CALCULATIONS OF ANGULAR DISTRIBUTIONS BACKSCATTERED PARTICLES FOR PLANAR CHANNELING FOR DIFFERENT POTENTIALS ION-PLANE

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The angular distributions for three different potentials for protons and He ions in Si, Ge, W have been calculated. The values of $\psi_{1/2}$ and $x_{\min}$ alter considerably according to the value of $V(r)$ in the region $\varrho_{\perp}$. The form of the angular distribution is influenced by the amorphous surface layer. In these cases the value of $\psi_{1/2}$ does not change but $x_{\min}$ increases as Δx approaches $B \times \Omega^2/\psi_p^2$. A comparison between calculated and experimental data is presented.

1. Introduction

In many recent experimental and theoretical studies the effect of planar channeling has been investigated to determine the critical angles, the energy losses and the minimum yield [1–8]. The interpretation of these phenomena is based on a classical theory [9], which assumes that a charged particle moving through a crystal lattice within a certain critical angle is steered by succesive collisions into coinciding with the aligned rows or planes. During its motion the particle approaches the lattice at the distance a_{TF}, i.e. the Thomas-Fermi screening distance. The experimental results agree rather well with Lindhard's predictions [9] for critical angles, but with regard to minimum yield this agreement is much worse. Picraux and Andersen [10] have calculated the angular distributions of planar channeling particles taking into account the effects of thermal vibrations. The minimum yield measured and calculated by them indicates only slight agreement. This paper shows the results of calculations for different types of average planar potentials taking adventage of the method given by Picraux and Andersen. Moreover, the effects of multiple scattering in the oxide surface layer are included.

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2. Calculation

The distribution of planar channeling particles given by Picraux and Andersen [10] is as follows:

$$P(E\psi^2) = \frac{1}{d_p}\int_0^{d_p} K(E\psi^2+V(y))Q(E\psi^2+V(y))dy,$$

where $Q(E_\perp)$ is the probability of emission of particles with the transverse energy $E_\perp (E_\perp = E\phi^2+V(y))$. This energy is conserved along the particle path. Here y and ϕ are the corresponding values of the distance from the plane and the angle of the particle velocity vector with respect to the plane.

$$Q(E_\perp) = \int_{y_{\min}}^{d_p/2} \left(\frac{E_\perp}{E_\perp - V(y)}\right)^{1/2} \left(\frac{2}{\pi}\right)^{1/2} \exp\left(-y^2/2\varrho_\perp^2\right) \frac{dy}{\varrho_\perp},$$

$\varrho_\perp^2$ — the mean-square displacement perpendicular to the plane obtained from the existing measurements of the Debye characteristic temperature θ, $y_{\min}$ — the minimum distance of approach for a particle with transverse energy $E_\perp$, $K(E_\perp)$ is a normalization constant for the spacial probability distribution

$$K(E_\perp) = \left[\frac{1}{d_p}\int_{y_{\min}}^{d_p/2} \left(\frac{E_\perp}{E_\perp - V(y)}\right)^{1/2} dy\right]^{-1},$$

$V(y)$ — the average planar potential, which is taken as zero for the distance $y = d_p/2$. In the presented results of calculation the three types of average planar potentials mentioned below were used

$$V(y) = 2\pi Z_1 Z_2 e^2 N d_p[(y^2+Ca^2)^{1/2} - y], \tag{1}$$

$$V(y) = 2\pi Z_1 Z_2 e^2 N d_p[(y^2+\varrho_\perp^2+Ca^2)^{1/2} - (y^2+\varrho_\perp^2)^{1/2}], \tag{2}$$

$$V(y) = 2\pi Z_1 Z_2 e^2 N d_p a \sum_{i=1}^{3} C_i \exp(-y/\alpha_i) \exp(\varrho_\perp^2/2\alpha_i) \left\{1 - 0.5\left[1 - \Phi\left(\frac{y}{\varrho_\perp\sqrt{2}} - \frac{\varrho_\perp}{\alpha_i\sqrt{2}}\right)\right] + 0.5\exp(2y/\alpha_i)\left[1 - \Phi\left(\frac{y}{\varrho_\perp\sqrt{2}} + \frac{\varrho_\perp}{\alpha_i\sqrt{2}}\right)\right]\right\}, \tag{3}$$

