate R_s as

$$A_s = \frac{R_{s-\max} - R_{s-\min}}{R_{s-\max} + R_{s-\min}}. \quad (7.24)$$

The total relative modulation amplitude A_T is defined in terms of the maximum $R_{T-\max}$ and minimum $R_{T-\min}$ total daily rates as

$$A_T = \frac{R_{T-\max} - R_{T-\min}}{R_{T-\max} + R_{T-\min}}. \quad (7.25)$$

The total rate consists of signal plus background, $R_T = R_s + R_b$. Assuming that there is no daily modulation in the background, $R_{T-\max} - R_{T-\min} = R_{s-\max} - R_{s-\min}$, and A_T is related to A_s as

$$A_T = A_s(R_s/R_T), \quad (7.26)$$

where the average total rate due to signal and background is $R_T = (R_{T-\max} + R_{T-\min})/2$ and the average rate due to the signal alone is $R_s = (R_{s-\max} + R_{s-\min})/2$.

Exploring the parameter space of WIMP mass and WIMP-proton cross section for different recoil energies we find that the relative modulation amplitudes A_s can be large, even more than 10% for some combination of parameters. We explored the range of WIMP masses from a few GeV to hundreds of GeV for recoil energies between 2 keV and a few MeV. We show some examples in Fig. 7.4, where we plot the signal rate (in events/kg/day/keVee) as function of the Universal Time (UT) during 24 hours. We find that the largest A_s happen when the signal is only due to channeling. This happens when there are no WIMPs in the galactic halo with large enough kinetic energy to provide the observed energy if the recoil is not channeled. The observed energies for which the rate is only due to channeling depend on the quenching factors Q , which are not well known. The smaller values of Q make channeling more important so we take $Q_{\text{Na}} = 0.2$ [97] for Na and the usual $Q_{\text{I}} = 0.09$ for I.

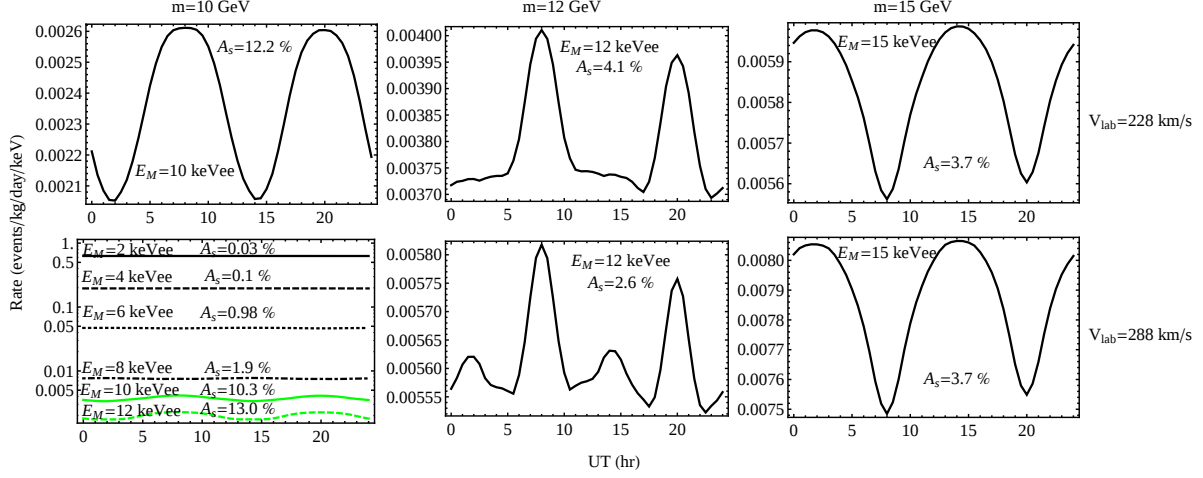


Figure 7.4: Signal rate (in events/kg-day-keV) as function of the Universal Time (UT) during 24 hours for $m = 10$ GeV, 12 GeV and 15 GeV for different energies. The parameters used are $\sigma_v = 300$ km/s, $Q_{\text{Na}} = 0.2$, $Q_{\text{I}} = 0.09$, $\sigma_p = 2 \times 10^{-40} \text{cm}^2$, $c = 1$ for temperature effects, a crystal temperature of $T = 293$ K and $V_{\text{lab}} = 228.4$ km/s (top row) or 288.3 km/s (bottom row).

7.3.2 Statistical Significance

The detectability of a particular amplitude of daily modulation depends on the exposure and background of a particular experiment. The former DAMA/NaI and the DAMA/LIBRA experiments (which we refer collectively as the DAMA experiment) have a very large cumulative exposure, $1.17 \text{ ton} \times \text{year}$. However even with this large exposure, we find that the daily modulations we predict are not observable. To observe the daily modulation, the total number of events N_T (N_s signal plus N_b background events) over the duration of the experiment should be divided into two bins, the “high-rate” bin with $N_{T-\text{max}}$ events and the “low-rate” bin with $N_{T-\text{min}}$ events, so that $N_T = N_{T-\text{max}} + N_{T-\text{min}}$. For the daily modulation to be observable at, say, the 3σ level one should have

$$N_{T-\text{max}} - N_{T-\text{min}} = A_T N_T > 3\sigma \simeq 3\sqrt{N_T/2}, \quad (7.27)$$

where $\sigma^2 \simeq N_T/2$ because, with a small modulation, on average $N_{T-\text{max}} \simeq N_{T-\text{min}} \simeq N_T/2$. In principle there are other errors associated with identifying the “high-rate” and “low-rate” bins which we do not include here. Thus we are underestimating the errors.

If the detector exposure is MT in kg-day and we take bins of width ΔE_M in keVee, then $N_{T-\max} = R_{T-\max}MT\Delta E_M/2$, $N_{T-\min} = R_{T-\min}MT\Delta E_M/2$, $N_T = R_TMT\Delta E_M$ and $N_s = R_sMT\Delta E_M$, where the rates are in events/kg-day-keVee. Thus $(N_s/N_T) = (R_s/R_T)$ and using Eq. 7.26, $A_T = A_s(N_s/N_T)$. Thus the condition in Eq. 7.27 becomes $A_sN_s > 3\sqrt{N_T/2}$ which implies

$$N_s^2/N_T > 9/(2A_s^2), \quad (7.28)$$

or

$$R_s^2/R_T > 9/(2A_s^2MT\Delta E_M). \quad (7.29)$$

The total rate of the DAMA experiment at low energies $4 \text{ keVee} < E_M < 10 \text{ keVee}$ is $R_T \simeq 1 \text{ events/kg/day/keVee}$ [98]. This rate is much larger than the signal rates we predict and is, therefore, dominated by background. With this value of R_T , Eq. 7.29 becomes

$$R_s^2A_s^2 > \frac{9}{2MT\Delta E_M \text{ kg day keVee}}. \quad (7.30)$$

We choose here a bin $\Delta E_M \simeq 1 \text{ keVee}$, narrow enough to assume the signal rate to be constant in it and compatible with the energy resolution of DAMA. The energy resolution of DAMA is $\sigma_E(E_M) = (0.448 \text{ keVee})\sqrt{E_M/\text{keVee}} + (0.0091)E_M \simeq 1 \text{ keVee}$ at low energies [99]. We consider the significance of the highest signal-to-noise energy bin that we found through inspection. With the cumulative exposure of DAMA, the condition in Eq. 7.30 for relative daily modulation amplitudes A_s observable at 3σ is

$$R_s A_s > 3.2 \times 10^{-3} \text{ events/kg/day/keVee}, \quad (7.31)$$

or

$$R_{s-\max} - R_{s-\min} > 6.4 \times 10^{-3} \text{ events/kg/day/keVee}. \quad (7.32)$$

For observability at the $n\sigma$ level we should multiply the right-hand side of Eq. 7.32 by $(n/3)$. Even the largest relative daily modulations we find, shown in Fig. 7.4, are not observable in the DAMA data according to Eq. 7.32.

The examples which we show here are for small WIMP masses and recoil energies. For large masses the value of σ_p must be chosen in the region of the cross section and mass plane

where XENON10/100 and CDMS impose σ_p to be smaller by four orders of magnitude than for light WIMPs. This amounts to corresponding smaller signal rates and $(R_{s-\max} - R_{s-\min})$ differences. For small WIMP masses and large energies, v_q is large and there are no WIMPs with the speed required for Na or I recoils. Thus, only small WIMP masses and recoil energies result in high modulation amplitudes.

Fig. 7.4 shows the signal rate during 24 hours for three different WIMP masses $m = 10$ GeV, 12 GeV and 15 GeV and different energies E_M between 2 and 15 keVee. The other relevant parameters are $\sigma_v = 300$ km/s, $\sigma_p = 2 \times 10^{-40} \text{cm}^2$ (close to the DAMA and CoGeNT regions [97, 8, 16]), $c = 1$, $T = 293$ K and two values of V_{lab} , 228.4 km/s (top row) and 288.3 km/s (bottom row). Recent bounds, e.g. those from XENON100 [15], impose smaller values of σ_p . In any event, changes in σ_p are easy to take into account because A_s is independent of σ_p and the rate is just proportional to it, $R_s \sim \sigma_p$.

We found the relative amplitude A_s to be as large as 12% in the examples shown in Fig. 7.4, but even those large values are not observable according to Eq. 7.32 (even at the 1σ level). With the choice of $V_{\text{lab}} = 228.4$ km/s (top row of Fig. 7.4) we get a signal rate difference $R_{s-\max} - R_{s-\min}$ of 0.56×10^{-3} events/kg/day/keVee for $m = 10$ GeV and $E_M = 10$ keVee (in this case $v_q = 454.8$ km/s and 790.5 km/s for channeled Na and I recoils, respectively), 3.17×10^{-4} events/kg/day/keVee for $m = 12$ GeV and $E_M = 12$ keVee (which corresponds to $v_q = 441.6$ km/s and 732.9 km/s for Na and I channeled recoils, respectively), and 4.25×10^{-4} events/kg/day/keVee for $m = 15$ GeV and $E_M = 15$ keVee (for which $v_q = 430.6$ km/s and 670.6 km/s for Na and I channeled recoils, respectively). With the choice of $V_{\text{lab}} = 288.3$ km/s (bottom row of Fig. 7.4), $R_{s-\max} - R_{s-\min}$ is 0.77×10^{-3} events/kg/day/keVee for $m = 10$ GeV and $E_M = 10$ keVee (one of the energies shown), 2.95×10^{-4} events/kg/day/keVee for $m = 12$ GeV and $E_M = 12$ keVee, and 0.58×10^{-5} events/kg/day/keVee for $m = 15$ GeV and $E_M = 15$ keVee. Because the minimum WIMP speeds v_q are large in these examples, a smaller velocity dispersion of the WIMP distribution leads to smaller rates (since a smaller amount of WIMPs have velocities larger than v_q). So the signal rate difference $R_{s-\max} - R_{s-\min}$ is even smaller for smaller values of σ_v .

The left-bottom panel of Fig. 7.4 shows the signal rate as function of UT for $m = 10$ GeV and $V_{\text{lab}} = 288.3$ km/s for several energies between 2 keVee and 12 keVee. The rate decreases but A_s increases with increasing energy and the best conditions for observability happen at some energy where neither the rate nor A_s are very small. The rates for low energies between 2 keVee and 6 keVee are dominated by the usual (i.e. non-channeled) rate and the daily modulation is due purely to the change in WIMP kinetic energy in the lab frame as the Earth rotates around itself. The rates for energies above 8 keVee (green/gray lines) are purely due to channeling, i.e. the usual rate is zero. For intermediate energies, 6 keVee to 8 keVee, the usual and channeled rates both contribute and thus the daily modulation is due to both the channeling effect and the daily change in the usual rate. For $E_M = 2, 4, 6, 8, 10$ and 12 keVee, the values of $R_{s\text{-max}} - R_{s\text{-min}}$ given in events/kg/day/keVee are respectively 4.3×10^{-4} , 0.5×10^{-3} , 0.92×10^{-3} , 2.8×10^{-4} , 0.77×10^{-3} and 0.52×10^{-3} . Notice that for all the energies shown the difference in rate is similar, but the largest A_s values happen at energies above 8 keVee, for which the rate is only due to channeling. The channeling daily modulation amplitude increases as the ratio of the velocity dispersion to the average speed of the WIMPs that contribute to the signal (i.e. with $v > v_q$) decreases. This ratio is small and thus A_s large for large values of v_q . Notice that the phase of the modulation due to channeling depends on the orientation of the crystal with respect to the Galaxy and the phase of the modulation in the usual rate does not, which would allow to distinguish both effects, if they were observable. The case of $m = 10$ GeV and $E_M = 6$ keVee has the largest rate difference, but is not observable at 3σ according to Eq. 7.32 (not even at the 1σ level). Choosing $\sigma_p = 4 \times 10^{-40} \text{cm}^2$ (still within the DAMA allowed region but not compatible with the recent XENON100 result) results in a rate difference of 1.84×10^{-3} events/kg/day/keVee for this case which would not be observable even at the 1σ level.

