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COMPUTER SIMULATION OF CHANNELLING MEASUREMENTS ON V_3Si SINGLE CRYSTALS

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A computer program has been developed to simulate the channelling process of He-ions in V_3Si with A15 crystal structure. The program considers the anisotropy of the thermal vibrations of the V-atoms and takes into account the interactions of an ion with all neighboured atoms in a plane. Angular scan curves through the [100]- and the [110]-channelling directions in the V- and the Si-sublattices are calculated with this computer program and found to be in good agreement with measured values. Calculated depth dependences of the critical angle and the minimum yield are in reasonable agreement with the measured results. Analytical treatments have also been applied but fail to describe the measured data.

1 INTRODUCTION

Channelling measurements on single crystals in connection with close encounter processes such as Rutherford large angle scattering, nuclear reactions and ion induced x-rays are widely used as a valuable tool for the study of impurities on regular lattice sites in crystals[1] and for the analysis of defect structures.[2] The analysis of such experiments is usually based on the following theoretical treatments:

a) an analytical treatment based on the continuum model[3]

b) a statistical analysis of ion trajectories generated by computer simulation based on the binary collision model[4,5,6]

c) empirical formulas derived as fits to computer calculations[5]

d) empirical formulas as mentioned in c) extended to the analysis of channelling results in compound crystals, where the mutual influence of neighbouring parallel atomic rows composed of atoms having large differences in atomic numbers has been taken into account by replacing the single row potential by a multi-row potential.[7]

The treatment as discussed in d) improves the analysis of channelling data for simple compound structures. With increasing crystal complexity the potential distribution and therefore the flux profile is in general no longer rotationally symmetric about the minimum potential energy. A detailed knowledge of the flux profile however is required for the quantitative analysis of channelling results. Therefore a computer simulation is expected to be the best solution for the simulation of channelling measurements in complex structures such as V_3Si.

The interest on channelling data of V_3Si is of different origin. Firstly, V_3Si is one of the well-known superconducting compounds with A15-structure. Compounds with this structure reveal the highest superconducting transition temperature, T_c, known up to now (Nb_3Ge with a T_c of 23 K[8]). T_c is related to the linear chain structure of transition metal atoms and is found to decrease strongly with an increasing number of defects produced by particle irradiation. The defect structure responsible for the drastic decrease of T_c has been explained by small atomic displacements with amplitudes of the order of 0.1 Å as judged from channelling measurements.[9–11] Therefore a more reliable quantitative analysis of the experimental data by computer simulation seems to be justified.

Secondly it is known from x-ray measurements[12] that the mean vibration amplitude of the V-atoms perpendicular to the chain is larger than parallel to the chain. This feature offers an interesting test possibility for the sensitivity of the channelling technique. Here a reliable simulation of this case can only be obtained with computer calculations.

In the following results from a computer calculation are compared with measured angular yield curves through the [100]- and [110]-channelling directions in V_3Si as a function of depth. Here the

experimental curves for the rows of V-atoms were obtained by elastic scattering of He-ions and those for the rows of Si-atoms by the $^{28}Si(d,p)\ ^{29}Si$-reaction. These results have already been analyzed previously[13] using the theoretical treatment described shortly under d) above. Large discrepancies between measured and calculated minimum yield values for the [100]-channelling direction indicated, that this analytical treatment is not satisfactory for the analysis of channelling data of crystals with A15-structure.

2 DESCRIPTION OF COMPUTER SIMULATION CALCULATIONS

The computer calculations are based on a program originally developed for the analysis of interstitial lattice sites for deuterium in niobium.[6] This program has been modified for a more convenient application to complex crystal structures especially for the A15-structure. Backscattering aligned and random spectra can be calculated. Different defect structure models can be inserted and the influence on backscattered spectra can directly be investigated. Results of an application to defect analysis in V_3Si will be discussed in a forthcoming paper.

The program has some features common with similar computer programs: the elastic interaction between incident ions and the lattice atoms is treated as series of independent binary collisions. For the calculation of the deflection at each interaction the classical scattering theory in momentum approximation is used.[14] The Molière-approximation[20] to the Thomas–Fermi potential has been used as scattering potential. The electronic energy loss is calculated from an impact-parameter-dependent term due to collisions with closed-shell electrons and from a constant part. This second contribution is due to collisions with valence electrons which are treated to be equally spread over the lattice, and to plasma excitations.[15] The energy loss due to nuclear interaction can be neglected, since the ion energies are in the MeV-region. The mean squared angular spread of the channelled beam due to multiple scattering from electrons, directly proportional to the inelastic energy loss rate,[16] has also been included in the program. Plasmon excitations are excluded from this energy loss term as they do not alter the transverse momentum of the particles. The influence of an amorphous surface layer on the divergence of the beam can also be simulated by choosing the transverse momentum of the starting ion from a Gaussian distribution.

Crystals of the type A_3B with A15-structure belong to the space group $P4_2/m\bar{3}2/n$ where the A-atoms occupy the following lattice positions: $(\frac{1}{4}, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{4}, 0; 0, \frac{1}{2}, \frac{1}{4}; \frac{3}{4}, 0, \frac{1}{2}; \frac{1}{2}, \frac{3}{4}, 0; 0, \frac{1}{2}, \frac{3}{4})$. The B atoms occupy the following sites: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Channelling experiments have been performed with 2 MeV ^{4}He-ions along the [100]- and [110]-directions. For simulation the unit cell is divided into slices perpendicular to the desired channelling directions in correspondence to the different atomic planes (Figure 1). For the [100]-direction the scattering cell chosen is a cubic cell with four lattice

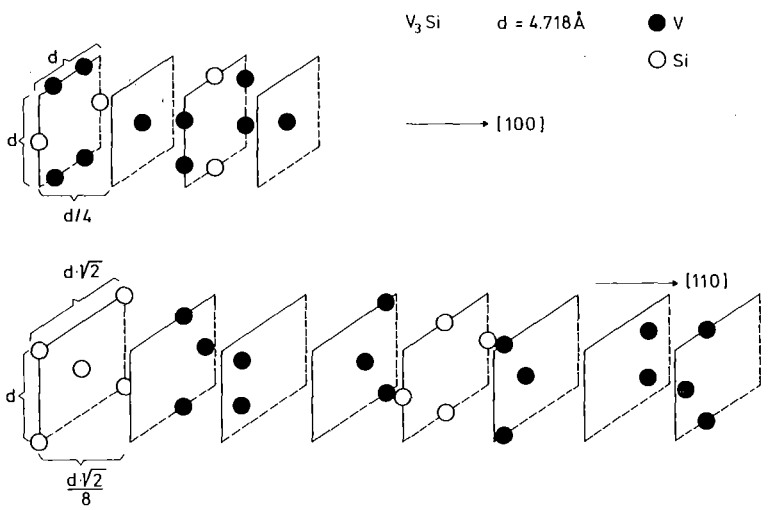

FIGURE 1 Scattering cells for the [100]- and the [110]-channelling directions in V_3Si sectionalized in isolated atomic planes.

planes at distances of $d/4$, with a lattice parameter d = 4.718 Å. For the [110]-channelling direction a parallelepiped has been chosen which contains the cubic unit cell. Here 8 lattice planes at a distance of $d\sqrt{2}/8$ must be considered. The first lattice plane is divided into 400 squares for the [100] and into 432 squares for the [110] channelling direction. The centers of the squares are taken as the starting points of the ions with fixed energy and momentum. The particle trajectories are then evaluated by calculating the deflection in this plane and by averaging the energy loss over the slice thickness.

