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Theoretical critical angels of ion channeling in carbon nanotubes

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ABSTRACT

We have developed a mass- and charge-dependent equation to predict theoretical critical angles for ion channeling in carbon nanotubes. We focus M (ion mass) effects how to reduce Ze (ion nucleus charge) effects on Ψ_C (critical angles). As an instance, we give theoretical critical angels of He, Ne, Ar, Kr, Xe and Rn ion channeling in carbon nanotubes. We find that for (10, 10) single-wall carbon nanotubes, $\Psi_C(\mathrm{He}) \approx \Psi_C(\mathrm{Ne}) \approx \Psi_C(\mathrm{Ar}) \approx \Psi_C(\mathrm{Kr}) \approx \Psi_C(\mathrm{Xe}) \approx \Psi_C(\mathrm{Rn}) \approx 23.3\,(\mathrm{keV}/E)^{1/2}$ deg. This is because $(Z/M)^{1/2} \approx 0.66\,[\mathrm{amu}]^{-1/2}$.

1. Introduction

In 1965, Lindhard proposed his classical equation for the critical angle, Ψ_C, from consideration of conservation of transverse energy; and he showed Ψ_C to obey $Z^{1/2}$ and $E^{-1/2}$ rules, for low energy ion channeling [1,2]. Before 2007, to our knowledge, none have studied mass effects on Ψ_C, for low energy ion channeling. In 2007, we found such effects on Ψ_C, for channeling of low energy light and heavy ions [3,4]. In 2008, we simulated channeling of low energy isotopic-ions and showed Ψ_C to obey $M^{-1/2}$ and $E^{-1/2}$ rules [5]. In this year, we generalized those ideas via consideration of transverse momentum, and proposed an improved equation including mass effects [6]. In the present work, we use the improved equation to study low energy ion channeling and show Ψ_C to obey $Z^{1/2}$, $M^{-1/2}$ and $E^{-1/2}$ rules. Here, E, M and Z are incident energy, mass and atomic number of the ion, respectively. One goal of us is to calculate critical angels of He, Ne, Ar, Kr, Xe and Rn ion channeling in carbon nanotubes.

2. Derivation of equations

Derivation of equations [6] is briefly introduced, below. Ion channeling was discovered mainly from computer simulations of ion beam propagation along atomic rows in crystals, based on binary ion–atom collisions [7]. After experimental confirmation of the effect, Lindhard [1,2] gave a simple explanation of the channeling: if an ion enters a single crystal at small enough angle Ψ with respect to an atomic row (or string), its motion is governed by the transverse continuum potential of the row (or string). Using considerations of conservation of transverse energy, defined by $E\sin^2\Psi$, he showed that the critical transverse energy $E\sin^2\Psi_C$ may be set equal to $U_C \equiv U(R_C)$, where $U(R_C)$ is the channeled ion potential energy at critical approach distance R_C, that is, he obtained

$$\Psi_C^2 \approx U_C/E, \tag{2.1}$$

In which the (good) approximation $\sin\Psi_C \approx \Psi_C$ has been used. He also obtained

$$U_C = 2zZe^2/d, \tag{2.2}$$

where Ze and ze are the ion nucleus and lattice atom charges, respectively (e is the charge on a proton), and d is the atomic separation in the row (or string). Although later work [8,9] used the continuum potential of an atomic plane instead of row (or string), (2.1) is still at least qualitatively useful. On perusing the form of (2.1), it is evident that only transverse energy effects are included, and transverse momentum effects ignored. For reference below, we substitute (2.2) into (2.1) to get

$$\Psi_C^2 \approx \frac{(ze)(Ze)}{E(d/2)}. \tag{2.3}$$

We now proceed (non-rigorously) to give a reasonable representation of transverse momentum effects, in order to improve (2.3) to include m (lattice atom mass) and M effects. We could argue in several ways, but the most straightforward (with no pretence of rigor) may be the following. In order to get (2.3), energy arguments were used to equate the critical transverse energy ($\approx E\Psi_C^2$) to the critical ion potential energy U_C, given by (2.2). We suggest that the momentum analogues of the energies $E\Psi_C^2$ and

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U_C are $(2ME)^{1/2}\Psi_C$ and $(2mU_C)^{1/2}$, respectively; on equating these two momenta, we get $\Psi_C^2 \approx (m/M)(U_C/E)$, which with (2.2) becomes

$$\Psi_C^2 \approx \frac{m(ze)(Ze)}{ME(d/2)}. \tag{2.4}$$

The equation that includes both (2.3) and (2.4) as special cases is

$$\Psi_C^2 \approx \prod_{j=1}^{6} x_j^{k_j}, \tag{2.5a}$$

where in vector form,

$$x \equiv (ze, Ze, E, d/2, m, M), \tag{2.5b}$$

and where each of the six k_j is equal to -1, 0 or 1. The Eqs. (2.3) and (2.4) are recovered from (2.5) via the choices of vector $k = (1, 1, -1, -1, 0, 0)$ and $(1, 1, -1, -1, 1, -1)$, respectively.