Finally, we would like to compare our results with those obtained in Ref. [22] by Creswick *et al.* They found a relative daily modulation amplitude $A_s = 0.85\%$ (their definition of amplitude differs by a factor of 2 from ours, so they quote 1.7%) for 5 GeV WIMP mass and 3.8 keVee measured energy (in which case $v_q = 471.2$ km/s and 936.6 km/s for channeled Na and I recoils, respectively). There are no WIMPs with the speed required for I recoils, thus

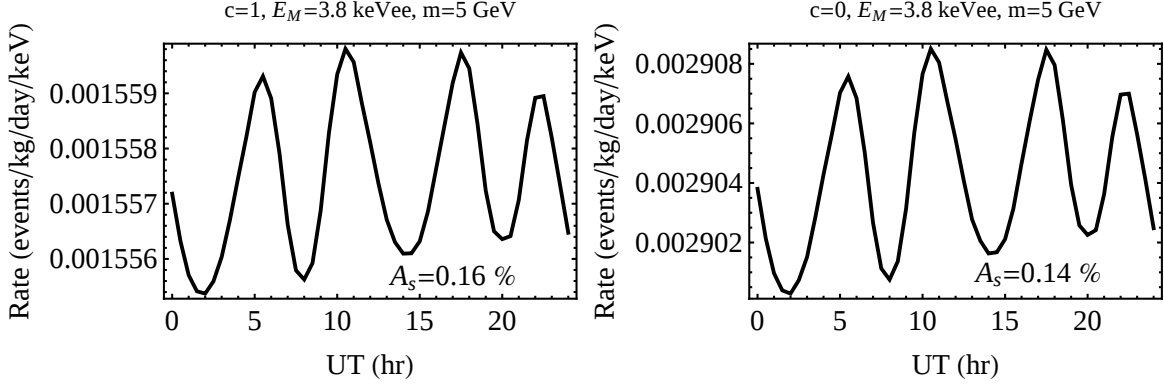


Figure 7.5: Signal rate as function of UT during 24 hours for $E_M = 3.8$ keVee and $m = 5$ GeV, with $V_{\text{lab}} = 228.4$ km/s, $\sigma_v = 300$ km/s, $\sigma_p = 2 \times 10^{-40} \text{cm}^2$, and $Q_{\text{Na}} = 0.2$, $Q_{\text{I}} = 0.09$ for (a) $c = 1$ and (b) $c = 0$. The daily modulation is not observable in both cases.

only Na recoils are possible). In order to compare our calculation with theirs, we compute the signal event rate as function of time for $c = 1$, $T = 293$ K (temperature corrections are not included in the calculation of Creswick *et al.*) and choosing all the other parameters very close to those used in Ref. [22], i.e. $V_{\text{lab}} = 228.4$ km/s and $\sigma_v = 300$ km/s. A WIMP mass of 5 GeV is outside the region of parameter space compatible with the annual modulation reported by DAMA [8]. Since A_s does not depend on σ_p , we choose an arbitrary value of $\sigma_p = 2 \times 10^{-40} \text{cm}^2$ to plot the signal rate as a function of UT (the upper bound given by TEXONO [100] and CoGeNT [2, 17] is five times larger, $\sigma_p < 1 \times 10^{-39} \text{cm}^2$). Our result is shown in Fig. 7.5.a. We find $A_s = 0.16\%$ ($R_{s-\text{max}} - R_{s-\text{min}} = 4.4 \times 10^{-6}$ events/kg/day/keVee). Even when we consider the extreme choice of $c = 0$ to compute temperature effects (an unrealistic value for which the channeling fractions are larger) with the same parameters, we get $A_s = 0.14\%$. This case is shown in Fig. 7.5.b.

7.3.3 Future Prospects for DAMA and other Experiments

The daily modulation might be detectable in other experiments with smaller background or WIMP halo components with a smaller dispersion such as streams or a thick disk. The amplitude of the daily modulation increases as the WIMP velocity distribution is narrower i.e. for larger values of the average velocity and smaller values of the velocity dispersion of

the detectable WIMPs (which is not σ_v), i.e. those with velocity larger than v_q . This is easy to understand since as the dispersion increases more channels are available for channeling of the recoiling ions. In the limit in which the velocity distribution would be isotropic with respect to the detector, the daily rotation would not introduce any difference in the rate due to channeling. Having a large relative signal modulation amplitude A_s is not sufficient for observability. In Eq. 7.32 what is important is $(A_s R_s) = (R_{s-\max} - R_{s-\min})/2$. However, the condition in Eq. 7.32 was derived considering the total rate in the DAMA experiment, which is dominated by background. For an experiment where the background is negligible, i.e. $R_T = R_s + R_b \simeq R_s$, we can derive a different observability condition (at the 3σ level) from Eq. 7.29,

$$R_s A_s^2 = A_s (R_{s-\max} - R_{s-\min})/2 > 9/(2MT \Delta E_M). \quad (7.33)$$

This condition might be easier to satisfy in future experiments.

One could ask which is the maximum level of total rate with the current DAMA exposure that would be needed to make the signal daily modulation observable. Inserting the current exposure of DAMA (1.17 ton-yr) in Eq. 7.29, we have

$$(A_s R_s)^2/R_T > 1.05 \times 10^{-5} \text{ events/kg/day/keVee}, \quad (7.34)$$

which using $A_s R_s = (R_{s-\max} - R_{s-\min})/2$, becomes

$$R_T < \frac{(R_{s-\max} - R_{s-\min})^2}{4.2 \times 10^{-5} \text{ events/kg/day/keVee}}. \quad (7.35)$$

Even in the case with the highest rate difference we found, i.e. $R_{s-\max} - R_{s-\min} = 0.98 \times 10^{-3}$ events/kg/day/keVee (the $m = 10$ GeV, $E_M = 6$ keVee, $V_{\text{lab}} = 288.3$ km/s example shown in the bottom-left panel of Fig. 7.4) observability would require

$$R_T < 0.023 \text{ events/kg/day/keVee}, \quad (7.36)$$

roughly 1/40 of what is now.

We could ask instead what exposure would be needed with the current total rate in the DAMA experiment to make the daily modulation observable. Setting $R_T \simeq 1$ events/kg/day/keVee

in Eq. 7.29, we obtain

$$\frac{MT\Delta E_M}{(\text{events/kg/day/keVee})} > \frac{9}{2(A_s R_s)^2} = \frac{18}{(R_{s\text{-max}} - R_{s\text{-min}})^2}. \quad (7.37)$$

Again, for the case with the highest rate difference we found ($m = 10$ GeV, $E_M = 6$ keVee and $V_{\text{lab}} = 288.3$ km/s) and with $\Delta E_M \simeq 1$ keVee we would require an exposure 40 times larger,

$$MT > 51.3 \text{ ton-yr}. \quad (7.38)$$

We have computed the daily modulation due to channeling in other material such as Ge, solid Xe and solid Ne, and we find that it will be very difficult to observe. For light WIMPs the cross section can be larger than for heavier ones without violating experimental bounds, $\sigma_p = 10^{-39}\text{cm}^2$ [100] and this favors the detection of the daily modulation. We find that for a WIMP mass $m = 5$ GeV the daily modulation due to channeling may be observable in solid Ne if the signal would be above threshold and assuming no background. The geometric channeling fraction reaches a maximum at around 10 keV for solid Ne (see Chapter 6), thus the largest modulation amplitude happens at that energy. For example for a solid Ne detector operating at 23 K at Gran Sasso, for $E_M = 10$ keV, assuming $Q_{\text{Ne}} = 0.25$ [101], $c = 1$ and with velocity distribution parameters $\sigma_v = 300$ km/s and $V_{\text{lab}} = 228.4$ km/s we find $R_s A_s^2 = 3.68 \times 10^{-5}$ events/kg/day/keVee. Using Eq. 7.33 we find that the exposure needed to observe this modulation at 3σ is $MT = 0.33$ ton-yr. For the same parameters but for $m = 7$ GeV and $\sigma_p = 2 \times 10^{-40}\text{cm}^2$ (parameters compatible with the possible dark matter signal found by CoGeNT and with DAMA according to Ref. [102]), we find $R_s A_s^2 = 7.2 \times 10^{-7}$ events/kg/day/keVee, and the exposure needed is $MT = 17.1$ ton-yr. The usual rate is zero in both cases, and the modulation is just due to channeling. The signal rate during 24 hours and the required exposures for the two cases are shown in Fig. 7.6 and Table 7.1, respectively.

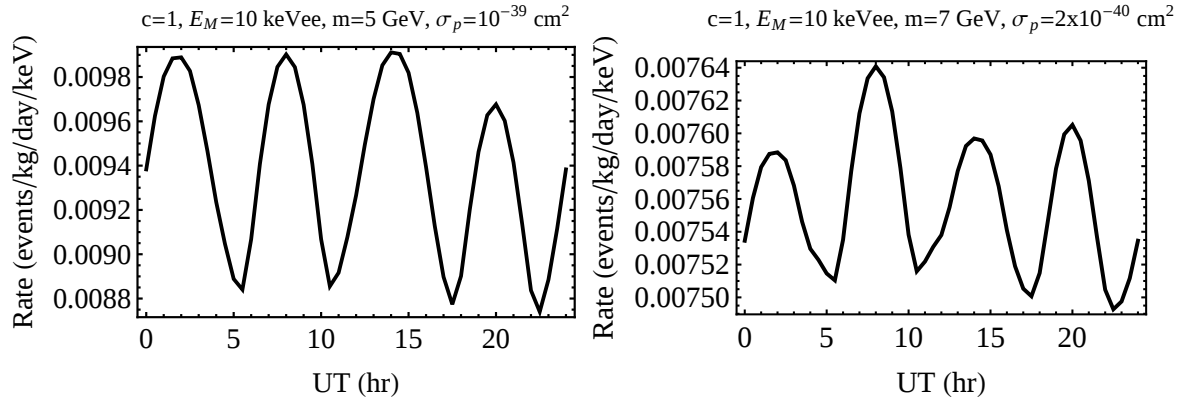


Figure 7.6: Signal rate as function of UT during 24 hours for a solid Ne detector operating at $T = 23$ K at Gran Sasso for $E_M = 10$ keVee, $Q = 0.25$, $c = 1$, $\sigma_v = 300$ km/s, $V_{\text{lab}} = 228.4$ km/s and for (a) $m = 5$ GeV and $\sigma_p = 10^{-39}\text{cm}^2$, and (b) $m = 7$ GeV and $\sigma_p = 2 \times 10^{-40}\text{cm}^2$.

Table 7.1: Observability in solid Ne detector

Case	σ_p (cm ²)	MT (ton-yr)
$m = 5$ GeV	10^{-39}	0.33
$m = 7$ GeV	2×10^{-40}	17.1

CHAPTER 8

Conclusions

We have studied the channeling of ions recoiling after collisions with WIMPs in NaI (Tl), Si, Ge, CsI, and solid Xe, Ar, and Ne crystals. Channeled ions move within the crystal along symmetry axes and planes and suffer a series of small-angle scatterings that maintain them in the open “channels” between the rows or planes of lattice atoms and thus penetrate much further into the crystal than in other directions. In order for the scattering to happen at small enough angles, the propagating ion must not approach a row or plane closer than a critical distance r_c for axial or x_c for planar channels. For a “static lattice” that here means a perfect lattice in which all vibrations are neglected, r_c and x_c are given in Eqs. 3.14 and 3.22 for NaI and CsI crystals and in Eqs. 4.8 and 4.13 for Si, Ge, and solid Xe, Ar, and Ne crystals.

The channeling of ions in a crystal depends not only on the angle their initial trajectory makes with rows or planes in the crystal, but also on their initial position. Ions which start their motion close to the center of a channel, far from a row or plane, at an initial angle ψ or ψ^p (see Eqs. 3.12 and 3.23), are channeled if the initial angle is smaller than the critical angle in Eqs. 3.17 and 3.25, respectively for NaI and CsI and in Eqs. 4.9 and 4.14, respectively for Si, Ge, solid Xe, Ar, and Ne, and are not channeled otherwise. We have found that the channeling of lattice ions recoiling after a collision with a WIMP is very different from the channeling of incident ions, and that the fraction of recoiling lattice ions that are channeled is smaller.

The nuclei ejected from their lattice sites by WIMP collisions are initially part of a row or plane. They start from lattice sites or very close to them, thus blocking effects are important. In fact, as argued originally by Lindhard [23], in a perfect lattice and in the

absence of energy-loss processes, the probability that a particle starting from a lattice site is channeled would be zero. This is what Lindhard called the “Rule of Reversibility.” However, any departure of the actual lattice from a perfect lattice due to vibrations of the atom, which are always present, violate the conditions of this argument and allow for some of the recoiling lattice nuclei to be channeled. Thus, the channeling fraction of recoiling ions is very temperature dependent.

The temperature corrected minimum distances of approach (given in Eqs. 3.29 and 3.30 for NaI and CsI and in Eq. 4.15 for Ge, Si, and solid Xe, Ar, and Ne) depend on the one dimensional rms vibration amplitude $u_1(T)$ (Eq. 3.26), which increases with the temperature, through the coefficients c_1 and c_2 . These dimensionless coefficients are found in the literature for different materials and propagating ions to take values between 1 and 2.

Due to vibrations in the crystal, the atom that interacts with a WIMP may be displaced from its position in a perfect lattice with a probability given in Eqs. 3.39 and 3.41. It is this displacement which allows for a non-zero probability of channeling, given in Eqs. 3.40 and 3.42. At high temperatures, the atoms vibrate with larger amplitudes, the recoiling ion can start further away from a row or plane (i.e u_1 in Eqs. 3.40 and 3.42 is larger), and the channeling fractions increase. However, there is a second temperature effect which makes the channeling fractions smaller as the temperature increases: the lattice vibrations (of all the other atoms in the crystal, besides the recoiling one) increase the critical distances of approach and reduce the critical angles for channeling (unless $c_1 = c_2 = 0$), which in turn decreases the channeling fractions as the temperature increases ($r_{i,\min}$ and $x_{i,\min}$ in Eqs. 3.40 and 3.42 increase). Depending on which of the two competing effects is dominant, the channeling fraction may either increase or decrease as the temperature increases. Increasing the temperature of a crystal usually increases the fraction of channeled recoiling ions, but when the values of c_1 and c_2 are large (i.e. close to 2) so the critical distances increase rapidly with the temperature, the opposite may happen.

