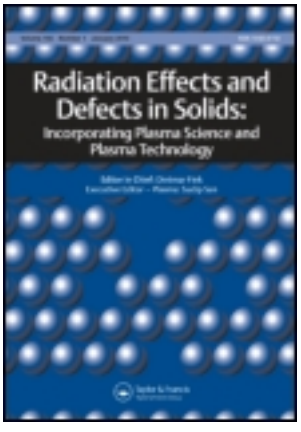

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Isotopic mass effects for low-energy channeling in a silicon crystal

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Isotopic mass effects for low-energy channeling in a silicon crystal

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Monte Carlo (MC) simulations have been used to study the low-energy channeling of ^{10}B and ^{11}B ions along the [100] axis in Si crystal. MC simulations show that the critical angle $\Psi_C \approx 15.3(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{10}B ions and $\Psi_C = 14.5(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{11}B ions, where E is the incident energy. This means that $(\Psi_{C\text{ for }10B\text{ ions}}/\Psi_{C\text{ for }11B\text{ ions}}) \approx (15.3/14.5) \approx (11/10)^{1/2}$.

Keywords: mass effect; channeling; silicon crystal

PACS: 61.46. Fg; 61.85. +p

1. Introduction

Theories, computer simulations and laboratory experiments have investigated the propagation of X-rays and thermal neutrons, as well as relativistic charged particles through carbon nanotubes, for over a decade (*1–11*). The first study (*3*) demonstrated the possibility of hard X-ray generation by relativistic charged particles channeled inside single-wall carbon nanotubes (SWCNTs). Zhevago and Glebov (*6*) expected the transverse motion of X-rays and neutrons in multi-wall carbon nanotubes (MWCNTs) to be better described with weakly localized Bloch waves leading to a band structure of the transverse momentum. Petroviæ et al. (*9*) exhibited the rainbow effect to enable the full explanation of the angular distributions of 1 GeV protons transmitted through the short straight and bent SWCNTs, and Greenenko and Shul'ga (*8*) showed the different deflection mechanisms of relativistic protons through bent SWCNTs.

Experiments and simulations have studied the phenomena of low-energy ion channeling in carbon nanotubes for several years (*12–19*). The first experiment (*12*) found the critical angle, Ψ_C, for channeling to be about 1.5° for incident energy $E = 2000$ keV He^+ channeling in MWCNTs. According to Equation (1) of (*5, 13*), the experimental results of (*12*) are described well by the formula $\Psi_C \approx 67(\text{keV}/E)^{1/2}$ (in degrees). Molecular dynamics simulations (*13*) gave

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$\Psi_C \approx 21(\text{keV}/E)^{1/2}$ (in degrees) for 1–10 keV Ar channeling in SWCNTs, and Monte Carlo (MC) simulations (*17*) gave $\Psi_C \approx 51((m/M)\text{keV}/E)^{1/2}$ (in degrees) for 10–550 keV channeling of natural- and pseudo-Ar ions in SWCNTs, where M and m are the ion and lattice atom masses, respectively. In particular, MC simulations (*18*) gave Ψ_C (^{12}C)/Ψ_C (^{13}C) $\approx (13/12)^{1/2}$ for the same values of E and for low-energy channeling of ^{12}C and ^{13}C ions in SWCNTs. Briefly, Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ions in carbon nanotubes, according to the conservations of transverse energy and transverse momentum, as suggested in (*17, 18*).

Low-energy channeling in ordinary crystals has been investigated since 1963 (*20–28*). Previous works (*23, 28*) have shown critical angles Ψ_C obey the $E^{-1/2}$ rule for B, P and As ions in Si crystals along the major channels; a more recent work (*27*) gave the modified master equation approach of axial dechanneling in perfect compound crystals. In the above investigations (and to date), to our knowledge no studies have shown isotopic mass effects. The present work attempts to show such effects.

2. Simulation program series

Our MC simulation program series has been already employed to investigate particle motion along straight-line trajectories in amorphous (*29, 30*) and crystalline (ordinary crystals or carbon nanotubes) (*16–18, 31, 32*) materials. It utilizes a binary collision model based on the Moliere potential for the ion–atom (or atom–atom) interactions and on the continuous slowing down approximation for electronic stopping, at low temperatures. Carbon nanotubes in a superlattice are kept in the position of equilibrium by van der Waals forces, and the gap between the walls of neighboring nanotubes is usually about 0.315 nm. In carbon nanotubes and ordinary crystals, the thermal vibration is modeled by giving each lattice atom a random displacement (commonly below 0.01 nm).

In the ordinary crystal, channeling phenomena are complicated; for example, dechanneling and rechanneling of ions, transition from the regime of the axial channeling to the planar channeling, etc. Thus, channeled and dechanneled ions should be defined. Each incident ion is given a random position in the initial plane, orthogonal to the crystal axis. The initial random positions of all incident ions define the initial beam size. The channeling tube (*16*) is defined to equal the cylinder, with its diameter being the initial beam size and its length being the crystal axis length. Based on the above definitions, the channeled ions are inside the channeling tube but the dechanneled ions are outside it when they arrive at the final orthogonal plane. The channeling critical angle, Ψ_C, is determined through simulating dechanneling probability data (the number of dechanneled ions per incident ion) (*13, 16*).