3. Results and discussion

Our Eq. (2.4) can exhibit m and M effects on Ψ_C, but Lindhard's equation (2.3) considered Ψ_C to be independent of mass effects, for low energy ion channeling in carbon nanotubes. In the present work, we focus M effects how to reduce Ze effects on Ψ_C. Thus, from Eq. (2.3), Lindhard obtained two formulas. If $\Psi_C = \Psi_C(E)$, he obtained

$$\Psi_C \approx CE^{-1/2}. \tag{3.1a}$$

If $\Psi_C = \Psi_C(Z, E)$, he obtained

$$\Psi_C \approx C_1 Z^{1/2} E^{-1/2}. \tag{3.1b}$$

From the Eq. (2.4), we obtain three formulas. If $\Psi_C = \Psi_C(E)$, we obtain

$$\Psi_C \approx C_2 E^{-1/2}. \tag{3.2a}$$

If $\Psi_C = \Psi_C(Z, M, E)$, we obtain

$$\Psi_C \approx C_3 Z^{1/2} M^{-1/2} E^{-1/2}. \tag{3.2b}$$

If $\Psi_C = \Psi_C(M, E)$, we obtain

$$\Psi_C \approx C_4 M^{-1/2} E^{-1/2}. \tag{3.2c}$$

where C, C_1, C_2, C_3 and C_4 are constants. Note $C = C_1 Z^{1/2}$ and $C_2 = C_3 Z^{1/2} M^{-1/2} = C_4 M^{-1/2}$. The formula (3.2b) is especially for studying ion channeling, and the formula (3.2c) is especially for studying isotopic-ion channeling.

Experiments and simulations have investigated the phenomenon of low energy ion channeling in carbon nanotubes for several years [3–6,10,11]. The first experiment [10] found the critical angle, Ψ_C, for channeling to be about 1.5 deg for incident energy $E = 2000$ keV He channeling in multi-wall carbon nanotube ropes. According to the formula (3.2a), the experimental results of Ref. [10] are described well by the formula $\Psi_C \approx 67\,(\mathrm{keV}/E)^{1/2}$ deg. Molecular dynamics (MD) simulations [11] gave $\Psi_C \approx 20\,(\mathrm{keV}/E)^{1/2}$ deg for 1–10 keV Ar channeling in single-wall carbon nanotubes (SWCNTs). In particular, Monte Carlo (MC) simulations [5] gave $\Psi_C(^{12}\mathrm{C})/\Psi_C(^{13}\mathrm{C}) \approx (13/12)^{1/2}$ for the same values of E, for low energy channeling of ^{12}C and ^{13}C ions in SWCNTs. Evidently, MC simulation results confirm our formula (3.2c).As analyzed before, Lindhard suggested $E\Psi_C^2 \approx U_C$ but we suggest $(2ME)^{1/2}\Psi_C \approx (2mU_C)^{1/2}$, for low energy ion channeling. Table 1 shows that U_C increases as Z increases, for low energy He, Ne, Ar, Kr, Xe and Rn ion channeling in (10, 10) SWCNTs. According to his suggestion, from Table 1, Ψ_C are given as follows:

Table 1
Z, $(m/M)^{1/2}$, $(Z/M)^{1/2}$ and U_C are, respectively, listed for low energy He, Ne, Ar, Kr, Xe and Rn ion channeling in (10, 10) SWCNTs.

Ion	Z	$(m/M)^{1/2}$	$(Z/M)^{1/2}$ [amu]$^{-1/2}$	U_C [eV]
He	2	1.73	0.71	63.6
Ne	10	0.77	0.70	318
Ar	18	0.55	0.67	572.4
Kr	36	0.38	0.66	1144.8
Xe	54	0.30	0.64	1717.2
Rn	86	0.23	0.62	2734.8

$$\Psi_C(\mathrm{He}) \approx 14.4\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.3a}$$
$$\Psi_C(\mathrm{Ne}) \approx 32.3\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.3b}$$
$$\Psi_C(\mathrm{Ar}) \approx 43.3\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.3c}$$
$$\Psi_C(\mathrm{Kr}) \approx 61.2\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.3d}$$
$$\Psi_C(\mathrm{Xe}) \approx 75.0\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.3e}$$
$$\Psi_C(\mathrm{Rn}) \approx 94.7\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}. \tag{3.3f}$$

However, according our suggestion, from Table 1, Ψ_C are given as follows:

$$\Psi_C(\mathrm{He}) \approx 24.9\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.4a}$$
$$\Psi_C(\mathrm{Ne}) \approx 24.8\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.4b}$$
$$\Psi_C(\mathrm{Ar}) \approx 23.8\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.4c}$$
$$\Psi_C(\mathrm{Kr}) \approx 23.3\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.4d}$$
$$\Psi_C(\mathrm{Xe}) \approx 22.5\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}, \tag{3.4e}$$
$$\Psi_C(\mathrm{Rn}) \approx 21.8\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}. \tag{3.4f}$$

We explain these two different results below.