We are already providing upper limits to the channeling fraction in NaI (Tl) and CsI due to our choice of x_c (see discussion after Eq. 3.22). In Figs. 3.13 and 5.10 we show absolute

upper bounds to this probability for NaI (Tl) and CsI, respectively in the unrealistic case in which temperature effects are only taken into account in the vibrations of the atom interacting with the WIMP, but not on the other atoms in the lattice (so $c_1 = c_2 = 0$). More realistic upper bounds to the channeling fractions for NaI (Tl) and CsI are given in Figs. 3.11 and 5.8, respectively, in which $c_1 = c_2 = 1$. The 20 °C curve from Fig. 3.11 is displayed again in Fig. 3.14, in which we show what we consider to be our best results for NaI (Tl). If $c_1 = c_2 = 2$, the channeling fractions are smaller, as shown in Fig. 3.12 for NaI (Tl) (from which the 20 °C curve is copied in Fig. 3.14), and in Fig. 5.9 for CsI.

Fig. 3.14.a shows what we consider to be our main predictions for the range expected as an upper limit to the channeling fraction in NaI (Tl), if dechanneling is ignored. Dechanneling happens when the channeled ion encounters impurities or defects. Fig. 3.14.b shows the channeling fraction for NaI (Tl) reduced by the probability of the channeling ion to not interact with a Tl atom (see Eq. 3.34). This way of taking into account dechanneling may be too extreme, as it neglects the probability that the ion after the collision with a Tl atom may reenter a channel (either the same channel or another one) and be again channeled. With dechanneling, the probability that the channeled ion does not interact with a Tl atom decreases with energy (since more energetic ions propagate further within channels). Thus, interactions with Tl atoms decrease the channeling fraction at high energies. This reduction may eventually prove to be too extreme and at present we do not have a better formalism to model dechanneling.

With the simple model of dechanneling we used for NaI (Tl) we could reproduce the channeling fractions computed by the DAMA collaboration which, however, apply to ions which start their motion close to the middle of a channel and not to the case of direct dark matter detection. Notice that we have not considered any mechanism of dechanneling of the channeled ions (due to irregularities in the crystals, for example) in Si, Ge, CsI, and solid Xe, Ar, and Ne which would decrease the channeling fractions.

Fig. 4.18 provides an upper limit to the channeling fractions in Si and Ge for $c_1 = c_2 = 0$. Similarly, Figs. 6.8.c, 6.9.c, and 6.10.c show the static lattice approximation for solid Xe,

Ar, and Ne, respectively. The $c_1 = c_2 = 1$ choice is shown in Fig. 4.19 for Si and Ge, and in Figs. 6.8.a, 6.9.a, and 6.10.a for solid Xe, Ar, and Ne, respectively. Fig. 4.20 shows the $c_1 = c_2 = 2$ choice in Si and Ge. If the values found by Hobler [7] and by us (see Fig. 4.11) to fit the measured channeling angles for B and P ions propagating in a Si crystal apply also to the propagation of Si ions in Si, then the case of $c_1 = c_2 = 2$ should be chosen. For Xe, Ar, and Ne, the $c_1 = c_2 = 2$ choice is shown in Figs. 6.8.b, 6.9.b, and 6.10.b, respectively.

The channeling fractions for all the crystals we studied would never be larger than a few percent at their maximum. This maximum occurs because the critical distances decrease with the ion energy E , making channeling more probable, and the critical angles also decrease with E , making channeling less probable.

Notice that a small change in the critical distances $r_c(T)$ or $x_c(T)$ and thus in the initial minimum distances of approach $r_{i,\min}$ or $x_{i,\min}$ is exponentially magnified in the channeling fractions χ_{axial} , Eq. 3.40, or χ_{planar} , Eq. 3.42. This constitutes the most important difficulty to evaluate channeling fractions in the models we use.

The result of our work has had important consequences on the compatibility of the DAMA results with other experiments. The effect of channeling on the regions in cross section versus mass of acceptable WIMP models is negligible, and in the absence of channeling, the DAMA region could be compatible with the CoGeNT region for light WIMPs [102]. Fig. 8.1 (reproduced from Ref. [8]) shows the regions in spin-independent cross section versus mass compatible with the DAMA modulation signal at the 7σ , 5σ , 3σ , and 90% level both with and without channeling included. The largest channeling fractions in Fig. 3.14.a were used to produce Fig. 8.1 as they provide the largest potential effect on the DAMA constraints. Even in this case there is negligible difference between the channeling and non-channeling cases except for regions incompatible with DAMA at greater than the 5σ level, in which the difference is only at masses below 4 GeV and at relatively high cross-sections.

The analytical approach used here can successfully describe qualitative features of the channeling and blocking effects, but should be complemented by data fitting of parameters and by simulations to obtain a good quantitative description too. Thus our results should in

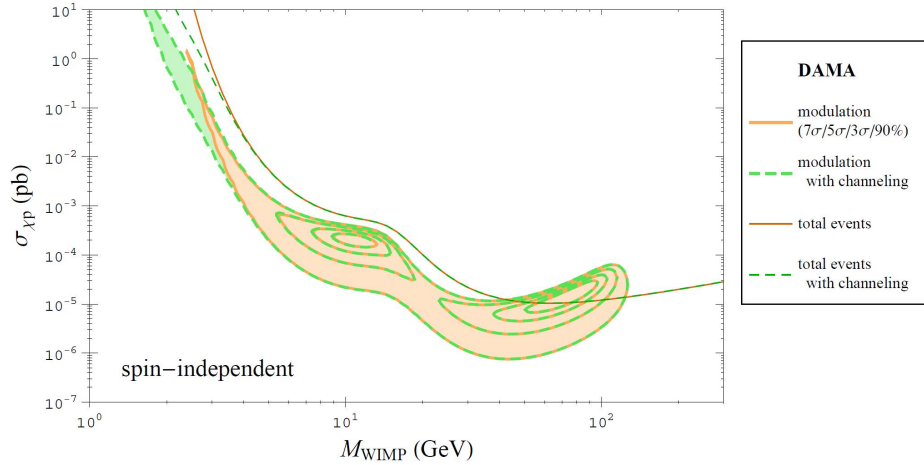


Figure 8.1: The range of masses and spin-independent cross sections compatible with the DAMA modulation signal and total number of events, determined with (dashed green) and without (solid orange) channeling. For the channeling case, the largest channeling fractions in Fig. 3.14.a are used. There is negligible difference in the DAMA modulation regions with and without channeling at the 90%, 3σ , and 5σ levels; only the 7σ contours differ and only for WIMP masses below 4 GeV. This figure is reproduced from Ref. [8].

the last instance be checked by using some of the many sophisticated Monte Carlo simulation programs implementing the binary collision approach or mixed approaches.

We have also studied the possibility of a daily modulation due to channeling, which would be a background free signature of dark matter. Channeling is a directional effect which depends on the velocity distribution of WIMPs in the dark halo of our Galaxy and could lead to a daily modulation of the signal. We have computed upper bounds to the daily modulation amplitudes expected in the data already collected by the DAMA experiment and found large modulation amplitudes of the signal rate, of the order of 10% in some instances, which are not observable at the 3σ level in the standard halo in the 13 years of data taken by the DAMA collaboration. For these to be observable the DAMA total rate should be 1/40 of what it is or the total DAMA exposure should be 40 times larger. The daily modulation due to channeling will be difficult to measure in future experiments. We find it could be observed for light WIMPs in solid Ne, assuming no background.

APPENDIX A

Crystal structures and other data

A.1 NaI

NaI is a diatomic compound that has two interpenetrating face-centered cubic (f.c.c.) lattice structures displaced by half of a lattice constant with 8 atoms per unit cell. The lattice constant a_{lat} of a cubic crystal system refers to the constant distance between unit cells of one of the f.c.c. lattices in the crystal, and for NaI it is $a_{\text{lat}} = 0.6473$ nm at room temperature (Table 3.4 in Appleton and Foti [64]). Fig. A.1 shows one eighth of the unit cell of the NaI crystal. The red and blue spheres represent Na and I ions respectively. The shortest distance between Na and I ions in Fig. A.1 is half the lattice constant, $a_{\text{lat}}/2$.

The atomic mass and atomic number of Na and I are $M_{\text{Na}} = 22.9$ amu, $M_{\text{I}} = 126.9$ amu, $Z_{\text{Na}} = 11$ and $Z_{\text{I}} = 53$. When computing ψ_1 in Eq. 3.2 for Na recoils, we take $Z_1 = Z_{\text{Na}}$ and Z_2 equal to an effective atomic number of the row or plane in the channel, which depends on the composition of the row or plane. “Mixed” channels, for example the rows $\langle 100 \rangle$ and $\langle 111 \rangle$, or the planes $\{100\}$ and $\{110\}$, contain both Na and I ions in alternation; they have $Z_2 = \bar{Z} = (Z_{\text{Na}} + Z_{\text{I}})/2$. “Pure” channels, for example the row $\langle 110 \rangle$ or the plane $\{111\}$, contain atoms of a single species, only Na or only I; they have $Z_2 = Z_{\text{Na}}$ or $Z_2 = Z_{\text{I}}$. Thus, for Na recoils from the row where it originally was, we have

$$\sin^2 \psi_1^{\text{Na}} = \frac{2Z_{\text{Na}}Z_2e^2}{Ed}. \quad (\text{A.1})$$

Similarly, for I recoils $Z_1 = Z_{\text{I}}$, and for mixed channels $Z_2 = \bar{Z} = (Z_{\text{Na}} + Z_{\text{I}})/2$ while for pure channels we use $Z_2 = Z_{\text{I}}$. We have

$$\sin^2 \psi_1^{\text{I}} = \frac{2Z_{\text{I}}Z_2e^2}{Ed}. \quad (\text{A.2})$$

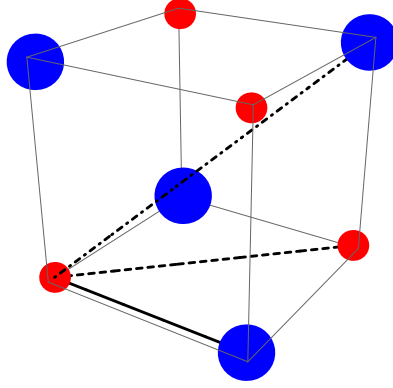


Figure A.1: One eighths of the NaI crystal unit cell with the red and blue spheres representing Na and I ions respectively. The solid, dashed and dot-dashed lines show the $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ axes respectively. The $\{100\}$, $\{110\}$ and $\{111\}$ planes are perpendicular to the respective axes with equal indices.

With respect to the Thomas-Fermi screening distance, for Na recoils from a mixed row or plane we use the average

$$\bar{a}_{\text{Na}} = (a_{\text{NaNa}} + a_{\text{NaI}})/2 = 0.01149 \text{ nm}, \quad (\text{A.3})$$

where $a_{\text{NaNa}} = 0.4685(Z_{\text{Na}}^{1/2} + Z_{\text{Na}}^{1/2})^{-2/3} = 0.01327 \text{ nm}$ and $a_{\text{NaI}} = 0.4685(Z_{\text{Na}}^{1/2} + Z_{\text{I}}^{1/2})^{-2/3} = 0.009711 \text{ nm}$ correspond to an Na scattering from an Na and an I lattice atom, respectively. On the other hand, for Na recoils from a pure row or plane we use a_{NaNa} because the row or plane from which the recoiling Na ion was emitted contains only Na atoms. Similarly, for I recoils from a mixed row or plane, we use

$$\bar{a}_{\text{I}} = (a_{\text{II}} + a_{\text{NaI}})/2 = 0.008784 \text{ nm}, \quad (\text{A.4})$$

where $a_{\text{II}} = 0.4685(Z_{\text{I}}^{1/2} + Z_{\text{I}}^{1/2})^{-2/3} = 0.007857 \text{ nm}$ and a_{NaI} correspond to an I ion scattering from an I and an Na lattice atom, respectively. For I recoils from a pure row or plane we use a_{II} , since the row or plane the recoiling ion is emitted from is made of I ions only.

Finally, to compute ψ_a for Na recoils

$$\sin \psi_a = \left(\frac{2\pi n Z_{\text{Na}} Z_2 e^2 a}{E} \right)^{\frac{1}{2}}, \quad (\text{A.5})$$

where $Z_2 = \bar{Z}$ and $a = \bar{a}_{\text{Na}}$ or $Z_2 = Z_{\text{Na}}$ and $a = a_{\text{NaNa}}$ for mixed or pure rows and planes respectively. For I recoils

$$\sin \psi_a = \left(\frac{2\pi n Z_{\text{I}} Z_2 e^2 a}{E_R} \right)^{\frac{1}{2}}, \quad (\text{A.6})$$

where $Z_2 = \bar{Z}$ and $a = \bar{a}_{\text{I}}$ or $Z_2 = Z_{\text{Na}}$ and $a = a_{\text{II}}$ for mixed or pure rows and planes respectively.

We here review the crystallographic notation for directions in the lattice. Once an origin of the coordinate system is fixed on a lattice point O , any position vector of a point on the crystal lattice can be written as $\mathbf{R} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$ with n_1 , n_2 , and n_3 specific integer numbers. The vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are the basis vectors of the crystal lattice, and are three noncoplanar vectors joining the lattice point O to its near neighbors. For the cubic lattice of NaI, the three vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ form a Cartesian frame and their length is $a_{\text{lat}}/2$ (they are the sides of the cube in Fig. A.1). The integers n_1 , n_2 , and n_3 can be positive, negative, or zero. The direction of a crystal axis pointing in the direction $\mathbf{R}$ is specified by the triplet $[n_1 n_2 n_3]$ written in square brackets, when n_1 , n_2 , and n_3 are positive or zero. Note that if there is a common factor in the numbers n_1 , n_2 , n_3 , this factor is removed. Moreover, negative integers are denoted with a bar over the number, e.g. -1 is denoted as $\bar{1}$ and the $-y$ axis is $[0\bar{1}0]$ direction. Fig. A.1 shows the directions of the $[100]$, $[110]$ and $[111]$ axes.