In the present work, the MC-simulated instances are the low-energy channeling of ^{10}B and ^{11}B ions along the [100] axis in Si crystal. A 10 nm diameter initial beam is chosen for study, and it is much larger than the lattice constant of Si (0.543 nm). This choice is similar to the experimental setup. In general, there are 1×10^3 incident ions when simulating dechanneling probability data. As the mass difference between ^{10}B and ^{11}B ions is very small, for better accuracy, 1×10^5 ions are statistically necessary for simulating the data in the present work.

3. Results and discussion

Figure 1 shows dechanneling probability as a function of the incident angle Ψ for the channeling of ^{10}B (a) and ^{11}B (b) ions along the [100] axis in Si crystal. The question is how to determine Ψ_C

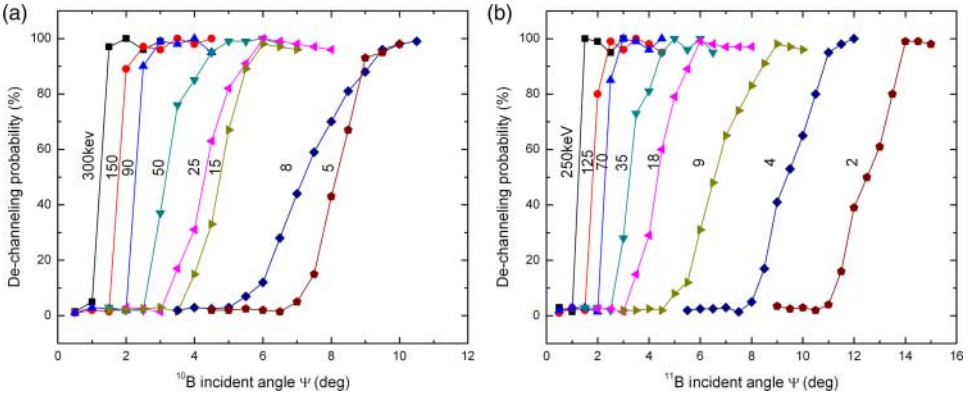

Figure 1. Dechanneling probability as a function of incident angle Ψ for the channeling of ^{10}B (a) and ^{11}B (b) ions along the [100] axis in Si crystal.

in relation to the incident angle Ψ and dechanneling probability (the number of dechanneled ions per incident ion) for a given incident energy? If $\Psi < \Psi_C$, dechanneling probability approximates 0%. If $\Psi > \Psi_C$, dechanneling probability rapidly reaches 100%. Therefore, Ψ_C can be determined by a sharp change between dechanneling probabilities, *i.e.* 0% and 100%. For example, when the ^{10}B incident energy = 90 keV, $\Psi_C = 2°$, because the sharp change begins at 2° (Figure 1(a)). In other words, Figure 1 gives the lower limit of the channeling critical angle Ψ_C.

Figure 2 shows the channeling critical angle Ψ_C as a function of ^{10}B (a) and ^{11}B (b) incident energies along the [100] axis in Si crystal. For the incident energy $E(i)$, the simulated critical angle $\Psi_C(i)$ is fitted by $CE(i)^{-1/2}$ (*22,23*). Here, the question is how to determine the best constant, C? If $\sum_{i=1}^{8}(\psi_C(i) - CE(i)^{-1/2})^2$ equals the minimum, the best C will be determined. Figure 2(a) shows the best $C = 15.3$, while Figure 2(b) shows the best $C = 14.5$.

Along the [100] axis in Si crystal, for channeling of B (20% ^{10}B and 80% ^{11}B) ions, previous works (*23, 25, 26, 28*) have shown the channeling critical angle $\Psi_C \approx 4.2°$ at the incident energy $E = 5$ keV, $\Psi_C \approx 3.4°$ at $E = 15$ keV, $\Psi_C \approx 2.8°$ at $E = 35$ keV and $\Psi_C \approx 2.1°$ at $E = 80$ keV, separately (Table 1). When compared with the above data, for the channeling of ^{11}B ions the present work shows $\Psi_C \approx 6.5°$ at $E = 5$ keV, $\Psi_C \approx 3.7°$ at $E = 15$ keV, $\Psi_C \approx 2.5°$ at $E = 35$ keV and $\Psi_C \approx 1.6°$ at $E = 80$ keV, respectively (Figure 2(b)). Evidently, these two angular-date ranks approximate each other.