For low energy He, Ne, Ar, Kr, Xe and Rn ion channeling in (10, 10) SWCNTs. Lindhard's formula (3.1b) showed $\Psi_C \approx C_1 Z^{1/2} E^{-1/2}$, so his formula (3.3) showed that Ψ_C increases as Z increases. However, our formula (3.2b) shows $\Psi_C \approx C_3 Z^{1/2} M^{-1/2} E^{-1/2}$. Table 1 shows $(Z/M)^{1/2} \approx 0.66\ [\mathrm{amu}]^{1/2}$. Therefore, our formula (3.4) shows

$$\Psi_C(\mathrm{He}) \approx \Psi_C(\mathrm{Ne}) \approx \Psi_C(\mathrm{Ar}) \approx \Psi_C(\mathrm{Kr}) \approx \Psi_C(\mathrm{Xe}) \approx \Psi_C(\mathrm{Rn}) \approx 23.3\,(\mathrm{keV}/E)^{1/2}\ \mathrm{deg}.$$

As mentioned above, for low energy Ar ion channeling in (10, 10) SWCNTs. Lindhard's formula (3.3C) showed $\Psi_C(\mathrm{Ar}) \approx 43.3\,(\mathrm{keV}/E)^{1/2}$ deg, our formula (3.4c) shows $\Psi_C(\mathrm{Ar}) \approx 23.8\,(\mathrm{keV}/E)^{1/2}$ deg, and MD simulations showed $\Psi_C(\mathrm{Ar}) \approx 20\,(\mathrm{keV}/E)^{1/2}$ deg [11]. Interestingly, our formula approximates the MD-simulated one.

4. Summary

We have developed a mass- and charge-dependent equation to predict theoretical critical angles for ion channeling in carbon nanotubes. We have employed this improved equation to exhibit several critical angle formulas. These obtained formulas can not only analyze previously experiment and simulation results, but also show other interesting ones. As the first instance, we give theoretical critical angels of He, Ne, Ar, Kr, Xe and Rn ion channeling in carbon nanotubes. We find that for (10, 10) SWCNTs, $\Psi_C(\mathrm{He}) \approx \Psi_C(\mathrm{Ne}) \approx \Psi_C(\mathrm{Ar}) \approx \Psi_C(\mathrm{Kr}) \approx \Psi_C(\mathrm{Xe}) \approx \Psi_C(\mathrm{Rn}) \approx 23.3\ (\mathrm{keV}/E)^{1/2}$ deg. This is because Table 1 shows $(Z/M)^{1/2} \approx 0.66\ [\mathrm{amu}]^{-1/2}$. As the second instance, our formula (3.4c) shows $\Psi_C(\mathrm{Ar}) \approx 23.8\,(\mathrm{keV}/E)^{1/2}$ deg, and MD simulations showed $\Psi_C(\mathrm{Ar}) \approx 20\,(\mathrm{keV}/E)^{1/2}$ deg. Interestingly, our formula approximates the MD-simulated one. As the third instance, MC simulations gave $\Psi_C(^{12}\mathrm{C})/\Psi_C(^{13}\mathrm{C}) \approx (13/12)^{1/2}$ for the same values of E, for low energy channeling of ^{12}C and ^{13}C

ions in SWCNTs. Evidently, MC simulation results confirm our formula (3.2c).

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Appendix

Theoretical formulas use [eV] and [radian] units, but experiments and simulations use [keV] and [deg] units. For convenient comparison, we give two formulas as follows. From conservation of transverse energy,

$$\begin{aligned}\Psi_C &\approx (U_C\ [\mathrm{eV}]/E\ [\mathrm{eV}])^{1/2}\ \mathrm{radian}\\ &= (U_C\ [\mathrm{eV}]/1000E\ [\mathrm{keV}])^{1/2}(180\ [\mathrm{deg}]/\pi\ [\mathrm{radian}])\\ &= 180/\pi/(1000)^{1/2}(U_C\ [\mathrm{eV}]/E\ [\mathrm{keV}])^{1/2}\ \mathrm{deg}\\ &= 1.81((U_C/\mathrm{eV})(\mathrm{keV}/E))^{1/2}\ \mathrm{deg}. \end{aligned} \quad (A1)$$

From conservation of transverse momentum,

$$\Psi_C \approx 1.81(m/M)^{1/2}((U_C/\mathrm{eV})(\mathrm{keV}/E))^{1/2}\ \mathrm{deg}. \quad (A2)$$

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