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x dt e^{-t^2},$$

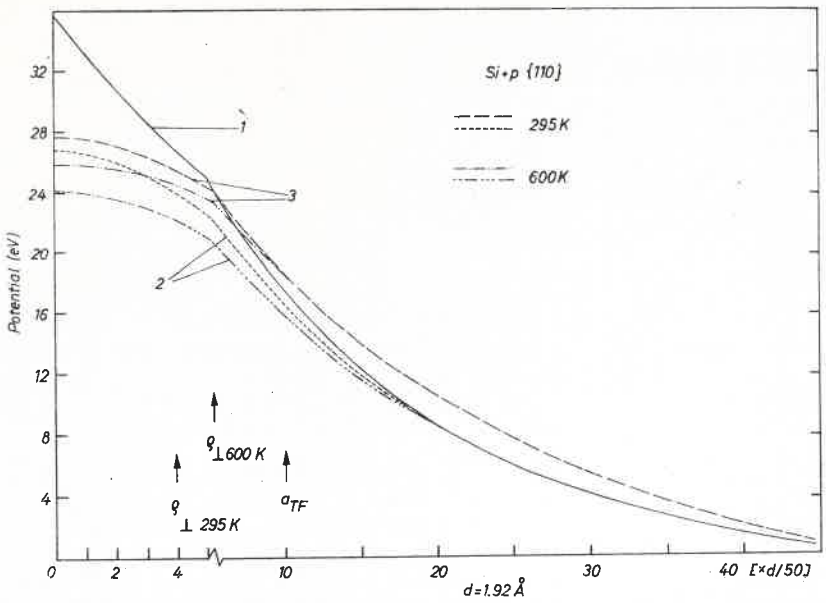

Fig. 1. Distance dependence of the potential given by Eqs (1), (2), (3) for different temperatures and for Si + p

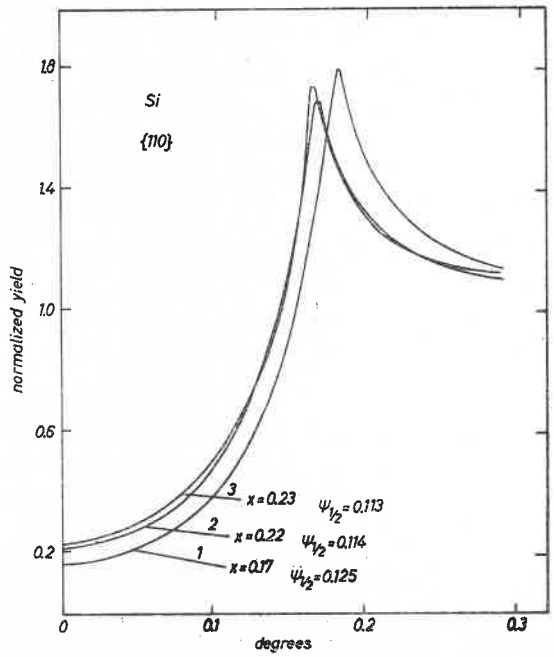

Fig. 2. Calculated normalized angular distribution $P(E\psi^2)$ for 3 MeV protons incident along the {110} plane in silicon for different potentials, Eqs (1), (2), (3), $T = 300$ K

TABLE I

Calculated values of $\psi_{1/2}$ and x_{min} for planar channeling for different potentials, a – Eq. (1), b – Eq. (2), c – Eq. (3)

Target	Plane, ion, energy [MeV]	Calculated		Measurement			
		$\psi_{1/2}$ [deg]	x_{min}	$\psi_{1/2}$ [deg]	Ref.	x_{min}	Ref.
Si	100 H 3	a. 0.093 b. 0.085 c. 0.086	0.22 0.27 0.33	0.070	[4]	0.42	[4]
	110 H 3	a. 0.125 b. 0.114 c. 0.113	0.17 0.22 0.24	0.087	[4]	0.31	[4]
	111 H 3	a. 0.144 b. 0.134 c. 0.132	0.14 0.20 0.21	0.092	[4]	0.36	[4]
	100 He 1	a. 0.28 b. 0.27 c. 0.28	0.17 0.22 0.24	0.22	[5]	0.27	[5]
W	100 H 3	a. 0.23 b. 0.22 c. 0.21	0.13 0.17 0.20	0.17	[4]	0.31	[4]
	110 H 3	a. 0.29 b. 0.27 c. 0.28	0.097 0.128 0.150	0.22	[4]	0.18	[4]
	111 H 3	a. 0.34 b. 0.31 c. 0.32	0.08 0.10 0.13				
	100 He 2	b. 0.38 c. 0.37	0.17 0.20	0.27	[4]		
	110 He 2	b. 0.47 c. 0.48	0.13 0.15	0.38	[4]	0.20	[12]
Au	100 Cl 20	c. 0.36	0.21	0.31	[4]		
Ge	112 He 1	b. 0.22 c. 0.18	0.31 0.34				

