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An improved critical angle equation for channeling

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ABSTRACT

Lindhard proposed his classical equation for the critical channeling angle from consideration of conservation of transverse energy. We generalize those ideas via consideration of conservation of transverse momentum, and propose an improved equation. A dimensional analysis of the problem is also presented, and that analysis puts our arguments and results on a firm footing.

1. Introduction

Experiments and simulations have investigated the phenomenon of low energy ion channeling in carbon nanotubes for several years [1–8]. The first experiment [1] 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 Eq. (1) of Refs. [2,3], the experimental results of Ref. [1] are described well by the formula $\Psi_C \approx 67(\mathrm{keV}/E)^{1/2}$ deg.

Molecular dynamics simulations [2,3] gave $\Psi_C \approx 21(\mathrm{keV}/E)^{1/2}$ deg for 1–10 keV Ar channeling in single-wall carbon nanotubes (SWCNTs), and Monte-Carlo (MC) simulations gave [7] $\Psi_C \approx 51((m/M)\mathrm{keV}/E)^{1/2}$ deg 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 [8] 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. Briefly, then, as suggested in Refs. [7,8] Ψ_C^2 is approximately proportional to m/ME according to the conservations of transverse energy and transverse momentum.

The classical equation, that is our (2.3), does not show the mass effects. In the present paper, we suggest an improved critical angle equation, that is our (2.4), for low energy ion channeling, which includes those effects. Both equations are special cases of our (2.5).

2. Derivation of equations

It is recognized that mass effects (that is, momentum effects) play important roles in the fields involving low energy ion–atom collisions [6–15]. It is clear that the mass effects include the "momentum asymmetry effect" in the sputtering of isotopically specific atoms [9–15] and the "incident momentum effect" in the channeling of isotopically specific ions [8].

Ion channeling was discovered mainly from computer simulations of ion beam propagation along atomic rows in crystals, based on binary ion–atom collisions [16–20]. After experimental confirmation of the effect, Lindhard [16,17] 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 [18,19] used

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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 effects of the masses m and M. 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 U_C are $(2ME)^{1/2}$ Ψ_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

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

A formula 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 formulas (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.

Our arguments and results are put on a firm footing by the rigorous dimensional analysis presented in the Appendix.

3. Summary

From considerations of conservation of transverse energy, Lindhard proposed (2.3) for the critical channeling angle Ψ_C. On generalizing those ideas via consideration of conservation of transverse momentum, we propose (2.4) as an improvement over (2.3). The generalized formula (2.5), which includes both (2.3) and (2,4) as special cases, is interesting in view of its close relationship to the results of the dimensional analysis presented in the Appendix; that analysis puts our arguments and results on a firm footing.

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Appendix. Dimensional analysis of the problem

We must first choose the "important quantities", which we label X_k with $X_0 = \Psi_C^2$. The six quantities x_k in (2.5b) seem reasonable choices, and we base our X_k (k = 1, 2, 3, 4, 5, 6) on them:

$$X_1 = (Ze)^2, \quad X_2 = (ze)^2, \quad X_3 = d/2, \quad X_4 = E, \quad X_5 = M, \quad X_6 = m. \tag{A1}$$

(We choose $(Ze)^2$ and $(ze)^2$ rather than Ze and ze in order that our resulting dimensional matrix contains only integers.) Where $[Q]$ means the dimensions of Q, we write $[X_k]$ in the style $M^{m_k}L^{l_k}T^{t_k}$, and get Table 1 for the dimensional matrix (M) calculation; (M) is the 7 × 3 array of integers in Table 1. The number P of independent

Table 1
The dimensional matrix.

k	X_k	m_k	l_k	t_k
0	Ψ_C^2	0	0	0
1	Ze^2	1	3	−2
2	ze^2	1	3	−2
3	$d/2$	0	1	0
4	E	1	2	−2
5	M	1	0	0
6	m	1	0	0

dimensional products Π_k is $P = N-r$, where $N = 7$ here (with k = 0, 1, 2, 3, 4, 5, 6) and r is the rank of (M); $r = 3$ gives $P = 4$, and a suitable set of Π_k (k = 0, 1, 2, 3) may be found by inspection:

$$\Pi_0 = \Psi_C^2, \quad \Pi_1 = \frac{(Ze)^2}{E(d/2)}, \quad \Pi_2 = \frac{z}{Z}, \quad \Pi_3 = \frac{m}{M}. \tag{A2}$$

The Buckingham Pi Theorem of dimensional analysis gives

$$G(\Pi_0, \Pi_1, \Pi_2, \Pi_3) = 0 \tag{A3}$$

where G is an unknown (as yet) function of four variables. The form of G may be studied using both experimental and theoretical considerations. We note that, given the choice (A1) of important quantities, the result (A3) is rigorously exact, and its exactness is not open to argument. It is reasonable to hope that (A3) may be "reasonably solved" for Π_0, so we write (perhaps with our fingers crossed for luck)

$$\Pi_0 = F(\Pi_1, \Pi_2, \Pi_3) \tag{A4}$$

where F is an unknown (as yet) function of three variables, which may also be studied using both experimental and theoretical considerations. It is worthwhile to hope that (A4) is useful, as it is a major simplification over (A3).

We note that, with the choice (A1) of important quantities (together with the choice $X_0 = \Psi_C^2$), the only rigorously exact result is (A3). At first sight, (A3) and (A4) may not look valuable, as they appear to say little. This attitude is entirely wrong, because (A3), and hopefully (A4) also, form excellent (invaluable) checks on all calculations, guesses, and so on. Our (2.3) gives

$$F \equiv F_1(\Pi_1, \Pi_2, \Pi_3) \approx \Pi_1\Pi_2, \tag{A5}$$

and our improved result (2.4) gives

$$F \equiv F_2(\Pi_1, \Pi_2, \Pi_3) \approx \Pi_1\Pi_2\Pi_3. \tag{A6}$$

The simplicity of the functions F_1 and F_2 is due both to luck and to a good choice of dimensionless products Π_k.

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