Assuming that the deflection takes place immediately in the planes and that the ions move linearly between two scattering events, the entrance coordinates for the next atomic plane are determined. Normally the binary collision model considers only one interaction at one time. In complicated structures however, like for V_3Si, several atoms in a plane may influence the deflection. Therefore, the deflection angles from interactions with all atoms in one plane neighboured to the ion have been calculated sequentially and the total deflection angle is determined by adding the single contributions. If the ion leaves the scattering cell laterally, then the ion coordinates are transformed back by one lattice parameter, causing the ion to stay in the cell. The energy of the ions is reduced due to the energy loss mechanisms mentioned above and the transverse components of momentum are spread due to electronic dispersion.

Thermal vibrations of the V- and Si-atoms are simulated by random numbers from a Gaussian distribution. It is essential to note that the V-atoms do not vibrate isotropically.[12] In this case, the vibrations of the atoms are characterized by a symmetric tensor[17] and it can be shown that the probability $W(\mathbf{u}^{\bar{r}})$ for an atom to be located on a certain position $\mathbf{u}^{\bar{r}} = (u_1, u_2, u_3)$ is represented by a product of three Gaussian distributions:

$$W(\mathbf{u}^r) = \frac{1}{\sqrt{2\pi u_{11}}} \exp\{-u_1^2/2u_{11}\} \frac{1}{\sqrt{2\pi u_{22}}} \times \exp\{-u_2^2/2u_{22}\} \frac{1}{\sqrt{2\pi u_{33}}} \exp\{-u_3^2/2u_{33}\}$$

In the program an ellipsoid of revolution with $u_{11} \neq u_{22} = u_{33}$ is considered for the V-atoms, whereas an isotropic distribution is assumed for the Si-atoms.

During channelling measurements in combination with Rutherford backscattering the number of backscattered particles is registered as function of energy. In order to calculate the probability of a backscattering event, the Rutherford cross section (at particle energy E and at a momentaneous angle between particle direction and particle detector times the solid angle of the detector) is multiplied by the probability density for a lattice atom at the position of each interaction. These backscattering probabilities are stored and accumulated in the corresponding energy and depth regions. The backscattering spectra are obtained by summing all calculated backscattering probabilities and by normalizing to the number of ions used in the experiment. The energy loss of backscattered particles on their way out via a random direction in the V_3Si-crystal to the detector has been calculated using a polynominal of fifth order.[18]

The calculation of the statistical error for the spectra is based on the number of ions that actually contribute to the backscattering during simulation. The number of backscattering events H per channel is given by $H = \delta E_1 (dE/dx)^{-1} d^{-1} n_0 F_s F_0^{-1}$ where δE_1 = energy/channel, d = lattice parameter, n_0 = number of particles used during simulation, F_s = effective impact area = $12\pi\langle u^2\rangle$ (if the Gaussian distribution is replaced by a rectangular distribution) and $F_0 = 4d^2$ in [100]. Averaging over $w = 16$ channels the statistical error is $\Delta H_w/H_w = \sqrt{w \cdot H}/w \cdot H$ = 7% for the random value of an angular scan curve. The statistical error under proper channelling conditions has been estimated from the registered random values and is about 50%.

3 COMPARISON WITH EXPERIMENT

Prior to the application of the program to the complicated A15-structure it was tested for the *bcc*-structure. Calculated angular scans through the [100]-channelling direction in V- and Mo-single crystals at depths of 400, 1300 and 2000 Å and for 2 MeV He-ions have been found in reasonable agreement with measured values.[21] The total energy loss as calculated from the formulae[15] used in the program for random incidence is in good agreement with measured values.[18] Random spectra were calculated by tilting the incident beam 15° off the [100]-channelling direction and by rotating the tilt plane by $\pi/2$ during acquisition. The main source of discrepancies between theoretical and measured angular scan curves is due to undefined tilt planes during experiment. From these results it is concluded that the channelling effect is reasonably

described by the models for the physical processes used in the program.

In order to simulate the channelling experiments for He-ions and deuterons in V_3Si, the following thermal vibration amplitudes as determined from x-ray measurements[12] were used: for $V\sqrt{u_{22}} = \sqrt{u_{33}} = 0.076$ Å and $\sqrt{u_{11}} = 0.067$ Å and for Si $\sqrt{\langle u^2 \rangle} = 0.075$ Å.

The spatial distribution of the channelling ions is known to be quite different from the uniform distribution of random incident particles. As an example for this effect Figure 2 shows calculated flux profiles for He-ions at various depths. The profiles are registered along the diagonals of the scattering planes in the [100]-direction. Each profile contains an average over 100 unit cells and is normalized to the total number of particles per unit area. As expected, the flux is zero at the position of the V-row in the middle of the [100]-scattering cell (Figure 1). The maximum of the flux profiles are about 1.5 Å displaced from the centre row. The relative flux minima at a distance of about 2.5 Å are due to saddle points of the potential caused by neighboured Si- and V-atoms. At the corner of the scattering cell the flux has a relative maximum according to the potential minimum here, which is however not as deep as that in the proper channel. It is seen that peaks in the spatial distribution have already been developed at a depth of 1180 Å, and statistical equilibrium is reached first at a depth of about 3000 Å.

Another result, the energy peaking effect, which is always combined with the flux peaking effect is shown in Figure 3. The energy distributions are registered under the same condition as described for the spatial distributions. It is seen that the energy

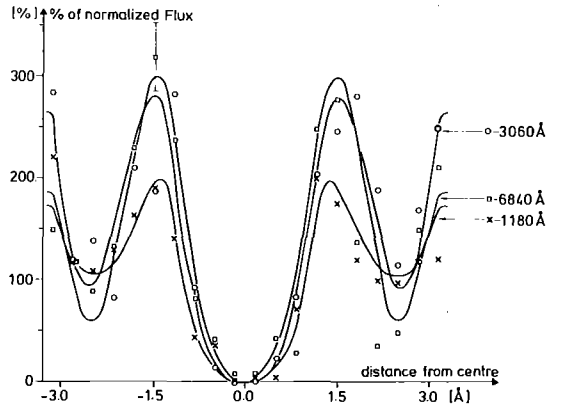

FIGURE 2 Flux profiles of channelled ^{4}He-ions at various depth. Spatial distributions are presented as registered along the diagonals of the scattering planes in the [100]-direction.