$\alpha_1 = 6, \alpha_2 = 1.2, \alpha_3 = 0.3, C_1 = 0.1/6, C_2 = 0.55/1.2, C_3 = 0.35/0.3$ [11], Z_1, Z_2 — atomic numbers of particle and lattice respectively, Nd_p — number of atoms per unit area in the lattice plane, $a = 0.529 \times 0.8852\ Z_2^{-1/3}$ [1] Thomas-Fermi screening distance, C — constant equal to $\sqrt{3}$. The average planar potential given by Eq. (2) is a modification of the potential in Eq. (1). We have assumed that in the region $\varrho_\perp$ the average planar potential should be nearly constant. Fig. 1 shows forms of these potentials for different temperatures for the Si+p and {110} plane. The differences between Eqs (1), (2) and (3) increase with temperature especially in the region $\varrho_\perp$. The difference in value between Eqs (2) and (3) is almost constant for various temperatures and it changes a little with distance from the plane. The typical angular distribution for 3 MeV protons and {110} Si is shown in Fig. 2. It can be seen that the curves are very similar. The differences between curves calculated by using the potential in Eqs (2) and (3) are very small. All the calculated results are displayed in Table I. In general, the agreement between the calculated and experimental result is better if the form of the potential is more "flat" in the region $\varrho_\perp$, but

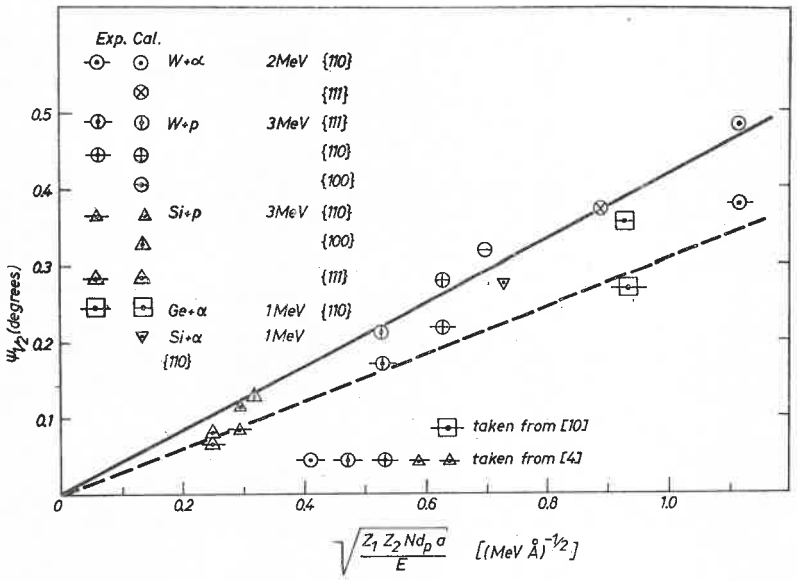

Fig. 3. Functional dependence of $\psi_{1/2}$ for different crystals, energy, planes and ions

the calculated values of $\psi_{1/2}$ ($\psi_{1/2}$ is defined as the half-way point between the normal and the minimum yield) are still too large as compared with the experimental ones. Fig. 3 shows a variation of a half-angle calculated by using the potential in Eq. (3) vs $(Z_1 Z_2 Nd_p/E)^{1/2}$ Assuming a linear dependence for $\psi_{1/2}$ vs $(Z_1 Z_2 Nd_p a/E)^{1/2}$, the full lines have been drawn as the best fit to the calculated and experimental points. In both cases the linear dependence can be only approximately true. It can be noted that both the experimental and corresponding calculated points are in a similar position, i.e., above or below the lines. So as

[1] for $Z_1 > 2$, $a = 0.529 \times 0.8852\ (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$.

to take into account the effects of multiple scattering in the oxide surface layer the angular distribution $P(E\psi^2)$ was transformed into a final distribution $R(E\psi^2)$ by using a Gaussian distribution:

$$p(\theta) = (2/\pi)^{1/2} \exp(-\theta^2/2\Omega^2) \frac{1}{\Omega},$$

where

$$(\Omega)^2 = \frac{2\pi Z_1^2 Z_2^2 e^4}{E^2} N\Delta R \ln 1.29\varepsilon, \qquad \varepsilon = \frac{E}{Z_1 Z_2 e^2} \times \frac{M_2}{M_1 + M_2},$$