In a cubic crystal, because of the symmetry of the unit cell, the directions $[100]$, $[010]$, and $[001]$ are equivalent. All directions equivalent to the $[n_1 n_2 n_3]$ direction are denoted by $\langle n_1 n_2 n_3 \rangle$ in angular brackets. For example, $\langle 100 \rangle$ indicates all six directions $[100]$, $[010]$, $[001]$, $[\bar{1}00]$, $[0\bar{1}0]$, and $[00\bar{1}]$. The plane perpendicular to the $[n_1 n_2 n_3]$ axis is denoted by $(n_1 n_2 n_3)$. For example, the plane perpendicular to the $[100]$ axis is denoted by (100) , and that perpendicular to $[101]$ by (101) . The integers n_1 , n_2 , and n_3 are called Miller indices.

When the unit cell has cubic symmetry, we can indicate all planes that are equivalent to the plane (hkl) by curly brackets $\{hkl\}$. For example, the indices $\{100\}$ refer to the six

planes (100), (010), (001), ($\bar{1}00$), ($0\bar{1}0$), and ($00\bar{1}$). The negative sign over a number denotes that the plane cuts the axis on the negative side of the origin.

We will only consider the lower index crystallographic axis and planes. For axial channeling we will consider the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ axes and for planar channeling we consider the $\{100\}$, $\{110\}$ and $\{111\}$ planes perpendicular to them.

To compute the interatomic spacing d in axial directions and the interplanar spacing d_{pch} in planar directions, we have to multiply the lattice constant by the following coefficients [33]:

- Axis: $\langle 100 \rangle : 1/2$, $\langle 110 \rangle : 1/\sqrt{2}$, $\langle 111 \rangle : \sqrt{3}/2$
- Plane: $\{100\} : 1/2$, $\{110\} : 1/2\sqrt{2}$, $\{111\} : 1/2\sqrt{3}$

For NaI, the Debye temperature is $\Theta = 165$ K, and the crystals in the DAMA experiment are at a temperature of 20 °C or 293.15 K.

A.2 Si and Ge

Silicon (Si) and Germanium (Ge) crystals have a diamond cubic type lattice structure which consists of two interpenetrating f.c.c. lattices, displaced along the body diagonal of the cubic cell by one quarter of the length of the diagonal. The unit cell, shown in Fig. A.2, has 8 atoms. The lattice constant, the side of the cube in Fig. A.2, is $a_{\text{lat}} = 0.5431$ nm for Si and 0.5657 nm for Ge (from the Table 3.4 of Ref. [64]).

The atomic mass and atomic number of Si and Ge are $M_{\text{Si}} = 28.09$ amu, $M_{\text{Ge}} = 72.59$ amu, $Z_{\text{Si}} = 14$ and $Z_{\text{Ge}} = 32$. The Thomas-Fermi screening distances for two Si atoms and two Ge atoms are $a_{\text{SiSi}} = 0.4685\text{\AA}(Z_{\text{Si}}^{1/2} + Z_{\text{Si}}^{1/2})^{-2/3} = 0.01225$ nm and $a_{\text{GeGe}} = 0.4685\text{\AA}(Z_{\text{Ge}}^{1/2} + Z_{\text{Ge}}^{1/2})^{-2/3} = 0.009296$ nm respectively.

For Si and Ge, the three basis vectors **a**, **b**, **c** form a Cartesian frame and their length is $a_{\text{lat}}/4$.

We only consider the most important channels, which are the $\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$, $\langle 211 \rangle$ and $\langle 311 \rangle$ axial channels and the $\{100\}$, $\{110\}$, $\{111\}$, $\{210\}$ and $\{310\}$ planar



Figure A.2: Unit cell of a Si or Ge crystal (a) in three dimensions, and (b) projected on a plane. The black spheres represent Si or Ge atoms.

channels. For example $\langle 211 \rangle$ and $\langle 311 \rangle$ indicate twelve different directions each. Similarly, $\{210\}$ and $\{310\}$ each indicate twelve different planes. Counting all the axes and planes, the total is 74.

The interatomic spacing d and the interplanar spacing d_{pch} in monatomic diamond crystals, are obtained by multiplying the respective lattice constant by the following coefficients [33]:

- Rows: $\langle 100 \rangle$: 1, $\langle 110 \rangle$: $1/\sqrt{2}$, $\langle 111 \rangle$: $3\sqrt{3}/4$, $\langle 211 \rangle$: $\sqrt{6}/2$, $\langle 311 \rangle$: $3\sqrt{11}/4$
- Planes: $\{100\}$: $1/4$, $\{110\}$: $1/2\sqrt{2}$, $\{111\}$: $\sqrt{3}/4$, $\{210\}$: $1/(4\sqrt{5})$, $\{310\}$: $1/(2\sqrt{10})$

The Debye temperatures for Si and Ge are $\Theta = 490$ K and $\Theta = 290$ K, respectively [33, 7, 49].

A.3 CsI

CsI is a diatomic compound that has two interpenetrating f.c.c. lattice structures displaced by half of a lattice constant with 8 atoms per unit cell. The lattice constant of CsI crystal is $a_{\text{lat}} = 0.45667$ nm at room temperature (Table 3.4 in Appleton and Foti [64]). The temperature dependence of a_{lat} is explained in Appendix D.

The atomic mass and atomic number of Cs and I are $M_{\text{Cs}} = 132.9$ amu, $M_{\text{I}} = 126.9$ amu, $Z_{\text{Cs}} = 55$ and $Z_{\text{I}} = 53$.

With respect to the Thomas-Fermi screening distance, for Cs recoils from a mixed row or plane we use the average

$$\bar{a}_{\text{Cs}} = (a_{\text{CsCs}} + a_{\text{CsI}})/2 = 0.007785 \text{ nm}, \quad (\text{A.7})$$

where $a_{\text{CsCs}} = 0.4685(Z_{\text{Cs}}^{1/2} + Z_{\text{Cs}}^{1/2})^{-2/3} = 0.007761$ nm and $a_{\text{CsI}} = 0.4685(Z_{\text{Cs}}^{1/2} + Z_{\text{I}}^{1/2})^{-2/3} = 0.007809$ nm correspond to a Cs scattering from a Cs and an I lattice atom, respectively. On the other hand, for Cs recoils from a pure row or plane we use a_{CsCs} . Similarly, for I recoils from a mixed row or plane, we use

$$\bar{a}_{\text{I}} = (a_{\text{II}} + a_{\text{CsI}})/2 = 0.007833 \text{ nm}, \quad (\text{A.8})$$

where $a_{\text{II}} = 0.4685(Z_{\text{I}}^{1/2} + Z_{\text{I}}^{1/2})^{-2/3} = 0.007857$ nm and a_{CsI} correspond to an I ion scattering from an I and a Cs lattice atom, respectively. For I recoils from a pure row or plane we use a_{II} .

To compute d and d_{pch} , we have to multiply the lattice constant by the following coefficients [33] which we also use for NaI:

- Axis: $\langle 100 \rangle : 1/2$, $\langle 110 \rangle : 1/\sqrt{2}$, $\langle 111 \rangle : \sqrt{3}/2$
- Plane: $\{100\} : 1/2$, $\{110\} : 1/2\sqrt{2}$, $\{111\} : 1/2\sqrt{3}$

The Debye temperature of CsI is $\Theta = 125$ K, and the crystals in the KIMS experiment are currently at a temperature of 293 K [87].

A.4 Solid Xe, Ar, and Ne

Solid Xe, Ar and Ne have f.c.c. lattice structures with 4 atoms per unit cell. The lattice constant of Xe, Ar and Ne crystals are $a_{\text{lat}}^{\text{Xe}} = 0.620$ nm at $T = 75$ K [103], $a_{\text{lat}}^{\text{Ar}} = 0.525$ nm and $a_{\text{lat}}^{\text{Ne}} = 0.442$ nm at $T = 4.2$ K and atmospheric pressure [104].

The atomic mass and atomic numbers of Xe, Ar, and Ne are $M_{\text{Xe}} = 131.29$ amu, $M_{\text{Ar}} = 39.948$ amu, $M_{\text{Ne}} = 20.1797$ amu, $Z_{\text{Xe}} = 54$, $Z_{\text{Ar}} = 18$ and $Z_{\text{Ne}} = 10$.

The Thomas-Fermi screening distance for an ion expelled from a lattice site in the crystal scattering on another atom in the same crystal is $a_{\text{XeXe}} = 0.4685(Z_{\text{Xe}}^{1/2} + Z_{\text{Xe}}^{1/2})^{-2/3} = 0.007808$ nm for Xe, $a_{\text{ArAr}} = 0.4685(Z_{\text{Ar}}^{1/2} + Z_{\text{Ar}}^{1/2})^{-2/3} = 0.01126$ nm for Ar and $a_{\text{NeNe}} = 0.4685(Z_{\text{Ne}}^{1/2} + Z_{\text{Ne}}^{1/2})^{-2/3} = 0.01370$ nm for Ne.

To compute d and d_{pch} , we have to multiply the lattice constant by the following coefficients [33]:

- Axis: $\langle 100 \rangle$: 1 , $\langle 110 \rangle$: $1/\sqrt{2}$, $\langle 111 \rangle$: $\sqrt{3}$
- Plane: $\{100\}$: $1/2$, $\{110\}$: $1/2\sqrt{2}$, $\{111\}$: $1/\sqrt{3}$

The Debye temperatures of Xe, Ar and Ne are $\Theta_{\text{Xe}} = 55$ K, $\Theta_{\text{Ar}} = 85$ K and $\Theta_{\text{Ne}} = 63$ K [105, 106], and the crystals in the Solid Xe R&D Project experiment will be operating at a temperature of 77.2 K or higher [90].

APPENDIX B

HEALPix Pixelization

The Hierarchical Equal Area iso-Latitude Pixelization (HEALPix) [76] provides a convenient way of dividing the surface of a sphere into equal area sectors. An integral over directions can then be performed as a simple Riemann sum. HEALPix has been introduced to pixelize data on a sphere and has been used by cosmic microwave background experiments like WMAP and BOOMERANG.

In HEALPix, the base resolution comprises 12 pixels in three rings: one ring around the north cap, one ring around the south cap, and one ring around the equator. At a higher resolution, each base pixel in each ring is divided into smaller pixels of equal area. The resolution parameter of the grid is N_{side} and it defines the number of divisions along the side of a base-resolution pixel which is needed to obtain a partition with higher resolution. We choose the resolution parameter of the grid to be $N_{\text{side}} = 50$.

A HEALPix map has $N_{\text{pixel}} = 12N_{\text{side}}^2$ pixels, each with the same area. The angular resolution of the map can be estimated by computing the solid angle covered by each pixel $\Omega = 4\pi/N_{\text{pixel}}$, and finding the typical diameter of each pixel as if it were small and of circular shape, $\theta_{\text{res}} = 2\sqrt{\Omega/\pi}$. This gives $\theta_{\text{res}} = 2/(\sqrt{3}N_{\text{side}}) = 66.2^\circ/N_{\text{side}}$. By choosing $N_{\text{side}} = 50$, we have 30,000 pixels on the sphere, and a resolution of 1.3 degrees. If the HEALPix is properly aligned with the cubic crystal so that there is a pixel in each $\langle 100 \rangle$ direction, this resolution should be sufficient for computing our integrals accurately. We have tried different values of N_{side} , up to $N_{\text{side}} = 400$ (for which the resolution is $\theta_{\text{res}} = 0.166^\circ$), and we found that the value of the channeling fraction already converges within one percent for $N_{\text{side}} = 20$. Thus, we used $N_{\text{side}} = 50$ as a safe value in our calculations.

The following algorithm [76] was used to generate a list of unit vectors on a sphere, with

each unit vector in the direction of one of the HEALPix pixels. Let p be the pixel index, with $p = 0, 1, \dots, N_{\text{pixel}} - 1$. We start with the definitions:

$$p_{\text{max}} = 12N_{\text{side}}^2 - 1, \quad p_{\text{max}}^{\text{north}} = \frac{p_{\text{max}} + 1}{2} + 2N_{\text{side}} - 1. \quad (\text{B.1})$$

If $p > p_{\text{max}}^{\text{north}}$, then $q = p_{\text{max}} - p$ otherwise $q = p$. Then we define

$$n_{\text{polar}} = N_{\text{side}} - 1, \quad n_{\text{equatorial}} = N_{\text{side}} + 1, \quad p_{\text{min}}^{\text{equatorial}} = 2N_{\text{side}}(N_{\text{side}} - 1). \quad (\text{B.2})$$

We proceed to compute the cylindrical coordinates z and φ of the direction of the p -th HEALPix pixel. If $q \geq p_{\text{min}}^{\text{equatorial}}$, the pixel belongs to one of the polar rings and we successively compute

$$h = p - p_{\text{min}}^{\text{equatorial}}, \quad (\text{B.3})$$

$$i = \left\lfloor \frac{ph}{4N_{\text{side}}} \right\rfloor + N_{\text{side}}, \quad (\text{B.4})$$

$$j = [h \bmod (4N_{\text{side}})] + 1, \quad (\text{B.5})$$

$$z = \frac{4}{3} - \frac{2i}{3N_{\text{side}}}, \quad (\text{B.6})$$

$$s = (i - N_{\text{side}} + 1) \bmod 2, \quad (\text{B.7})$$

$$\varphi = \frac{\pi}{2N_{\text{side}}} \left(j - \frac{s}{2} \right). \quad (\text{B.8})$$