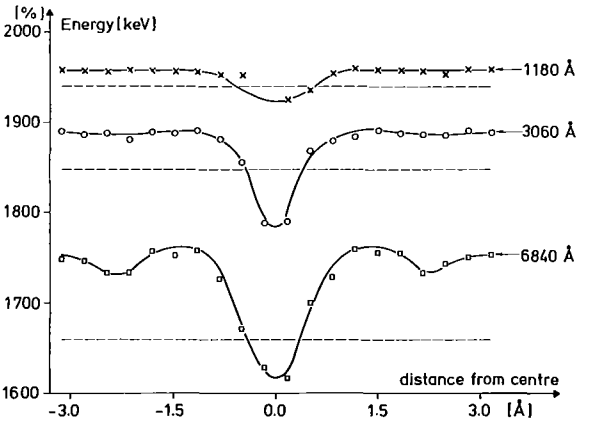

FIGURE 3 Energy distributions at various depth as registered along the diagonals of the scattering planes in the [100]-direction.

profile has a sharp minimum at the position of the V-row in the middle of the scattering cell and two minima at about 2.5 Å from the centre row which are mainly developed at greater depth.

This phenomenon can easily be understood if one takes into account the trajectory-dependent term of the electronic energy loss: ions moving very close to the lattice atoms are additionally slowed down by collisions with closed shell electrons, whereas for particles moving in the centre of a channel this contribution can be neglected. Thus the latter have higher kinetic energies compared to those moving near atomic rows. It is notable that for greater depths an increasing energy loss is observed in the region of the potential saddle points. This is due to an enhanced influence of core electrons between close lying atoms.

The primary object of this investigation was to compare calculated angular yield curves with measured data. The minimum yield in the angular scan normalized to the random yield, χ_{min}, and the critical angle, $\psi_{1/2}$, which is the half-angular width at half height between the minimum yield and the random yield are to be determined from calculated angular yield curves as a function of depth and should also be compared to measured data. Additionally the influence of the tilt plane on the shape of the angular scan curves should be explored since this effect is a well-known source of discrepancies between theory and experiment.

Therefore angular scan curves have been calculated for different tilt planes. Even in the worst case when the tilt plane coincided with a planar channel, $\psi_{1/2}$ was still measurable and showed a maximum deviation of only about 0.03° from values

measured for other tilt planes. For other tilt planes no deviations have been found within the accuracy of the calculations which is about 0.02°. The reason for this surprising result is thought to be due to the rather low symmetry of the A15-structure which does not allow the formation of pronounced lateral focusing effects on the ion trajectories.[19] The channel is limited by rather high potentials at the saddle points. In the calculation and in the experiment the tilt planes chosen were 30° against the horizontal for the [100)-direction and 5° for the [100]-direction, respectively.

As mentioned in Chapter 2 the original binary collision model was replaced here by considering the interactions of the He-ions with all neighbouring atoms in one plane. In order to examine the influence of this effect, calculations have been performed considering the interaction of the He-ions with only one nearest neighbour atom in a plane. As a result $\psi_{1/2}$ was found to increase by 0.03° and χ_{min} by 0.005. This clearly demonstrates that the influence of other neighboured atoms on the particle trajectories can not be neglected in the A15-structure.

Angular scan measurements through the [100]- and [110]-channelling directions for the V-rows were performed by using 2 MeV He-particles elastically scattered from V-atoms and well separated in energy from those scattered from Si-atoms.[13] The calculated angular scan curves together with the measured values are shown in Figure 4. The agreement between theory and experiment at $\psi_{1/2}$ is within 0.02°. For the [100]-direction the theoretical curve is steeper than the experimental values at tilt angles above 0.8°. For the [110]-direction the theoretical curve is slightly above the measured values for tilt angles below 0.4°. This deviation is however within the statistical accuracy of both the calculated and measured values.

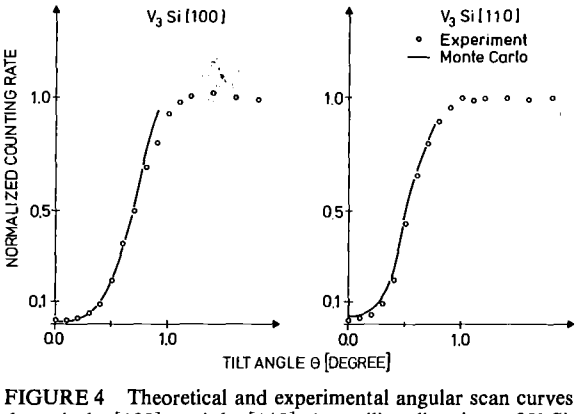

FIGURE 4 Theoretical and experimental angular scan curves through the [100]- and the [110]-channelling directions of V_3Si. The He-ions are scattered from V-atoms at a depth of 470 ± 250 Å.

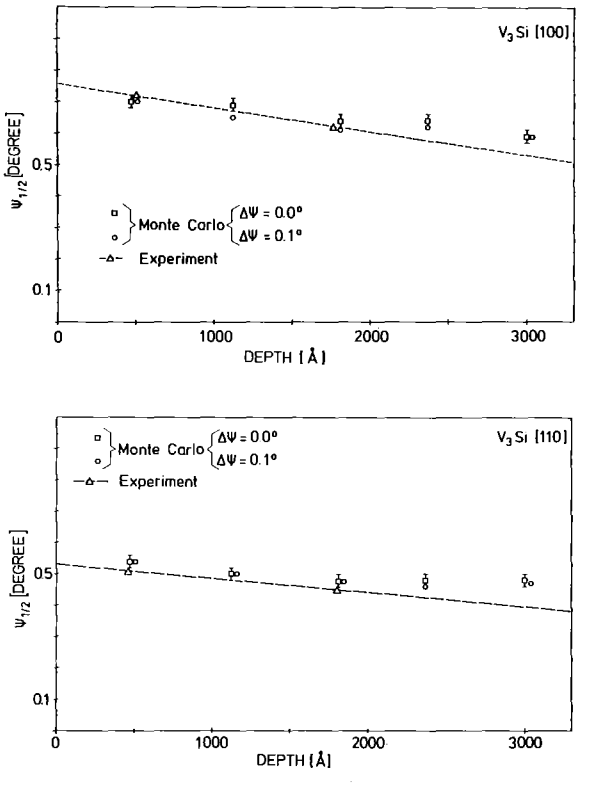

FIGURE 5 Depth dependence of calculated and measured critical angles, $\psi_{1/2}$, for the [100]- and the [110]-channelling directions (Figure 5a and Figure 5b respectively). As a parameter, the beam divergence of the incident beam has been varied. With a divergence of 0.1° the influence of a 20 Å thick amorphous surface layer on $\psi_{1/2}$ is simulated.