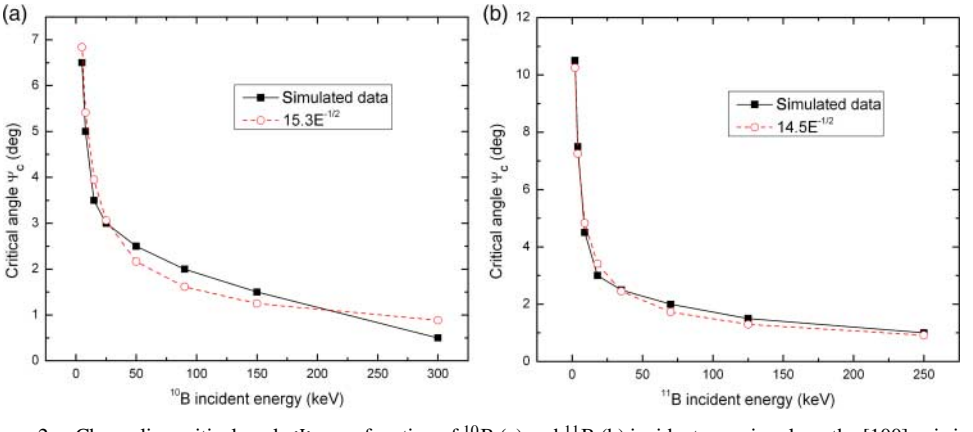

Figure 2. Channeling critical angle Ψ_C as a function of ^{10}B (a) and ^{11}B (b) incident energies along the [100] axis in Si crystal.

Table 1. Channeling critical angle Ψ_C as a function of B (20% ^{10}B and 80% ^{11}B) incident energies along the [100] axis in Si crystal.

Ref.	Ion	Incident energy (keV)	Ψ_C
(*24*)	B	5	4.2°
(*25*)	B	15	3.4°
(*25*)	B	35	2.8°
(*25*)	B	80	2.1°

Our recent work (*18*) showed that in the (30,30) SWCNT, $\Psi_C \approx 21.3(\text{keV/E})^{1/2}$ (in degrees) for the channeling of isotopic ^{12}C ions, and $\Psi_C \approx 20.2(\text{keV/E})^{1/2}$ (in degrees) for the channeling of isotopic ^{13}C ions. This means that $(\Psi_{\text{C for 12C ions}}/\Psi_{\text{C for 13C ions}}) \approx (21.3/20.2) \approx (13/12)^{1/2}$. In other words, Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ^{12}C and ^{13}C ions in the (30,30) SWCNT. Thus, the question arises whether Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ^{10}B and ^{11}B ions along the [100] axis in Si crystal. This is the goal of the present work.

Figure 2 shows that along the [100] axis in Si crystal, $\Psi_C \approx 15.3(\text{keV/E})^{1/2}$ (in degrees) for the channeling of isotopic ^{10}B ions and $\Psi_C \approx 14.5(\text{keV/E})^{1/2}$ (in degrees) for the channeling of isotopic ^{11}B ions. This means that $(\Psi_{\text{Cfor 10B ions}}/\Psi_{\text{C for 11B ions}}) \approx (15.3/14.5) \approx (11/10)^{1/2}$. In other words, Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ^{10}B and ^{11}B ions along the [100] axis in Si crystal. A simple explanation of the above rules is as follows.

We emphasize that low-energy ion channeling should obey both the transverse energy and transverse momentum conservations. $E\Psi_C^2$ approximates the conserved transverse energy and $(2ME)^{1/2}\Psi_C$ approximates the conserved transverse momentum. Note that $\Psi_C \approx \sin(\Psi_C)$ if Ψ_C is small. Because $E\Psi_C^2$ approximates one constant, $\Psi_C \approx C(E)^{-1/2}$, as shown in (*5, 13*). Also, because $(2ME)^{1/2}\Psi_C$ approximates another constant, $\Psi_C \approx C_1(ME)^{-1/2}$, as shown in (*18*), where C and C_1 are constants. This is why Ψ_C might obey the $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ions in carbon nanotubes and ordinary crystals.

As pointed out during this paper's review, in the cases of proton and deuterium low-energy channeling in silicon crystal, the isotopic mass effect should be, of course, much more pronounced and much more easily tested in the experiment. Therefore, as suggested by the reviewer, we will perform the calculation in the above case in the future.

4. Summary

Our recent work (*18*) showed that in the (30,30) SWCNT, $\Psi_C \approx 21.3(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{12}C ions and $\Psi_C \approx 20.2(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{13}C ions. This means that $(\Psi_{\text{C for 12C ions}}/\Psi_{\text{C for 13C ions}}) \approx (21.3/20.2) \approx (13/12)^{1/2}$. In other words, Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ^{12}C and ^{13}C ions in the (30,30) SWCNT. The present work shows that along the [100] axis in Si crystal, $\Psi_C \approx 15.3(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{10}B ions, and $\Psi_C \approx 14.5(\text{keV}/E)^{1/2}$ (in degrees) for the channeling of isotopic ^{11}B ions. This means that $(\Psi_{\text{C for 10B ions}}/\Psi_{\text{C for 11B ions}}) \approx (15.3/14.5) \approx (11/10)^{1/2}$. In other words, Ψ_C might obey $E^{-1/2}$ and $M^{-1/2}$ rules for the channeling of isotopic ^{10}B and ^{11}B ions along the [100] axis in Si crystal.

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