Here $\lfloor x \rfloor$ is the minimum integer less or equal to x , and $x \bmod y$ is the remainder of the integer division of x by y . If $q < p_{\text{min}}^{\text{equatorial}}$, the pixel belongs to the equatorial ring and we successively compute

$$h = \frac{q + 1}{2}, \quad (\text{B.9})$$

$$i = \left\lfloor \sqrt{h - \sqrt{[h]}} \right\rfloor + 1, \quad (\text{B.10})$$

$$j = q + 1 - 2i(i - 1), \quad (\text{B.11})$$

$$\text{If } p > p_{\text{max}}^{\text{north}} \text{ then } j = 4i - j + 1, \quad (\text{B.12})$$

$$z = 1 - \frac{i^2}{3N_{\text{side}}^2}, \quad (\text{B.13})$$

$$\text{If } p > p_{\text{max}}^{\text{north}} \text{ then } z = -z, \quad (\text{B.14})$$

$$\varphi = \frac{\pi}{2i} \left(j - \frac{1}{2} \right). \quad (\text{B.15})$$

Finally, the direction vector of the p -th pixel is given by

$$\hat{\mathbf{n}}_p = \left(\sqrt{1 - z^2} \cos \varphi, \sqrt{1 - z^2} \sin \varphi, z \right). \quad (\text{B.16})$$

APPENDIX C

Matyukhin model of planar channeling

Matyukhin in Ref [67] uses a different condition for planar channeling than we used previously which consists of Eq. 3.6 written in terms of the planar potential, namely $U_p''(x) < 8E/d_p^2$ (where $''$ denotes the second derivative with respect to x). We have not been able either to derive this condition for the planar potential or to find the derivation of this condition anywhere. We have not found the results derived from this condition compared with data either, but we mention the model for completeness. For Lindhard's planar potential, the condition used by Matyukhin becomes

$$E > \frac{d_p^2}{8} \frac{C^2 a E_2}{[x_{\min}^2 + C^2 a^2]^{3/2}}, \quad (\text{C.1})$$

where $x_{\min}$ is the minimum distance of approach to the plane, $d_p = 1/\sqrt{Nd_{\text{pch}}}$ and

$$E_2 = E\psi_a^2 = 2\pi N d_p Z_1 Z_2 e^2 a. \quad (\text{C.2})$$

From Eq. C.1, the smallest possible value of $x_{\min}$ is now

$$x_c^M(E) = Ca \sqrt{\left(\frac{d_p^2 E_2}{8Ca^2 E}\right)^{2/3} - 1}. \quad (\text{C.3})$$

For all the energies we consider here ($\sim$ keV and above), x_c^M is smaller than $d_{\text{pch}}/2$, thus $U_p(d_{\text{pch}}/2)$ can be neglected in the definition of the critical planar angle ψ_c^p , Eq. 3.25. At low energies $E \leq d_p^2 E_2 (8Ca^2)^{-1}$ we have $x_c^M(E) \simeq Ca(d_p^2 E_2 / 8Ca^2 E)^{1/3} = (C^2 \pi Z_1 Z_2 e^2 a^2 / 4E)^{1/3}$ and

$$\psi_c^{pM}(E) \simeq \left(\frac{C^2 a E_2}{d_p E}\right)^{1/3} = \left(\frac{2 C^2 \pi Z_1 Z_2 e^2 (Nd_{\text{pch}})^{3/2} a^2}{E}\right)^{1/3}, \quad (\text{C.4})$$

where $\psi_c^{pM}(E) = (6\pi)^{1/3} \theta_{pl}$ and θ_{pl} is the critical angle used by DAMA.

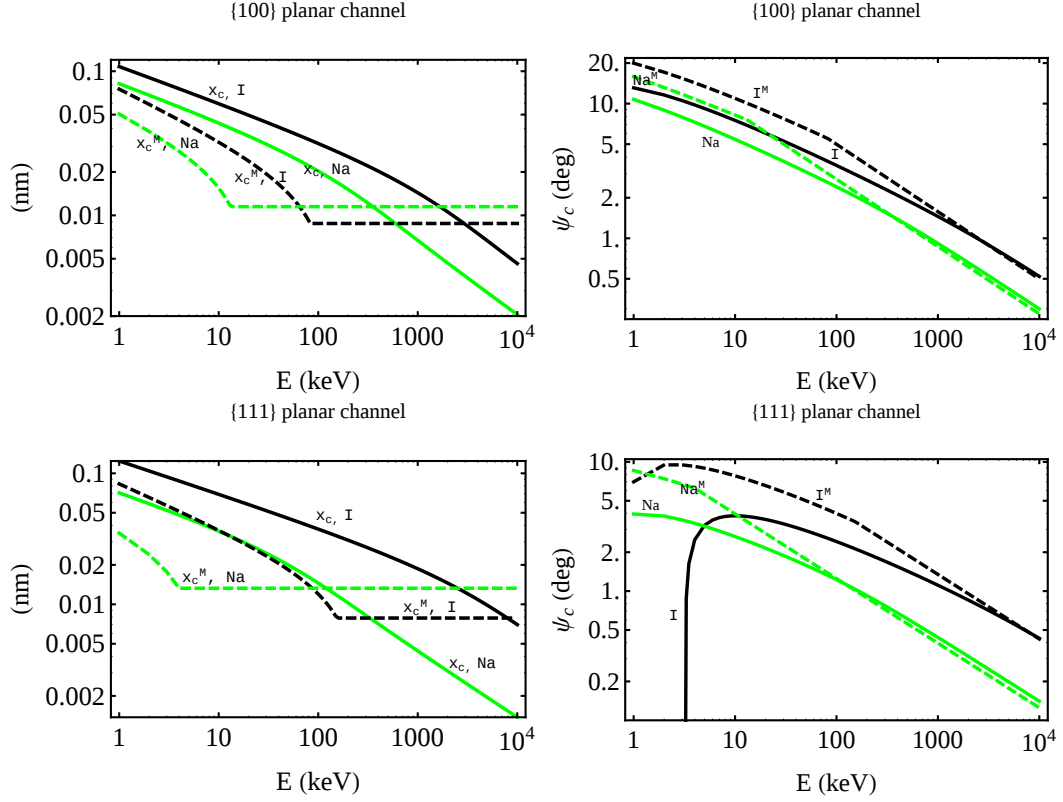


Figure C.1: Comparison of (a) (top left) critical distances of approach and (b) (top right) critical angles at 20 °C with $c_1 = c_2 = 1$ in the {100} planar channel predicted by our main model (solid lines, see Figs. 3.4, 3.5) and by Matyukhin's (dashed lines). (c) (bottom left) and (d) (bottom right), same for the {111} planar channel. Green/gray lines are for Na and black for I propagating ions.

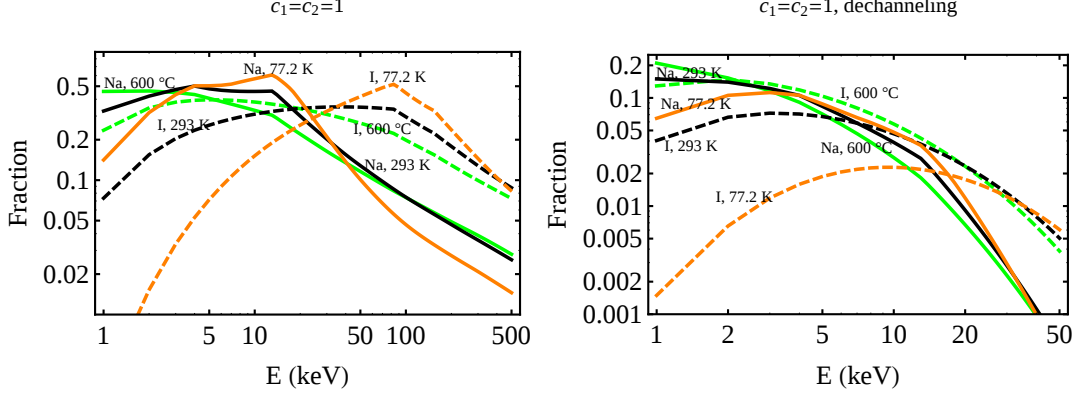


Figure C.2: Channeling fractions using Matyukhin's model for the planar channel as a function of the energy of recoiling Na and I ions for $T=600$ °C (green/light gray), 293 K (black) and 77.2 K (orange/dark gray) for T-corrections included in the lattice with $c_1 = c_2 = 1$, (a) without and (b) with dechanneling included as in Eq. 3.34. The probabilities are larger than in our main method, but we do not trust Matyukhin's approach.

As E approaches the value $d_p^2 E_2 (8Ca^2)^{-1}$, $x_c^M(E)$ approaches zero. At larger energies, $E > d_p^2 E_2 (8Ca^2)^{-1}$, $x_c^M(E)$ in Eq. C.3 becomes imaginary, but $x_c^M(E)$ is by definition real and positive thus one could take it to be zero. Matyukhin takes in this case $x_c^M(E) = a$ instead. Either way, in this energy range $\psi_c^{pl}(E) \simeq \psi_a$ which is the value given by Lindhard for the “breakthrough” angle [40] necessary to have $E_{\text{perp}} = U_p(0)$. We take $x_c^M(E) = a$ wherever the prediction of Eq. C.3 is smaller than a . Including temperature corrections due to the thermal and zero point energy vibrations of the atoms in the lattice, we have $x_c(T)$ as in Eq. 3.30.

The equations of Matyukhin coincide with those presented here if $C = 1$ (but, following Lindhard, we take $C = \sqrt{3}$ instead).

A comparison of the static critical distances of approach $x_c(E)$ in our method (using Eq. 3.22 and 3.25) and in Matyukhin's model, and of the critical angles for $c_1 = c_2 = 1$ in both models is shown in Figs. C.1(a) and C.1(c) and in Figs. C.1(b) and C.1(d) respectively for the $\{100\}$ and $\{111\}$ planar channels respectively. The Matyukhin critical distances of approach are smaller (and thus the critical angles larger) than those in our main method at

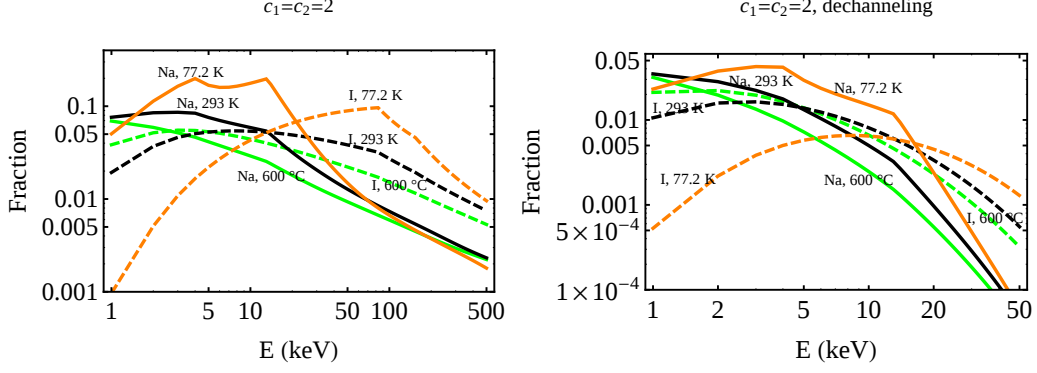


Figure C.3: Same as Fig. C.2 (for Matyukhin's model) but for $c_1 = c_2 = 2$.

low energies, which leads to higher channeling fractions, as shown in Figs. C.2 and C.3 for $c_1 = c_2 = 1$ and for $c_1 = c_2 = 2$ respectively. In these figures the left panels are without and the right panels with dechanneling as in Eq. 3.34 included. The channeling fractions using Matyukhin's model are much higher than the fractions we obtain with our method, but, as explained above, we do not trust Matyukhin's model. The critical distances in Matyukhin's model (see Figs. C.1(a) and C.1(c)) have a discontinuous slope at the energy where they become constant and this shows in the channeling fraction curves also as discontinuities in slope (at the values of E at which different important channels have a sharp change in x_c^M).

APPENDIX D

Probability of correlated channels

In Eq. 3.50 we treat channeling along different channels as independent events. Here we prove that this procedure is adequate for our purpose of providing upper bounds to the channeling fractions.

For an axial channel when $\phi < \psi_c$ (otherwise $\chi_{\text{axial}} = 0$), the integration region in Eq. 3.40 is the exterior of an infinitely long cylinder of radius $r_{i,\min}(E, \phi)$ and axis coincident with the channel axis. Similarly, for a planar channel when $\phi < \psi_c^p$ (otherwise $\chi_{\text{planar}} = 0$), the integration region in Eq. 3.42 is the exterior of an infinite slab of half-thickness $x_{i,\min}(E, \phi)$. Let us consider the complements of the integration regions, i.e. the regions excluded in the integrals. These are the regions interior to a cylinder (for an axial channel) or a slab (for a planar channel).

Note that only channels making angles with the direction $\hat{\mathbf{q}}$ (of the initial momentum) smaller than their respective critical angles contribute to the union of integration regions. Therefore the problem of combining channels arises only when a recoil direction belongs to more than one channel, and this happens if the channels overlap for some directions of $\hat{\mathbf{q}}$. For the cases we consider (cubic lattices), only axial channels overlap with a subset of planar channels, or two or more planar channels overlap with each other. Notice that two different planar channels crossing at an angle, overlap in a parallelepiped of very long length on one side, thus one can define an inscribed cylinder within the parallelepiped, whose diameter is equal to the smallest of the two widths of both planar channels.