Calculated and measured $\psi_{1/2}$-values as a function of depth are shown for the [100]-direction in Figure 5a and for the [110]-direction in Figure 5b respectively. The influence of a 20 Å thick amorphous layer on the critical angle, simulated by an incident beam divergence of 0.1°, has been included in Figure 5. The agreement between simulation and experiment is up to a depth of 2000 Å within the range of statistical error. These errors were calculated by interpolation of discrete calculated normalized yield values as function of ψ. At depths below 2000 Å, the simulated values are larger than the measured ones. This discrepancy may be due to defects in the crystal which cause an enhanced increase of the transverse energy of the channelled beam and therefore an enhanced decrease of $\psi_{1/2}$. A further possible reason may be an

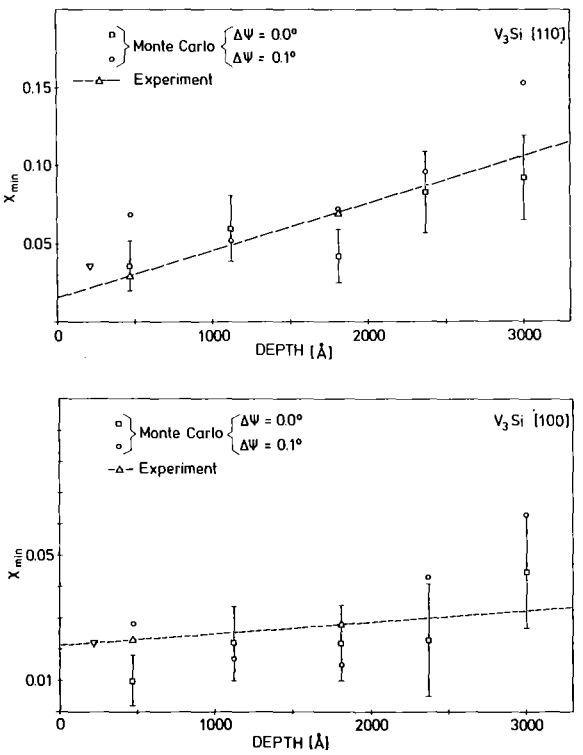

FIGURE 6 Depth dependence of calculated and measured minimum yields, χ_{min}, for the [100]- and the [110]-channelling directions (Figure 6a and Figure 6b respectively). With a beam divergence of 0.1° the influence of a 20 Å thick amorphous surface layer on $\psi_{1/2}$ is simulated. Experimental values ▽ from Ref. 10 have been included.

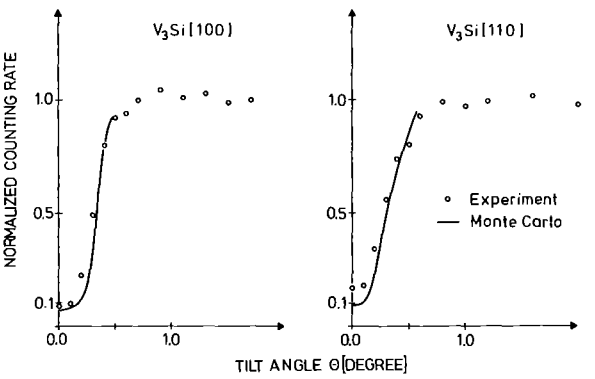

FIGURE 7 Theoretical and experimental angular scan curves through the [100]- and [110]-channelling directions. Protons from the $^{28}Si(d,p_{10})^{29}Si$-reaction have been used to measure the channelling data from the Si-rows.

enhanced beam spread caused by multiple scattering being stronger than considered in the program. It is notable in this connection that an incident beam divergence of 0.1° does not strongly affect the calculated $\psi_{1/2}$-values. This result would favour the first explanation for the deviations discussed above.

Calculated and measured χ_{min}-values as a function of depth are shown from the [100]-channelling direction in Figure 6a and for the [110]-direction in Figure 6b. χ_{min}-values have been calculated at five depth values averaged over intervals of 500 Å in correspondence to the experiment. The influence of a 20 Å thick amorphous layer simulated by an incident beam divergence of 0.1° has been included. χ_{min}-values as measured by Testardi *et al.*[10] have also been included in Figure 6. The error bars of the calculated values have been obtained as described earlier. In general, the measured depth dependences of χ_{min} are reproduced by the calculated values. The large increase of χ_{min} observed as function of depth for the [110]-channelling direction (the slope is about 3 times the slope of the [100]-direction) is reproduced by the calculated values. The large error bars of the calculated values are due to the small number of particles used for calculation. A comparison with other theoretical evaluations however can still be given and will be discussed in detail in Chapter 4. No influence of a surface layer on χ_{min} is observed within the statistical accuracy.

The $^{28}Si(d,p)^{29}Si$-reaction with an incident beam energy of 1.7 MeV was used for angular scan measurements from the Si-rows. Due to the relative small energy loss of the protons the measurements have been performed in a depth region close to the surface with a width of about 3000 Å. Angular scan curves through the [100]- and [110]-channelling directions have been calculated and compared to the measured results in Figure 7. The agreement is good for the $\psi_{1/2}$-values, however a large discrepancy is found by comparing the χ_{min}-values for the [110]-direction. If an amorphous layer of 20 Å was simulated in the calculations then the following results have been obtained: no change has been found for the $\psi_{1/2}$ [100]-value however, the value for $\psi_{1/2}$ [110] was found to decrease by 0.03°. χ_{min} [100] was found to increase from 7% to 10% and χ_{min} [110] from 9% to 12%. This result is supported by the experimental observation that low χ_{min}-values are obtained after careful surface treatment only, whereas $\psi_{1/2}$-values are less sensitive in this respect.

In the computer calculations we have used up to now an ellipsoid of revolution to describe the thermal vibrations of the V-atoms whereas the vibrations of the Si-atoms have been assumed to be isotropic. The question arises about the sensitivity of channelling measurements to detect anisotropy

effects of lattice vibration. Therefore, the ellipsoid has been replaced by a sphere using $\sqrt{\langle u^2 \rangle} = \sqrt{u_{11} + 2u_{22}/3}$. The square root of the averaged vibrational amplitude for the V-atoms then is $\sqrt{\langle u^2 \rangle} = 0.073$ Å. Using this value in the program the angular scan curves have been recalculated and the results are given in Figure 8 as dashed curves. It is seen that the $\psi_{1/2}$ [100]-value is not affected whereas the $\psi_{1/2}$ [110]-value decreased by 0.04°. A possible influence on the χ_{min}-values is within statistical errors.