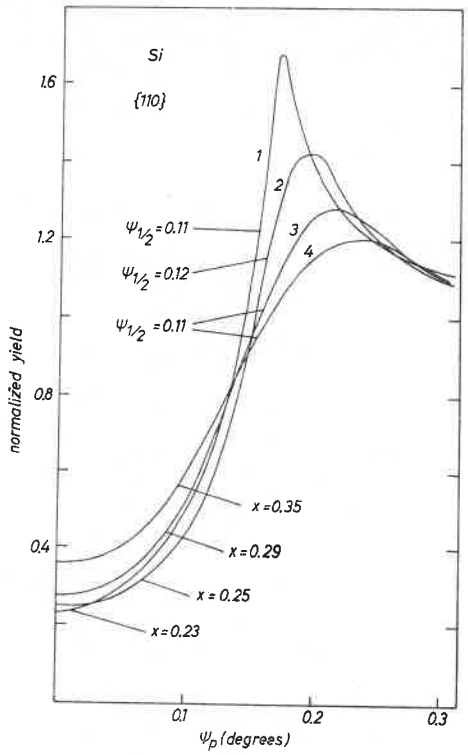

Fig. 4. Calculated distribution of $R(E\psi^2)$ for 3 MeV protons incident along the {110} plane in silicon for different values Ω^2/ψ_p^2, (0.0), (0.04), (0.16), (0.36)

$N\Delta R$ — number of oxygen or target atoms in an amorphous surface layer;

$$R(E\psi^2) = \int_{-\infty}^{\infty} p(\theta) P(E(\psi+\theta)^2) d\theta. \tag{4}$$

The final angular distribution calculated in this way is shown in Fig. 4. It was calculated by using the potential in Eq. (3) for the {110} plane Si and 3 MeV protons for a different values Ω^2/ψ_p^2 (ψ_p is defined by Picraux and Andersen as $E\psi_p^2 = V(0)/\pi$). It was found that for different target, energy, and incident particles for $\Omega^2/\psi_p^2 < 0.5$ the angular width is

almost constant (changes are less than 5%), x_{min} increases slowly, so that $\Delta x_{min} = B \times \Omega^2/\psi_p^2$, $B = 0.3$–0.4. The value of B depends on d_p, for larger d_p is 0.3 rather than 0.4. Fig. 5 shows the results calculated and measured by Picraux and Andersen compared to the calculated distribution $R(E\psi^2)$ for a 30 Å oxide layer. The influence of oxide layer has caused the growth in x_{min} of about 0.1 in comparison with the value of x_{min} calculated by Picraux and Andersen.

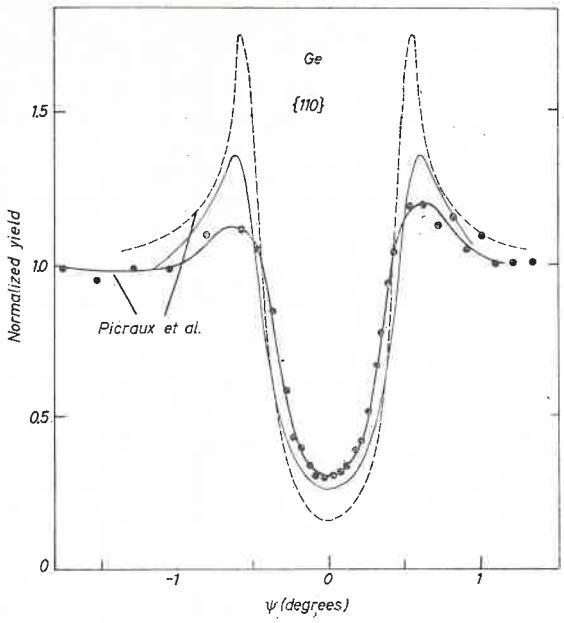

Fig. 5. Comparison of the calculated distribution of $R(E\psi^2)$ for a 30 Å oxide surface layer and calculated and measured results from Ref. [10]. (1 MeV He ions, {110} plane in germanium $T = 295$ K, $\theta = 290$ K)

3. *Conclusion*

In all cases in which knowledge of the derivatives of the planar potential is necessary, potential (2) can be used because the difference between (2) and (3) is almost constant in distance from the plane and amounts to about 0.1 $V(0)$. The value of x_{min} calculated by using the method given in [10] strongly depends on the form of the potential in the region $\varrho_\perp$. The calculated and experimental results are similar if the potential in the region $\varrho_\perp$ changes slowly together with increasing distance from the plane. Taking into consideration the oxide surface layer or any other impurity leads to better agreement between the experimental and calculated results particularly for the value x_{min}. Simultaneously, the shoulder region becomes lower and much broader. The calculated value of $\psi_{1/2}$ is still too large by about 15–20% than the measured critical angles, but in the presented calculations electronic multiple scattering has not been taken into account. This leads to non-conservation of the transverse energy $E_\perp$ and consequently to the reduction of the effective planar potential vs path.

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