We can obtain an upper limit to the channeling probability of overlapping channels by replacing the intersection of the complements of the integration regions with the inscribed circle of radius r_{MIN} equal to the minimum of the $r_{i,\min}$ or $x_{i,\min}$ among the overlapping

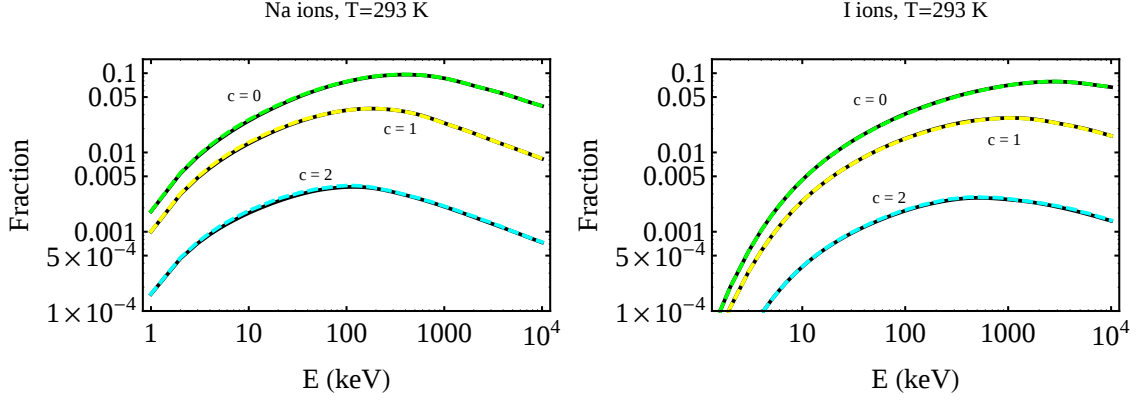


Figure D.1: Maximum channeling fractions using Eq. D.1 for $c_1 = c_2 = c$ and $c = 0$ (dashed green), $c = 1$ (dashed yellow) and $c = 2$ (dashed cyan) compared with the results of our method of Section 3.3.3 (solid black lines) for the same models for (a) Na ions and (b) I ions propagating in NaI crystal at $T = 293$ K. Notice that the lines overlap.

channels. Then an upper bound to the probability $\chi_{\text{rec}}(E, \hat{\mathbf{q}})$ in Eq. 3.52 is

$$\chi_{\text{rec}}(E, \hat{\mathbf{q}}) \leq \int_{r_{\text{MIN}}}^{\infty} dr g(r) = \exp(-r_{\text{MIN}}^2/2u_1^2). \quad (\text{D.1})$$

When only one channel is open (i.e. $\phi < \psi_c$ for only one channel), we still use Eq. 3.40 or 3.42 for the channeling probabilities.

Fig. D.1 shows the comparison of this upper limit with the fractions we computed using Eq. 3.50 for NaI crystal. The two are practically indistinguishable. This proves that the method we used (see Section 3.3.3) is adequate for our purpose of providing upper bounds to the channeling fractions in NaI.

We find that the two methods give practically indistinguishable results for Si and Ge also, as clearly shown in Fig. D.2 for some particular examples.

Fig. D.3 shows the channeling fractions of Si ions propagating in a Si crystal and Ge ions propagating in a Ge crystal for individual channels with $c_1 = c_2 = 1$ and $T = 293$ K. The black and green (or gray) lines correspond to single axial and planar channels respectively.

Fig. D.3 shows that at low energies channeling is dominated by axial channels which do not overlap, so treating them as independent is strictly correct. However, at the transition

energy of 1 to 10 MeV at which axial and planar channels are both equally important, and at higher energies at which planar channels dominate, the overlap of one axial and two or more planar channels, or the overlap of two or more planar channels among themselves, makes the channeling along them not necessarily uncorrelated. Still we find that considering channeling along different channels as independent is a good approximation if we are interested in providing upper bounds to the channeling fractions.

APPENDIX E

Temperature dependence of lattice constant

In general the lattice constant, a_{lat} is temperature dependent. The change in a_{lat} with temperature depends on the thermal expansion coefficient, β of a crystal. For NaI, $\beta_{\text{NaI}} = 47.4 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$. To find the change in the lattice constant at a temperature T and the lattice constant at $20 \text{ }^\circ\text{C}$, we have

$$[a_{\text{lat}}(T) - a_{\text{lat}}(20 \text{ }^\circ\text{C})]/a_{\text{lat}}(20 \text{ }^\circ\text{C}) = \beta(T - 20 \text{ }^\circ\text{C}), \quad (\text{E.1})$$

where $a_{\text{lat}}(20 \text{ }^\circ\text{C})$ is the lattice constant at $20 \text{ }^\circ\text{C}$. When T changes from $20 \text{ }^\circ\text{C}$ to $600 \text{ }^\circ\text{C}$, the change in the lattice constant of NaI (using Eq. E.1) is only 2.75%. This change in a_{lat} between $20 \text{ }^\circ\text{C}$ and $600 \text{ }^\circ\text{C}$ results in a negligible change in the channeling fractions. As an example the Na channeling fractions with $c_1 = c_2 = 1$ and $c_1 = c_2 = 2$ for the two choices of $a_{\text{lat}}(20 \text{ }^\circ\text{C})$ and $a_{\text{lat}}(600 \text{ }^\circ\text{C})$ are shown in Fig. E.1.a. As the two curves are very similar, we use $a_{\text{lat}}(20 \text{ }^\circ\text{C})$ for all three crystal temperatures we considered for NaI in Chapter 3.

We can use Eq. E.1 to find the temperature dependent lattice constant for CsI, Si and Ge crystals. For these three crystals, the coefficient of thermal expansion is $\beta_{\text{CsI}} = 54 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$, $\beta_{\text{Si}} = 2.6 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$, and $\beta_{\text{Ge}} = 5.9 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$. When T changes from $20 \text{ }^\circ\text{C}$ to $600 \text{ }^\circ\text{C}$, the change in the lattice constant of CsI (Tl) is 3.1%. In Si and Ge, we can go to higher temperatures, and the maximum temperature that we considered in Chapter 4 was $900 \text{ }^\circ\text{C}$. When T changes from $20 \text{ }^\circ\text{C}$ to $900 \text{ }^\circ\text{C}$, the change in the lattice constant of Si and Ge is 0.23% and 0.52% respectively.

The Cs channeling fractions with $c_1 = c_2 = 1$ and $c_1 = c_2 = 2$ for the two choices of $a_{\text{lat}}(20 \text{ }^\circ\text{C})$ and $a_{\text{lat}}(600 \text{ }^\circ\text{C})$ are shown in Fig. E.1.b for a CsI crystal. Fig. E.2 shows the channeling fractions for Si and Ge for the two choices of $a_{\text{lat}}(20 \text{ }^\circ\text{C})$ and $a_{\text{lat}}(900 \text{ }^\circ\text{C})$. Clearly,

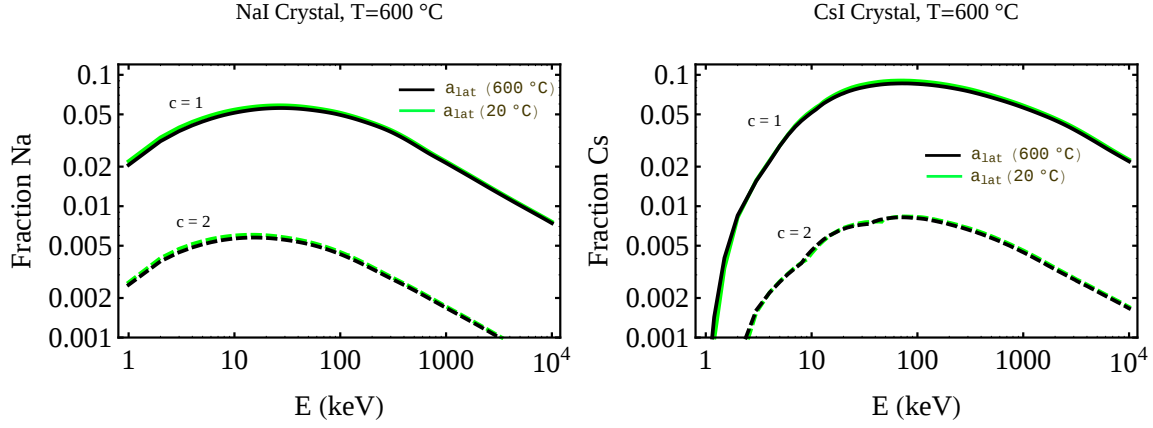


Figure E.1: Channeling fraction of (a) Na ions propagating in an NaI crystal and (b) Cs ions propagating in a CsI crystal as a function of the recoil energy E for $T = 600\text{ °C}$ with $a_{\text{lat}}(600\text{ °C})$ (black) and $a_{\text{lat}}(20\text{ °C})$ (green/gray) for the two choices of $c_1 = c_2 = 1$ or 2.

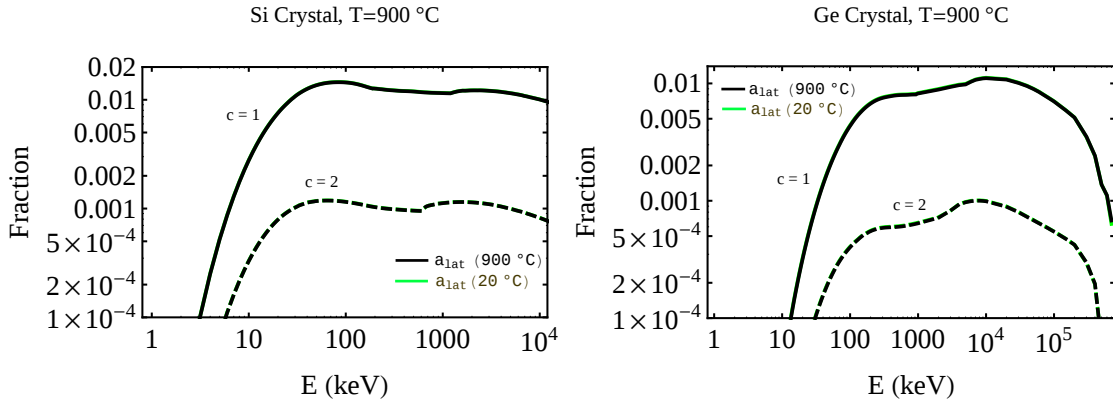


Figure E.2: Channeling fraction of (a) Si ions propagating in a Si crystal and (b) Ge ions propagating in a Ge crystal as a function of the recoil energy E for $T = 900\text{ °C}$ with $a_{\text{lat}}(900\text{ °C})$ (black) and $a_{\text{lat}}(20\text{ °C})$ (green/gray) for the two choices of $c_1 = c_2 = 1$ or 2.

the change in the curves is negligible. Thus we always used the value of a_{lat} measured at 20 °C for CsI, Si and Ge.

APPENDIX F

Crystal Orientation

We need to orient the crystal with respect to the laboratory. We define a reference frame fixed with the laboratory and orient its axes so that the xy plane is horizontal, the x -axis points North, the y -axis points West, and the z -axis points to the zenith. We denote its unit coordinate vectors as $\hat{\mathcal{N}}$, $\hat{\mathcal{W}}$ and $\hat{\mathcal{Z}}$, respectively. We also define the crystal frame with X, Y, Z cartesian axes fixed with the crystal. The unit coordinate vectors of the crystal frame are $\hat{\mathbf{X}}$, $\hat{\mathbf{Y}}$ and $\hat{\mathbf{Z}}$.

We now want to connect the laboratory frame to the crystal frame. Let the standard orientation correspond to the configuration in which $\hat{\mathbf{X}} = \hat{\mathcal{N}}$, $\hat{\mathbf{Y}} = \hat{\mathcal{W}}$, and $\hat{\mathbf{Z}} = \hat{\mathcal{Z}}$. We start with the crystal in the standard orientation, and we turn it into any other orientation $\hat{\mathbf{X}}$, $\hat{\mathbf{Y}}$, $\hat{\mathbf{Z}}$. In this new orientation, each of the unit coordinate vectors of the crystal frame can be written in terms of unit coordinate vectors of the lab frame,

$$\begin{aligned}\hat{\mathbf{X}} &= \alpha_X \hat{\mathcal{N}} + \beta_X \hat{\mathcal{W}} + \gamma_X \hat{\mathcal{Z}}, \\ \hat{\mathbf{Y}} &= \alpha_Y \hat{\mathcal{N}} + \beta_Y \hat{\mathcal{W}} + \gamma_Y \hat{\mathcal{Z}}, \\ \hat{\mathbf{Z}} &= \alpha_Z \hat{\mathcal{N}} + \beta_Z \hat{\mathcal{W}} + \gamma_Z \hat{\mathcal{Z}},\end{aligned}\tag{F.1}$$

where α_i , β_i and γ_i are the “direction cosines” between the two sets of cartesian coordinates of the lab and crystal frames, for $i = X, Y, Z$. For example, the coordinate vector $\hat{\mathbf{X}}$ of the crystal has a particular angle with each of the lab frame coordinate vectors $\hat{\mathcal{N}}$, $\hat{\mathcal{W}}$, $\hat{\mathcal{Z}}$. Let a_X be the angle between $\hat{\mathbf{X}}$ and $\hat{\mathcal{N}}$, b_X the angle between $\hat{\mathbf{X}}$ and $\hat{\mathcal{W}}$, and c_X the angle

between $\hat{\mathbf{X}}$ and $\hat{\mathbf{Z}}$. The direction cosines of the unit vector $\hat{\mathbf{X}}$ are given by,

$$\begin{aligned}\alpha_X &\equiv \cos a_X = \hat{\mathbf{X}} \cdot \hat{\mathcal{N}}, \\ \beta_X &\equiv \cos b_X = \hat{\mathbf{X}} \cdot \hat{\mathcal{W}}, \\ \gamma_X &\equiv \cos c_X = \hat{\mathbf{X}} \cdot \hat{\mathbf{Z}}.\end{aligned}\tag{F.2}$$

We can find the direction cosines for $\hat{\mathbf{Y}}$ and $\hat{\mathbf{Z}}$ unit vectors in a similar way. From these definitions it follows that $\alpha_i \alpha_j + \beta_i \beta_j + \gamma_i \gamma_j = \delta_{ij}$ where $i, j = X, Y, Z$. We prefer using direction cosines over Euler angles because the direction cosines can easily be measured for any known orientation of a crystal in a laboratory, whereas it may be difficult to specify the Euler angles.