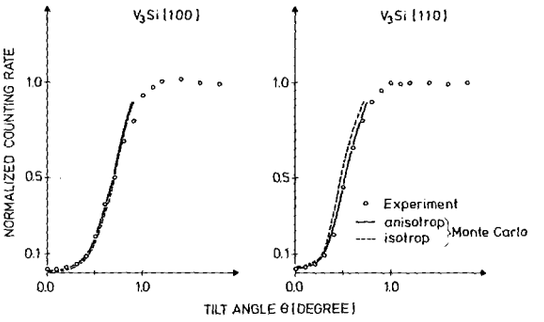

FIGURE 8 Theoretical and experimental angular scan curves through the [100]- and [110]-channelling directions. Calculations have been performed using isotropic (dashed curves) and anisotropic thermal vibration amplitudes of the V-atoms.

4 SUMMARY AND DISCUSSION

In Tables I and II the experimental values for the critical angle and the minimum yield obtained for the [100]- and the [110]—channelling directions for the V- and Si-sublattices are summarized together with the results of different analytical treatments. The experimental values have been measured at depths of 500 and 3000 Å, for the V- and Si-sublattices respectively.

Results given in column A in Table I were obtained by using a formula derived from a fit to computer calculations for tungsten with *bcc*-structure.[5] For a compound crystal with parallel rows of different scattering potentials a multirow potential has been inserted by following a treatment given in.[17] The results from such a treatment for the $\psi_{1/2}$- as well as for the χ_{min}-values are given in columns B in Tables I and II. In contrast to results reported earlier[13] the vibrational amplitudes used here are taken from x-ray results,[12] without considering anisotropy ($\sqrt{\langle u^2 \rangle}$(V) = 0.073 Å and $\sqrt{\langle u^2 \rangle}$(Si) = 0.075 Å). For the Monte-Carlo calculation results given in the columns C of Tables I and II the anisotropy has been considered for the V-atoms using values of $\sqrt{u_{11}}$(V) = 0.067 Å and $\sqrt{u_{22}}(V)$ = 0.076 Å and Si has been treated isotropically with a value of $\sqrt{\langle u^2 \rangle}$(Si) = 0.075 Å.

It is obvious from Table I that the computer calculations are in excellent agreement with the experimental results, whereas results from analytical treatments given in column A deviate by 11% and in column B by 8% from experimental values for the V-sublattices. For the Si-sublattice agreement is found between all theoretical treatments and experiment.

TABLE I

Experimental $\psi_{1/2}$-values compared to values obtained from different theoretical treatments

Experiments in V_3Si	$\psi_{1/2}^{exp}$ (degrees)	A $\psi_{1/2}^{calc}$ Barrett[5] single row pot.	B $\psi_{1/2}^{calc}$ Multi-row pot.[7]	C $\psi_{1/2}^{calc}$ Monte Carlo
V(α, α) [100] 2 MeV	0.72 ± 0.01	0.81	0.78	0.70 ± 0.02
V(α, α) [110] 2 MeV	0.52 ± 0.01	0.49	0.47	0.54 ± 0.02
Si(d, p) [100]	0.35 ± 0.01	0.35	0.35	0.36 ± 0.02
Si(d, p) [110]	0.29 ± 0.01	0.29	0.29	0.31 ± 0.02

TABLE II

Experimental and calculated χ_{min}-values

Experiments in V_3Si	χ_{min}^{exp}	B χ_{min}^{calc} Multi-row pot.[7]	C χ_{min}^{calc} Monte Carlo
V(α, α) [100] 2 MeV	0.023 ± 0.004	0.048	0.01 ± 0.008
V(α, α) [110] 2 MeV	0.028 ± 0.004	0.04	0.035 ± 0.016
Si(d, p) [100]	0.09	0.04	0.07 ± 0.013
Si(d, p) [110]	0.18	0.07	0.09 ± 0.015

The experimental $\psi_{1/2}$-values for the [100]-direction are smaller and for the [110]-direction larger than the analytical values from columns A and B. This discrepancy had been attributed to the anisotropy of the V-atom vibrations.[13] Monte-Carlo calculations did not confirm this statement. Replacing the anisotropic vibrations by an isotropic vibration amplitude in the program was found to influence mainly the $\psi_{1/2}$-value for the [110]-direction. This result is not obvious from analytical treatments A and B where it has been observed that the $\psi_{1/2}$-values in both directions responded with similar sensitivity to variations of the vibration amplitude. A possible reason for this result, which is not yet studied in detail may stem from different densities of trajectories in [100] and [110] as function of transverse energy being larger for the [110]-channelling direction. Thus the response of a close encounter probability on variations of the thermal vibration amplitude will be more sensitive in [110]-direction.

The second parameter used for comparison between theory and experiment is the minimum yield. Although the statistical error for the computer calculated values in column C is large, it can be seen from Table II that the agreement with the experimental values is superior to that of column B. The χ_{min}-values for the V-sublattice in both directions as obtained with the multi-row potential treatment (column B) are found to be larger than the experimental values. As the contribution of the Si-rows to the χ_{min}-values of the [110]-channelling direction is small and can be neglected, agreement with experiment is obtained by setting the structural dependent fit parameter C[5] equal to 2.2. However, this reduced number does not explain the total difference between theory and experiment in the [100]-direction. This may indicate that the procedure as developed to calculate χ_{min}-values for compounds[7] is not quite applicable for the A15-structure. The mutual contributions of parallel V-rows in [100] having strong and weak scattering potentials seems to be overestimated.

From the good agreement between measured and calculated angular scan curves and depth dependence of $\psi_{1/2}$ and χ_{min} it is concluded that the models for the physical processes used in the computer program are sufficient to describe the channelling process in complicated crystal structures such as the A15-structure. In contrast to the binary collision model the interactions of the ion with all neighboured atoms in one plane has to be considered. This effect probably leads to an increase of beam divergence and thus to a decrease of $\psi_{1/2}$. The influence on χ_{min} is within statistical accuracy. As already expected[5] it is not possible to apply formulae derived from fits to computer results for a certain crystal structure to other crystal structures. Some improvements in agreement between analytical and experimental results is obtained by replacing the fitted single row potential by a multi-row potential.

The influence of anisotropy in the thermal vibrations of the transition metal atom on the angular scan curves is only slightly above the limit of accuracy of current measurements and calculations. Clearly, the computer calculation is the only possible way to study this influence on the channelling process. Further improvements in program evaluation and in considering the temperature dependence of measured and calculated angular scan curves will enlighten the role of channelling measurements for the study of lattice vibrations.

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COMPUTER SIMULATION OF CHANNELING MEASUREMENTS IN He-IRRADIATED V_3Si SINGLE CRYSTALS

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A previously developed computer program has been extended to simulate the channeling process in V_3Si after irradiation at room temperature with $4 \cdot 10^{16}$ and $1.5 \cdot 10^{16}$ He/cm^2 at energies of 300 and 50 keV respectively. The best agreement with measured results in the transmission region of the ions with 300 keV was obtained by assuming an average static displacement of 0.05 Å of all V-atoms from their lattice sites. In order to study the radiation damage in the region where the 50 keV-He-ions came to rest depth profiles of defects as well as lateral profiles perpendicular to the channels have been simulated in the program. The number and the lateral distribution of the defects have been varied until the measured backscattering aligned yields in dependence of the incident beam angle could be reproduced by the calculation. By this method the assumption is preferred that about 50% of the V-atoms are displaced with a maximum displacement length of 0.5 Å.

1 INTRODUCTION

The channeling technique in combination with a close encounter process such as Rutherford backscattering is widely used for the investigations of damage depth distributions as produced by ion irradiation and implantation in materials.[1] The depth profile is obtained by comparing the normalized aligned yield from the undamaged to the normalized aligned yield from the damaged crystal. Two components contribute mainly to the aligned yield of a damaged crystal: firstly, ions from the channeled beam are directly backscattered from atoms being more than about 0.2 Å displaced from their lattice sites and secondly, ions from the channeled beam are transferred to the random beam by deflections from these displaced atoms with deflection angles larger than the critical angle. In semiconductors it has been observed that the first contribution prevails[2] whereas in metals this contribution can often be omitted in the analysis.[3] The dechanneling process in metals can be caused by structural distortions due to strain fields connected to point defect clusters.[4] The dependence of the dechanneling yield on the probing beam energy then may provide further information on the nature of these extended defects.[5] The defect distribution in transverse direction perpendicular to the channel can be explored by utilizing the angular dependence of the spatial distribution of the channeling ion flux.[6]

In the present work the lateral defect distribution produced by He-ion irradiation in V_3Si is examined. V_3Si belongs to the group of superconductors with A15-crystal structure which have the highest known superconducting transition temperatures T_c. In crystals with this structure, T_c is strongly suppressed by ion induced defects.[7,8] Channeling measurements have been performed in He-irradiated V_3Si single crystals in order to get more information on the nature of this damage structure in the transmission region.[9–11] An appreciable narrowing of the angular scan curves has been observed and was attributed to small displacements of the V-atoms from the atomic rows.[9] In order to get a more quantitative analysis of these measurements a computer simulation has been used to calculate the normalized aligned yield of the damaged crystal as a function of the incident beam angle.

Similar to semiconductors, V_3Si reveals a direct backscattering component after implantation of low energy Zr-, Kr- and He-ions.[11] The lateral distribution of displaced atoms after low energy He-ion irradiation have also been evaluated with the program.

2 COMPUTER CALCULATIONS

A Monte-Carlo-program had been developed in order to simulate channeling measurements in V_3Si with A15 structure.[12] The depth dependence of

angular scan curves as measured in V_3Si single crystals are well reproduced by this computer simulation indicating that the models of the physical processes used in the program are able to describe the channeling process in a good approximation.[12] Special features included in the program are the anisotropic thermal vibrations of the V-atoms and the consideration of the interactions between an incident ion and all neighboured atoms in one plane. The influence of an amorphous layer causing an angular spread of the incident beam can also be simulated with the program. The program calculates the backscattered aligned and random spectra which then can directly be compared with measured spectra as a function of incident beam angle.

In order to calculate the aligned backscattering spectra of a damaged crystal two parameters have been used in the program: the number of defects as a function of depth and the lateral distribution of displaced atoms perpendicular to the channel. For the depth distribution a theoretical energy deposition profile for He-ions in V_3Si was inserted.[13] The number of defects and their lateral distribution was varied until the measured aligned spectra in dependence of the incident ion beam angle have been well reproduced by the calculated spectra. This procedure has several obvious advantages as compared to analytical treatments usually used:[1] it takes into account all the details in the distribution of the channeled particles with depth such as flux peaking, flux oscillations, beam spread due to scattering from defects and the difference in specific energy loss for random and channeled particle trajectories. In the defect model it has been assumed that atoms do not change their vibrational amplitude after being displaced and that the displacements are perpendicular to the atomic rows. The influence of different tilt planes on the calculated angular yield curves are small as has been shown previously.[12]

3 COMPARISON WITH EXPERIMENT

3.1 Lateral Defect Distribution in the Transmission Region

In experiments described previously[9] disorder produced by $4 \cdot 10^{16}$ He/cm^2 at an energy of 300 keV in V_3Si had been analysed by 2 MeV He-ion channeling measurements. The He-ions penetrate a surface region of about 4000 Å with low energy loss (transmission region). The particles are stopped at a depth of approximately 6000 Å where a direct backscattering contribution from displaced V- and Si-atoms had been observed. Angular yield curves from V-rows in the [100]- as well as in the [110]-channeling direction performed in the transmission region revealed an appreciable narrowing after implantation of $4 \cdot 10^{16}$ He/cm^2 at room temperature.

As a defect model for the computer simulation it was assumed that all V-atoms are displaced from their lattice sites. The displacements have a Gaussian distribution with a rms-amplitude of 0.05 Å perpendicular to the [100] and [110] channeling directions. The results of the computer calculation are presented in Figure 1 together with the measured angular scan curves. In general the measured values are reproduced within the statistical accuracy limit of calculations and measurements.

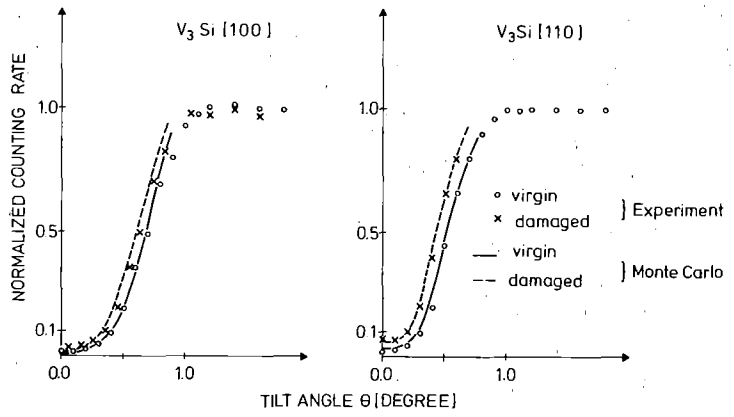

FIGURE 1 Normalized angular scan curve at 500 Å below the surface through the [100]- and the [110]-channeling directions using 2 MeV He-ions scattered from V-atoms. Results are presented prior to and after irradiation with $4 \cdot 10^{16}$ He/cm^2, 300 KeV at room temperature and are compared to calculated angular scan curves.