Eq. F.1 gives the transformation from the lab frame to the crystal frame. We can also find the lab coordinate vectors in terms of the crystal coordinate vectors,

$$\begin{aligned}\hat{\mathcal{N}} &= \alpha_X \hat{\mathbf{X}} + \alpha_Y \hat{\mathbf{Y}} + \alpha_Z \hat{\mathbf{Z}}, \\ \hat{\mathcal{W}} &= \beta_X \hat{\mathbf{X}} + \beta_Y \hat{\mathbf{Y}} + \beta_Z \hat{\mathbf{Z}}, \\ \hat{\mathbf{Z}} &= \gamma_X \hat{\mathbf{X}} + \gamma_Y \hat{\mathbf{Y}} + \gamma_Z \hat{\mathbf{Z}}.\end{aligned}\tag{F.3}$$

In the results we show in Chapter 7, we took $\alpha_X = \beta_Y = \gamma_Z = 1$ and all the other α_i , β_i and γ_i equal to zero. Choosing a different orientation for the crystal does not change the average rate, but A_s may change by a factor of 2 for NaI depending on the orientation of the crystal. The observability condition is still not satisfied.

F.1 Lab to equatorial transformation

To connect the laboratory frame to the equatorial coordinate frame, we recall the definition of the geocentric equatorial inertial (GEI) frame: its origin is at the center of the Earth, its x_e -axis points in the direction of the vernal equinox, its y_e -axis points to the point on the celestial equator with right ascension 90° (so that the cartesian frame is right-handed), and its z_e -axis points to the north celestial pole. We denote its unit coordinate vectors as $\hat{\mathbf{x}}_e$, $\hat{\mathbf{y}}_e$, and $\hat{\mathbf{z}}_e$. We want to find the transformation formulas from the laboratory frame to the GEI

frame.

This transformation can be achieved by two successive rotations. The first rotation is by an angle of $(90^\circ - \lambda_{\text{lab}})$ counterclockwise about the laboratory y -axis to align the new $x'y'$ plane with the plane of the celestial equator. Here λ_{lab} is the latitude of the laboratory in degrees, with northern latitudes taken as positive and southern latitudes taken as negative. With this rotation, the new z' -axis points to the north celestial pole. The second rotation is by an angle $(15t_{\text{lab}} + 180)$ degrees clockwise about the new z' -axis to bring the x' -axis in the direction of the vernal equinox. Here t_{lab} is the laboratory Local Apparent Sidereal Time (LAST) in hours (the LAST is the hour angle of the vernal equinox at the location of the laboratory). One has

$$t_{\text{lab}} = t_{\text{GAST}} + l_{\text{lab}}/15, \quad (\text{F.4})$$

where t_{GAST} is the Greenwich Apparent Sidereal Time (GAST) in hours and l_{lab} is the longitude in degrees measured positive in the eastward direction (e.g. $l_{\text{lab}} = +110^\circ$ for 110° E and $l_{\text{lab}} = -110^\circ$ for 110° W).

The current local apparent sidereal time for any specified longitude l_{lab} can be computed online, for example on the website of the US Naval Observatory at <http://tycho.usno.navy.mil/sidereal.html> (accessed Sept 19, 2010). As an alternative, one can use the following formula [107, 108] for the Greenwich mean sidereal time (which differs from the Greenwich apparent sidereal time by less than 1.2 seconds, completely negligible for our purposes),

$$t_{\text{GAST}} = (101.0308 + 36000.770 T_0 + 15.04107 \text{ UT})/15, \quad (\text{F.5})$$

where

$$T_0 = \frac{[\text{MJD}] - 55197.5}{36525.0}. \quad (\text{F.6})$$

Here UT is the Universal Time in hours, $[\text{MJD}]$ is the integer part of the modified Julian date (MJD), which is the time measured in days from 00:00 UT on 17 November 1858 (Julian date 2400000.5). Note that T_0 is the time in Julian centuries (36525 days) from 12:00 UT on 1 January 2010 to the previous midnight. At 12:00 UT on 1 January 2010, the Julian date is 2455198, and the MJD is 55197.5. Also the $15.04107/15$ in Eq. F.5 corrects from

solar time (UT) to sidereal time. Sidereal day is shorter than Solar day by 3.9 minutes. In Chapter 7, all our results are computed for the particular arbitrary day of 25 September 2010, for which $T_0 = 0.00729637$.

Note also that UT is different from coordinated Universal Time (UTC) which is the time scale usually used for data recording. UTC is atomic time adjusted by an integral number of seconds to keep it within 0.6 s of UT. For our purposes the difference between UT and UTC is negligible.

Taking into account the two rotations explained above, one can find the transformation equations of the unit vectors,

$$\begin{aligned}\hat{\mathbf{x}}_e &= -\cos(t_{\text{lab}}^\circ) \left[\sin(\lambda_{\text{lab}}) \hat{\mathcal{N}} - \cos(\lambda_{\text{lab}}) \hat{\mathcal{Z}} \right] + \sin(t_{\text{lab}}^\circ) \hat{\mathcal{W}}, \\ \hat{\mathbf{y}}_e &= -\sin(t_{\text{lab}}^\circ) \left[\sin(\lambda_{\text{lab}}) \hat{\mathcal{N}} - \cos(\lambda_{\text{lab}}) \hat{\mathcal{Z}} \right] - \cos(t_{\text{lab}}^\circ) \hat{\mathcal{W}}, \\ \hat{\mathbf{z}}_e &= \cos(\lambda_{\text{lab}}) \hat{\mathcal{N}} + \sin(\lambda_{\text{lab}}) \hat{\mathcal{Z}},\end{aligned}\tag{F.7}$$

where $t_{\text{lab}}^\circ = 15t_{\text{lab}}$ is the laboratory LAST converted to degrees.

As a check, for a laboratory on the equator at local sidereal time 0, i.e. $\lambda_{\text{lab}} = 0^\circ$ and $t_{\text{lab}}^\circ = 0^\circ$, one has $\hat{\mathbf{x}}_e = \hat{\mathcal{Z}}$, $\hat{\mathbf{y}}_e = -\hat{\mathcal{W}}$, and $\hat{\mathbf{z}}_e = \hat{\mathcal{N}}$; six sidereal hours later at the same laboratory, i.e. $\lambda_{\text{lab}} = 0^\circ$ and $t_{\text{lab}}^\circ = 90^\circ$, one has $\hat{\mathbf{x}}_e = \hat{\mathcal{W}}$, $\hat{\mathbf{y}}_e = \hat{\mathcal{Z}}$, and $\hat{\mathbf{z}}_e = \hat{\mathcal{N}}$; for a laboratory at the South Pole ($\lambda_{\text{lab}} = -90^\circ$), using the direction of the Greenwich meridian in place of the "North" axis $\hat{\mathcal{N}}$ so that the local sidereal time at the South Pole by convention coincides with the Greenwich sidereal time, one has $\hat{\mathbf{x}}_e = \hat{\mathcal{N}}$, $\hat{\mathbf{y}}_e = -\hat{\mathcal{W}}$, and $\hat{\mathbf{z}}_e = -\hat{\mathcal{Z}}$ at $t_{\text{lab}}^\circ = 0^\circ$ and $\hat{\mathbf{x}}_e = \hat{\mathcal{W}}$, $\hat{\mathbf{y}}_e = \hat{\mathcal{N}}$, and $\hat{\mathbf{z}}_e = -\hat{\mathcal{Z}}$ at $t_{\text{lab}}^\circ = 90^\circ$. All of these are correctly given by Eq. F.7.

The formulas in Eq. F.7 can be inverted, and the transformation from the equatorial frame to the lab frame is achieved:

$$\begin{aligned}\hat{\mathcal{N}} &= -\sin(\lambda_{\text{lab}}) [\cos(t_{\text{lab}}^\circ) \hat{\mathbf{x}}_e + \sin(t_{\text{lab}}^\circ) \hat{\mathbf{y}}_e] + \cos(\lambda_{\text{lab}}) \hat{\mathbf{z}}_e, \\ \hat{\mathcal{W}} &= \sin(t_{\text{lab}}^\circ) \hat{\mathbf{x}}_e - \cos(t_{\text{lab}}^\circ) \hat{\mathbf{y}}_e, \\ \hat{\mathcal{Z}} &= \cos(\lambda_{\text{lab}}) [\cos(t_{\text{lab}}^\circ) \hat{\mathbf{x}}_e + \sin(t_{\text{lab}}^\circ) \hat{\mathbf{y}}_e] + \sin(\lambda_{\text{lab}}) \hat{\mathbf{z}}_e.\end{aligned}\tag{F.8}$$

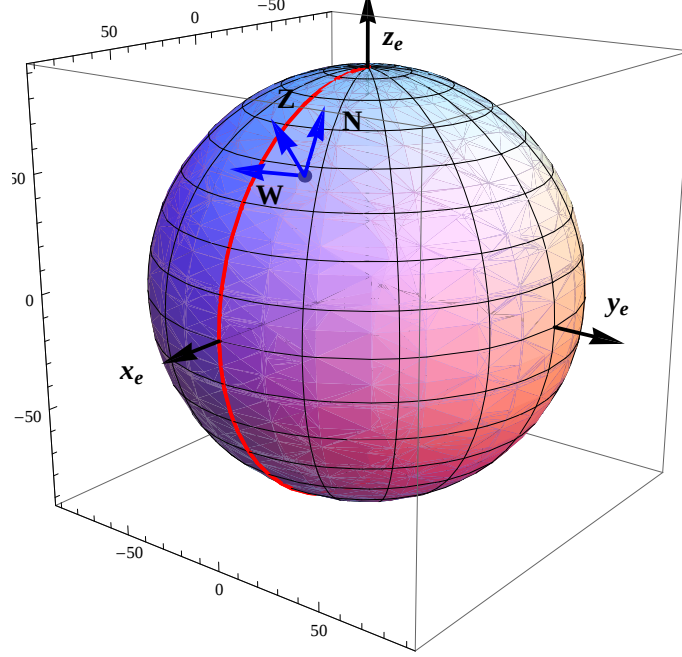


Figure F.1: (Color online) Earth's sphere in the equatorial frame $(\hat{\mathbf{x}}_e, \hat{\mathbf{y}}_e, \hat{\mathbf{z}}_e)$ specified with black arrows. The laboratory frame (N,W,Z) specified with blue/dark gray arrows is also shown.

The latitude and longitude of Gran Sasso are $\lambda_{\text{lab}} = 42.45^\circ$ and $l_{\text{lab}} = 13.7^\circ$, respectively.

Fig. F.1 shows the laboratory frame $(\hat{\mathcal{N}}, \hat{\mathcal{W}}, \hat{\mathcal{Z}})$ and the equatorial coordinate frame $(\hat{\mathbf{x}}_e, \hat{\mathbf{y}}_e, \hat{\mathbf{z}}_e)$ plotted on the Earth's sphere at $UT = 0$ using Eq. F.8.

F.2 Equatorial to galactic transformation

To connect the equatorial frame to the galactic coordinate frame, we recall the definition of the galactic coordinate system: its origin is at the position of the Sun, its x_g -axis points towards the galactic center, its y_g -axis points in the direction of the galactic rotation, and its z_g -axis points to the north galactic pole.

For the epoch of January 1950.0 the transformation from the equatorial frame $(\hat{\mathbf{x}}_e, \hat{\mathbf{y}}_e, \hat{\mathbf{z}}_e)$

to the galactic frame $(\hat{\mathbf{x}}_g, \hat{\mathbf{y}}_g, \hat{\mathbf{z}}_g)$ is given by [109]:

$$\begin{aligned}\hat{\mathbf{x}}_g &= \hat{\mathbf{x}}_e (-0.06699) + \hat{\mathbf{y}}_e (-0.8728) + \hat{\mathbf{z}}_e (-0.4835), \\ \hat{\mathbf{y}}_g &= \hat{\mathbf{x}}_e (0.4927) + \hat{\mathbf{y}}_e (-0.4503) + \hat{\mathbf{z}}_e (0.7446), \\ \hat{\mathbf{z}}_g &= \hat{\mathbf{x}}_e (-0.8676) + \hat{\mathbf{y}}_e (-0.1883) + \hat{\mathbf{z}}_e (0.4602).\end{aligned}\tag{F.9}$$

The transformation from the galactic frame to the equatorial frame is given by

$$\begin{aligned}\hat{\mathbf{x}}_e &= \hat{\mathbf{x}}_g (-0.06699) + \hat{\mathbf{y}}_g (0.4927) + \hat{\mathbf{z}}_g (-0.8676), \\ \hat{\mathbf{y}}_e &= \hat{\mathbf{x}}_g (-0.8728) + \hat{\mathbf{y}}_g (-0.4503) + \hat{\mathbf{z}}_g (-0.1884), \\ \hat{\mathbf{z}}_e &= \hat{\mathbf{x}}_g (-0.4835) + \hat{\mathbf{y}}_g (0.7446) + \hat{\mathbf{z}}_g (0.4602).\end{aligned}\tag{F.10}$$

The change of Eqs. F.9 and F.10 from the epoch of January 1950.0 to 25 September 2010 is small and would not affect the final results in Chapter 7.

APPENDIX G

Laboratory motion

The velocity of the lab with respect to the center of the Galaxy can be divided into four components (as in Eq. 7.9): $\mathbf{V}_{\text{GalRot}}$, $\mathbf{V}_{\text{Solar}}$, $\mathbf{V}_{\text{EarthRev}}$ and $\mathbf{V}_{\text{EarthRot}}$.

We take $V_{\text{GalRot}} = 220 \text{ km/s}$ or 280 km/s [95], $V_{\text{Solar}} = 18 \text{ km/s}$ [110], $V_{\text{EarthRev}} = 29.8 \text{ km/s}$ and $V_{\text{EarthRot}} = (0.465102 \text{ km/s}) \cos \lambda_{\text{lab}}$, where λ_{lab} is the latitude of the lab. Values of $V_{\text{GalRot}} = 220 \text{ km/s}$ or 280 km/s results in $V_{\text{lab}} = 228.4 \text{ km/s}$ or 288.3 km/s , respectively (see Appendix F.5 for the equation of $\mathbf{V}_{\text{lab}}$). Thus, $\mathbf{V}_{\text{lab}}$ is dominated by the galactic rotation velocity.

We need to compute $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}$, where $\hat{\mathbf{q}}$ is given in the crystal reference frame ($\hat{\mathbf{q}} = q_X \hat{\mathbf{X}} + q_Y \hat{\mathbf{Y}} + q_Z \hat{\mathbf{Z}}$). Therefore, we need to also write $\mathbf{V}_{\text{lab}}$ in the crystal frame. We have,

$$\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}} = \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{GalRot}} + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{Solar}} + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRev}} + \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRot}}. \quad (\text{G.1})$$

We will compute each term on the right-hand side of Eq. G.1 individually.

G.1 Galactic rotation

The velocity of the galactic rotation $\mathbf{V}_{\text{GalRot}}$ is defined in the galactic reference frame,

$$\mathbf{V}_{\text{GalRot}} = V_{\text{GalRot}} \hat{\mathbf{y}}_g, \quad (\text{G.2})$$

where V_{GalRot} is the galactic rotation speed (i.e. the local circular speed), and $\hat{\mathbf{y}}_g$ is in the direction of the galactic rotation. Following Ref. [95], we take $V_{\text{GalRot}} = 220 \text{ km/s}$ or 280 km/s . Using the conversions in Eq. F.9, we can write $\hat{\mathbf{y}}_g$ in the equatorial reference frame in terms of $(\hat{\mathbf{x}}_e, \hat{\mathbf{y}}_e, \hat{\mathbf{z}}_e)$. Then, we use Eq. F.7 to transform from the equatorial frame to the lab

frame $(\hat{\mathcal{N}}, \hat{\mathcal{W}}, \hat{\mathcal{Z}})$, and finally we use Eq. F.3 to transform from the lab frame to the crystal frame $(\hat{\mathbf{X}}, \hat{\mathbf{Y}}, \hat{\mathbf{Z}})$.

Thus, we can use Eq. F.3 to write $\mathbf{V}_{\text{GalRot}}$ in terms of the crystal frame coordinates, and compute $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{GalRot}}$,

$$\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{GalRot}} = q_X V_{\text{GalRot},X} + q_Y V_{\text{GalRot},Y} + q_Z V_{\text{GalRot},Z}. \quad (\text{G.3})$$

We have

$$\begin{aligned} \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{GalRot}} = V_{\text{GalRot}} & \left\{ \left([-0.4927 \cos(t_{\text{lab}}^\circ) + 0.4503 \sin(t_{\text{lab}}^\circ)] \sin(\lambda_{\text{lab}}) \right. \right. \\ & + 0.7446 \cos(\lambda_{\text{lab}}) \Big) (\alpha_X q_X + \alpha_Y q_Y + \alpha_Z q_Z) + \left(0.4927 \sin(t_{\text{lab}}^\circ) \right. \\ & + 0.4503 \cos(t_{\text{lab}}^\circ) \Big) (\beta_X q_X + \beta_Y q_Y + \beta_Z q_Z) + \left([0.4927 \cos(t_{\text{lab}}^\circ) \right. \\ & - 0.4503 \sin(t_{\text{lab}}^\circ)] \cos(\lambda_{\text{lab}}) + 0.7446 \sin(\lambda_{\text{lab}}) \Big) \\ & \left. \left. (\gamma_X q_X + \gamma_Y q_Y + \gamma_Z q_Z) \right\}. \end{aligned} \quad (\text{G.4})$$

Eq. G.4 has a time dependence through t_{lab}° and would be responsible for any daily modulation in the rate.

G.2 Solar motion

The velocity of the Sun's motion in the galactic rest frame is,

$$\mathbf{V}_{\text{Solar}} = U \hat{\mathbf{x}}_g + V \hat{\mathbf{y}}_g + W \hat{\mathbf{z}}_g, \quad (\text{G.5})$$

where $(U, V, W)_\odot = (11.1, 12.2, 7.3)$ km/s [110]. Using Eq. F.9, we can transform from the galactic frame to the equatorial frame, and using Eq. F.7 we can transform from the equatorial frame to the lab frame. Then we can use Eq. F.3 to write $\mathbf{V}_{\text{Solar}}$ in terms of the crystal frame coordinates.

Thus, we can compute $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{Solar}}$ as

$$\begin{aligned}
\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{Solar}} = & \left([(1.066 \text{ km/s}) \cos(t_{\text{lab}}^\circ) + (16.56 \text{ km/s}) \sin(t_{\text{lab}}^\circ)] \sin(\lambda_{\text{lab}}) \right. \\
& \left. + (7.077 \text{ km/s}) \cos(\lambda_{\text{lab}}) \right) (\alpha_X q_X + \alpha_Y q_Y + \alpha_Z q_Z) \\
& + \left(-(1.066 \text{ km/s}) \sin(t_{\text{lab}}^\circ) + (16.56 \text{ km/s}) \cos(t_{\text{lab}}^\circ) \right) \\
& (\beta_X q_X + \beta_Y q_Y + \beta_Z q_Z) + \left(-[(1.066 \text{ km/s}) \cos(t_{\text{lab}}^\circ) \right. \\
& \left. + (16.56 \text{ km/s}) \sin(t_{\text{lab}}^\circ)] \cos(\lambda_{\text{lab}}) + (7.077 \text{ km/s}) \sin(\lambda_{\text{lab}}) \right) \\
& (\gamma_X q_X + \gamma_Y q_Y + \gamma_Z q_Z). \tag{G.6}
\end{aligned}$$

Clearly, Eq. G.6 has a time dependence through t_{lab}° and would be responsible of any daily modulation in the rate.

G.3 Earth's revolution

The velocity of the Earth's revolution around the sun is given in terms of the Sun ecliptic longitude λ as [111]

$$\begin{aligned}
\mathbf{V}_{\text{EarthRev}} = & V_\oplus(\lambda) [\cos \beta(x) \sin(\lambda - \lambda_x) \hat{\mathbf{x}}_g \\
& + \cos \beta(y) \sin(\lambda - \lambda_y) \hat{\mathbf{y}}_g + \cos \beta(z) \sin(\lambda - \lambda_z) \hat{\mathbf{z}}_g], \tag{G.7}
\end{aligned}$$

where $V_\oplus = 29.8 \text{ km/s}$ is the orbital speed of the Earth, $V_\oplus(\lambda) = V_\oplus[1 - e \sin(\lambda - \lambda_0)]$, $e = 0.016722$, and $\lambda_0 = 13^\circ + 1^\circ$ are the ellipticity of the Earth's orbit and the ecliptic longitude of the orbit's minor axis, respectively, and $\beta_i = (-5^\circ.5303, 59^\circ.575, 29^\circ.812)$ and $\lambda_i = (266^\circ.141, -13^\circ.3485, 179^\circ.3212)$ are the ecliptic latitudes and longitudes of the $(\hat{\mathbf{x}}_g, \hat{\mathbf{y}}_g, \hat{\mathbf{z}}_g)$ axes, respectively.

The Sun's ecliptic longitude λ can be expressed as (p. 77 of Ref. [112] and Ref. [111]),

$$\lambda = L + (1^\circ.915 - 0^\circ.0048T_0) \sin g + 0^\circ.020 \sin 2g, \tag{G.8}$$

where $L = 281^\circ.0298 + 36000^\circ.77T_0 + 0^\circ.04107UT$ is the mean longitude of the Sun corrected

for aberration, $g = 357^\circ.9258 + 35999^\circ.05T_0 + 0^\circ.04107UT$ is the mean anomaly (polar angle of orbit).

Using Eq. F.9, we can transform from the galactic frame to the equatorial frame, and using Eq. F.7 we can transform from the equatorial frame to the lab frame ($\hat{\mathcal{N}}, \hat{\mathcal{W}}, \hat{\mathcal{Z}}$). Then we can use Eq. F.3 to write $\mathbf{V}_{\text{Solar}}$ in terms of the crystal frame coordinates.

Thus, we can compute $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRev}}$ as

$$\begin{aligned} \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRev}} = V_{\oplus}(\lambda) & \left\{ \left[-\cos(t_{\text{lab}}^\circ) \sin(\lambda_{\text{lab}}) \mathcal{A} - \sin(t_{\text{lab}}^\circ) \sin(\lambda_{\text{lab}}) \mathcal{B} \right. \right. \\ & + \cos(\lambda_{\text{lab}}) \mathcal{C} \left. \right] (\alpha_X q_X + \alpha_Y q_Y + \alpha_Z q_Z) \\ & + \left[\sin(t_{\text{lab}}^\circ) \mathcal{A} - \cos(t_{\text{lab}}^\circ) \mathcal{B} \right] (\beta_X q_X + \beta_Y q_Y + \beta_Z q_Z) \\ & + \left[\cos(t_{\text{lab}}^\circ) \cos(\lambda_{\text{lab}}) \mathcal{A} + \sin(t_{\text{lab}}^\circ) \cos(\lambda_{\text{lab}}) \mathcal{B} \right. \\ & \left. \left. + \sin(\lambda_{\text{lab}}) \mathcal{C} \right] (\gamma_X q_X + \gamma_Y q_Y + \gamma_Z q_Z) \right\}, \end{aligned} \quad (\text{G.9})$$

where

$$\begin{aligned} \mathcal{A} &= (-0.06699) \cos \beta(x) \sin(\lambda - \lambda_x) + (0.4927) \cos \beta(y) \sin(\lambda - \lambda_y) \\ &+ (-0.8676) \cos \beta(z) \sin(\lambda - \lambda_z), \\ \mathcal{B} &= (-0.8728) \cos \beta(x) \sin(\lambda - \lambda_x) + (-0.4503) \cos \beta(y) \sin(\lambda - \lambda_y) \\ &+ (-0.1883) \cos \beta(z) \sin(\lambda - \lambda_z), \\ \mathcal{C} &= (-0.4835) \cos \beta(x) \sin(\lambda - \lambda_x) + (0.7446) \cos \beta(y) \sin(\lambda - \lambda_y) \\ &+ (0.4602) \cos \beta(z) \sin(\lambda - \lambda_z). \end{aligned} \quad (\text{G.10})$$

Eq. G.9 has a time dependence through t_{lab}° and λ and would be responsible for any daily modulation in the rate.

G.4 Earth's rotation

Finally, we want to compute $\mathbf{V}_{\text{EarthRot}}$, the velocity of Earth's rotation around itself. We have

$$\mathbf{V}_{\text{EarthRot}} = -V_{\text{RotEq}} \cos \lambda_{\text{lab}} \hat{\mathcal{W}}, \quad (\text{G.11})$$

where V_{RotEq} is the Earth's rotation speed at the equator, and is defined as $V_{\text{RotEq}} = 2\pi R_{\oplus}/(1 \text{ sidereal day})$. The Earth's equatorial radius is $R_{\oplus} = 6378.137 \text{ km}$, and one sidereal day is $23.9344696 \text{ hr} = 86164 \text{ s}$. therefore $V_{\text{RotEq}} = 0.465102 \text{ km/s}$.

Using Eq. F.3 to write $\hat{\mathcal{W}}$ in terms of the crystal frame coordinates, we can easily find $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRot}}$ as

$$\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{EarthRot}} = -V_{\text{RotEq}} \cos \lambda_{\text{lab}} (\beta_X q_X + \beta_Y q_Y + \beta_Z q_Z). \quad (\text{G.12})$$

There is no time dependence in Eq. G.12, because it is written in the crystal frame, and both the lab and the crystal are rotating with the Earth.

G.5 Total Velocity

Now we can insert Eqs. G.4, G.6, G.9 and G.12 into Eq. G.1 to compute $\hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}}$. Inserting the values of $V_{\oplus} = 29.8 \text{ km/s}$, $\epsilon = 23.439^\circ$ and $V_{\text{RotEq}} = 0.465 \text{ km/s}$, we have (in km/s):

$$\begin{aligned} \hat{\mathbf{q}} \cdot \mathbf{V}_{\text{lab}} = & \left\{ \left[-\cos(t_{\text{lab}}^\circ) A + \sin(t_{\text{lab}}^\circ) B \right] \sin \lambda_{\text{lab}} + C \cos \lambda_{\text{lab}} \right\} \\ & (\alpha_X q_X + \alpha_Y q_Y + \alpha_Z q_Z) + \left\{ \sin(t_{\text{lab}}^\circ) A + \cos(t_{\text{lab}}^\circ) B \right. \\ & \left. - 0.465 \cos \lambda_{\text{lab}} \right\} (\beta_X q_X + \beta_Y q_Y + \beta_Z q_Z) + \left\{ \left[\cos(t_{\text{lab}}^\circ) A \right. \right. \\ & \left. \left. - \sin(t_{\text{lab}}^\circ) B \right] \cos \lambda_{\text{lab}} + C \sin \lambda_{\text{lab}} \right\} (\gamma_X q_X + \gamma_Y q_Y + \gamma_Z q_Z), \end{aligned} \quad (\text{G.13})$$

where

$$\begin{aligned} A &= 0.4927 V_{\text{GalRot}} - 1.066 \text{ km/s} + V_{\oplus}(\lambda) \mathcal{A}, \\ B &= 0.4503 V_{\text{GalRot}} + 16.56 \text{ km/s} - V_{\oplus}(\lambda) \mathcal{B}, \\ C &= 0.7445 V_{\text{GalRot}} + 7.077 \text{ km/s} + V_{\oplus}(\lambda) \mathcal{C}. \end{aligned} \quad (\text{G.14})$$

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