TABLE I

Critical angles, $\psi_{1/2}$, and minimum yields, χ_{min}, as obtained from angular scan curves through the [100]- and the [110]-channeling directions in V_3Si prior to and after an irradiation of $4 \cdot 10^{16}$ He/cm^2, 300 KeV at room temperature

	Experiment		Monte Carlo	
	χ_{min}	$\psi_{1/2}$ (degree)	χ_{min}	$\psi_{1/2}$ (degree)
[100] virgin	0.023 ± 0.004	0.72 ± 0.01	0.010 ± 0.008	0.70 ± 0.02
damaged	0.040 ± 0.005	0.64 ± 0.01	0.021 ± 0.01	0.63 ± 0.02
[110] virgin	0.026 ± 0.005	0.52 ± 0.01	0.036 ± 0.016	0.54 ± 0.02
damaged	0.065 ± 0.005	0.44 ± 0.01	0.058 ± 0.018	0.46 ± 0.02

The experimental values for the critical angles and minimum yields from the angular yield curves as obtained for the V-sublattice in [100]- and [110]-channeling direction prior to and after irradiation compared with results from the computer calculation are summarized in Table I. The agreement between measured and calculated $\psi_{1/2}$-values is within the accuracy limit whereas discrepancies are observed for the χ_{min}-values mainly in [100]-channeling direction. Here the measured values for the damaged crystal are larger than the calculated values. This is not astonishing as in the calculation only a single defect structure is considered namely small static displacements (0.05 Å) of all V-atoms from their lattice sites. Some defect clusters, however, will be produced in the transmission region by high energy recoil atoms. These extended defects will also contribute to the dechanneling rate as discussed in Ref. 11.

3.2 *Lateral Damage Profile at the End of the He-ion Range*

A direct backscattering component as observed at the end of the He-ion range indicated that a large amount of lattice atoms had been displaced with displacement amplitudes larger than about 0.2 Å. The lateral distribution of these displacements can be conveniently explored if the damage depth profile is close to the surface. Therefore $1.5 \cdot 10^{16}$ He/cm^2 with a low energy of 50 keV have been implanted in V_3Si at random direction. The He-implanted V_3Si single crystal has been analysed with 2 MeV He-particles. The random and [100]-aligned backscattering spectra prior to and after He-implantation are shown in Figure 2 together with aligned spectra of the damaged crystal for various incident angles of the probing beam. A peak is observed in the range of the implanted He-ions due to 2 MeV He-ions directly backscattered from displaced atoms. The peak area whose shape reflects the depth profile of the

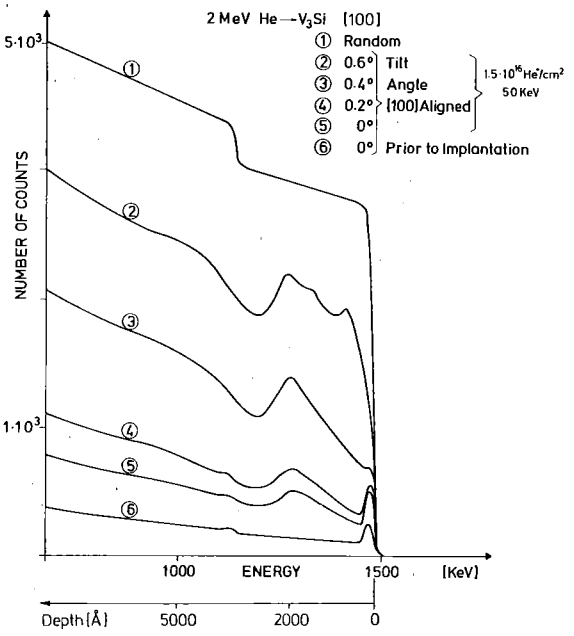

FIGURE 2 Energy spectra of 2 MeV He-ions backscattered from a V_3Si single crystal. Spectra are given for random and [100]-aligned beam incident on the virgin crystal and in dependence of the incident beam angle after implantation of $1.5 \cdot 10^{16}$ He/cm^2, 50 KeV at room temperature.

displaced atoms is a function of the tilt angle and the lateral defect distribution.[6] Increasing the transverse energy of the probing beam by increasing the angle of incidence changes the spatial distribution of the channeled beam such that the flux peak in the minimum potential decreases and the density of trajectories close to the rows increases. Thus if the main number of displaced atoms has small displacement amplitudes the direct backscattering peak area will increase with increasing angle of incidence. This is the case as can be seen in Figure 2. A quantitative analytical analysis, however, is difficult as it is necessary to know the dechanneled fraction of the

beam in order to extract the peak area. This dechanneled fraction is due to ions being scattered from displaced atoms and thus being transferred from the channeled to the random beam.

In order to simulate the measured spectra with the computer program two different models for the lateral defect distributions have been used: in a first model lattice atoms have been assumed to be randomly distributed across the channel with an amount of 10% in the maximum of the damage depth profile and in a second model lattice atoms have been assumed to be displaced according to a rectangular distribution with a width of 0.5 Å from the atomic rows with an amount of 50%. The profile used as a damage depth distribution has been calculated with a computer program from Brice.[13] The maximum of the disorder was at 2000 Å, in good agreement with the depth of the measured damage peak as shown in Figure 2.

With the first defect distribution the aligned backscattering spectra have been calculated for various angles of incidence up to a depth of 5000 Å. The results of these calculations are shown in Figure 3. The spectra at tilt angles of 0.0 and 0.2 degrees agree with the measured spectra, however, with increasing tilt angle at 0.4 degrees the calculated damage peak disappears because of the enhanced dechanneling yield. Behind the peak region the measured dechanneling curve is reproduced by the calculated curve. This result indicates that the assumption of displaced atoms being randomly distributed across the channel does not reproduce the measured results at large incident beam angles. Therefore the second model was used and the result of these calculations are

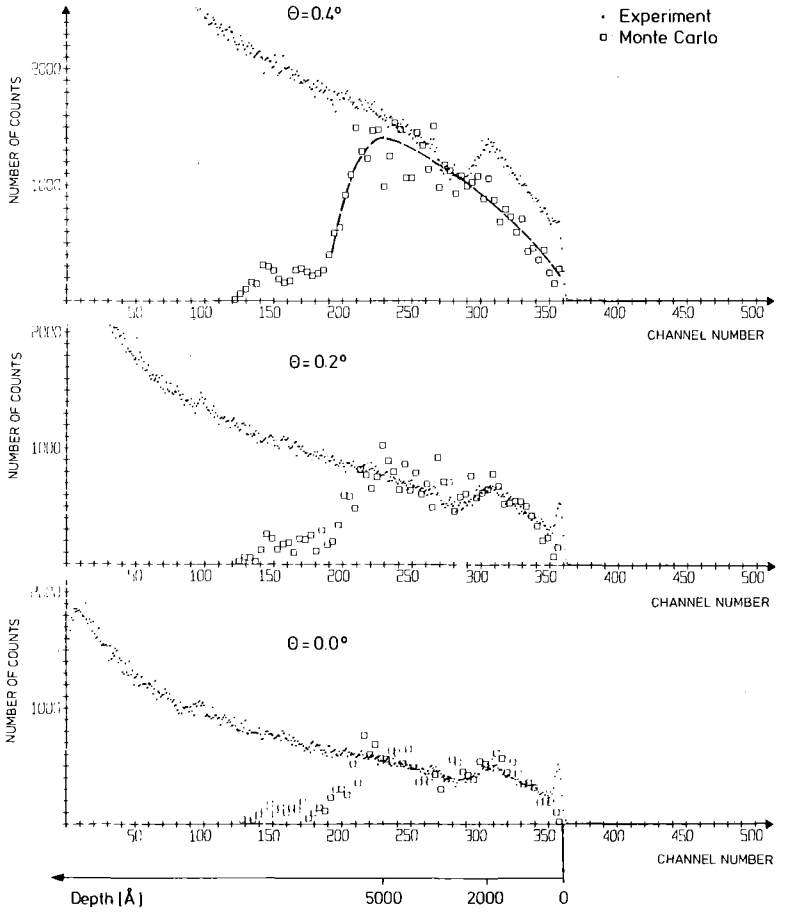

FIGURE 3 Calculated and measured aligned spectra at various tilt angles between the [100]-direction and incident beam from a V_3Si single crystal after implantation of $1.5 \cdot 10^{16}$ He/cm², 50 KeV at room temperature. As a defect model 10% displaced atoms have been assumed randomly distributed across the channel. The dashed line represents a smooth curve through the calculated results.

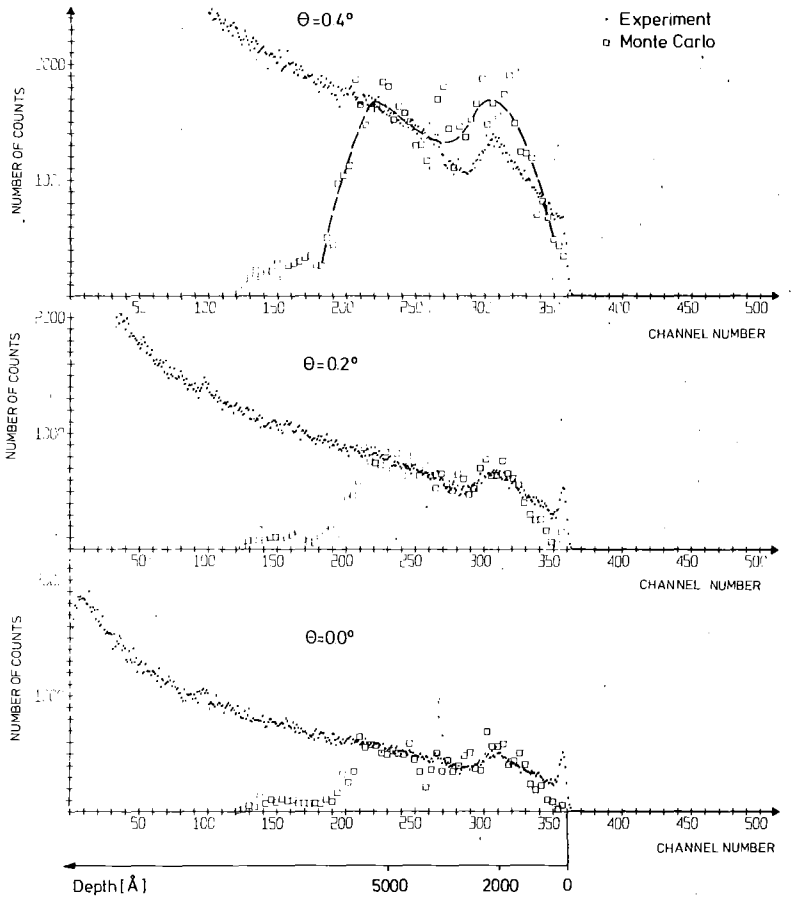

FIGURE 4 Calculated and measured aligned spectra at various tilt angles between the [100]-direction and incident beam from a V_3Si single crystal after implantation of $1.5 \cdot 10^{16}$ He/cm^2, 50 KeV at room temperature. As a defect model 50% displaced atoms have been assumed having a lateral rectangular distribution with a maximum displacement amplitude of 0.5 Å. The dashed line represents a smooth curve through the calculated results.

shown in Figure 4. At tilt angles of 0.0 and 0.2 degrees good agreement between measured and calculated spectra is achieved. The increase of the damage peak area at a tilt angle of 0.4 degrees is reproduced by the calculation. The absolute height of the calculated spectrum lies above the measured values. This is due to the fact that the lateral defect distribution model is not yet optimized in width and height. The appearance of the damage peak at larger tilt angles, however, favours the inhomogeneous lateral defect distribution assumed in this model.

4 SUMMARY

The effect of an irradiation experiment on V_3Si single crystals with $4 \cdot 10^{16}$ He/cm^2 at an energy of 300 keV has been studied in the transmission region of about 2000 Å below the surface by using the channeling method. The observed narrowing of the angular yield curves after the He-ion bombardment can be reproduced in the Monte-Carlo-simulation by inserting static displacements of the V-atoms from their lattice sites perpendicular to the channels. The displacement length was found to be 0.05 Å.

In order to study the damage caused by irradiation in the region where the ions come to rest [100]-aligned backscattering spectra from V_3Si single crystals irradiated with $1.5 \cdot 10^{16}$ He/cm^2 at an energy of 50 keV were analysed. The spectra were taken at different tilt angles and show a significant damage peak at a depth of about 2000 Å. The area under this peak is increasing with increasing tilt angle. For simulation of the channeling experiment damage profiles in depth[13] as well as in lateral

direction perpendicular to the channel were inserted into the Monte-Carlo-program. The latter were varied until the simulated spectra showed the same behaviour of the increasing peak area with increasing tilt angle as the measured ones. The resulting profile was a rectangular distribution with a width of 0.5 Å from the atomic rows. Yet the defect model is not optimized with regard to the most appropriate shape of the lateral distribution and is clearly not unique.

The results indicate the usefulness of computer simulation to analyse aligned backscattering spectra from damaged crystals with complicated crystal structures, improvements are necessary mainly in increasing statistics.

A still open question is whether there exists a continuous transition from small to large displacement lengths of the kind that with increasing ion fluence the average lateral displacement length increases.

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