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Discussion

Reply to "Comment on an improved critical angle equation for channeling"

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Carbon nanotubes have super-lattice structures. As new phenomena, high-energy ion channeling and low-energy ion channeling in carbon nanotubes are very different from those in compact crystals [1–18]. We proposed a generalized critical angle equation (2.5) [9], including Lindhard's classical equation (2.3) [10,11], and an improved equation (2.4) [9], for low-energy ion channeling. Where E is the incident energy and M is the ion mass, we note that (2.3) implies that the E effects dominate over the incident momentum $(2ME)^{1/2}$ effects on channeling critical angles Ψ_C, whereas (2.4) implies that the $(2ME)^{1/2}$ effects dominate over the E effects on Ψ_C. Our (2.3) commonly applies to compact crystals [19–22], whereas (2.4) commonly applies to carbon nanotubes. In other words, (2.5) is generally valid, but (2.3) and (2.4) are of limited validity.

From (2.3), if $\Psi_C \equiv \Psi_C(Z,E)$, Lindhard obtained

$$\Psi_C \approx C_{F1} Z^{1/2} E^{-1/2} \tag{F1}$$

where Z is the ion atomic number. From (2.4), if $\Psi_C \equiv \Psi_C(Z,M,E)$, we get

$$\Psi_C \approx C_{F2} Z^{1/2} M^{-1/2} E^{-1/2} \tag{F2}$$

where C_{F1} and C_{F2} are constants.

Our (2.4) comes from the momentum analogues $(2ME)^{1/2}\Psi_C$ and $(2mU_C)^{1/2}$, where m is the lattice-atom mass and U_C is the channeled ion potential energy at critical approach distance. For small Ψ_C, $(2ME)^{1/2}\Psi_C$ is the conserved transverse momentum, so its use is rigorous; use of the momentum analogue $(2mU_C)^{1/2}$ is straightforward and reasonable. Our (2.4) shows how the M effects reduce the Z effects on Ψ_C owing to the rigorous $(2ME)^{1/2}\Psi_C$ and the reasonable $(2mU_C)^{1/2}$. Essentially, the authors of the Comment say that applying (2.4) to the case of 3 MeV protons channeling in a tungsten crystal gives an incorrect (unreasonably large) critical angle of 12.5°, and we thank them for bringing to our attention that this is not stated in our paper.

Approximately 15 years ago, more experimental data showed that Lindhard's (2.3) is of limited validity, such as for the cases of B, P and As ion channeling in silicon crystals along the major channels [12]. For example, for channeling of 15 keV B ($Z = 5$, $M \approx 10.81$u) and As ($Z = 33$, $M \approx 74.92$u) ions along the [100] axis in silicon crystals, [12] gives $\Psi_C(\mathrm{As})/\Psi_C(\mathrm{B}) \approx (4.2^\circ/3.4^\circ) \approx 1.2$. Our (F2) gives $\Psi_C(\mathrm{As})/\Psi_C(\mathrm{B}) \approx (10.81/74.92)^{1/2}(33/5)^{1/2} \approx 1.0$, but Lindhard's (F1) gives $\Psi_C(\mathrm{As})/\Psi_C(\mathrm{B}) \approx (33/5)^{1/2} \approx 2.6$. Thus, an argument arises as to whether the M effects strongly reduce the Z effects on Ψ_C for low-energy ion channeling in compact crystals.

For low-energy ion channeling in carbon nanotubes, experiments and simulations [13–18] show that Ψ_C is much smaller for the heavier ion (Ar) than for the lighter one (He); that is, Ψ_C depends strongly on M. The experiments and simulations disagree with Lindhard's classical (2.3), because it predicts Ψ_C to be independent of M. In particular, Monte-Carlo simulations [15] give $\Psi_C(^{12}\mathrm{C})/\Psi_C(^{13}\mathrm{C}) \approx (13/12)^{1/2}$ for low-energy channeling of ^{12}C and ^{13}C ions at the same value of E. This is the important information, which shows that Ψ_C obeys $M^{-1/2}$ rules. Thus, we proposed (2.4) from consideration of conservation of transverse momentum.

Just as, for small Ψ_C, $(2ME)^{1/2}\Psi_C$ is approximately the conserved transverse momentum, so $E\Psi_C^2$ is approximately the conserved transverse energy. Because $E\Psi_C^2$ = one constant,

$$\Psi_C = C_1 E^{-1/2} \tag{1}$$

and, because $(2ME)^{1/2}\Psi_C$ = another constant,

$$\Psi_C = C_2 M^{-1/2} E^{-1/2} \tag{2}$$

where C_1 and C_2 are constants. We note that, in (1), the E effects dominate over the $(2ME)^{1/2}$ effects, whereas, in (2), the $(2ME)^{1/2}$ effects dominate over the E effects. By combining (1) and (2), we obtain the simplest generalized critical angle equation for channeling, that is,

$$\Psi_C = C M^{-K} E^{-1/2} \tag{3}$$

where C and K are constants. We have $C = C_1$ when $K = 0$, and $C = C_2$ when $K = 1/2$.

Our (3) may be applied to compact crystals if $K = 0$, that is, the E effects dominate. Of course, (3) may be applied to carbon nanotubes if $K = 1/2$, that is, the $(2ME)^{1/2}$ effects dominate. In principle, (1) is similar to Lindhard's (2.3), whereas (2) is similar to our (2.4).

For low-energy Ar ion channeling in (10,10) single-wall carbon nanotubes, (2.3) shows that Lindhard's formula gives $\Psi_C(\mathrm{Ar}) \approx 43.3^\circ(\mathrm{keV}/E)^{1/2}$, (2.4) shows that our formula gives $\Psi_C(\mathrm{Ar}) \approx 23.8^\circ(\mathrm{keV}/E)^{1/2}$, and MD (molecular dynamics) simulations imply the formula $\Psi_C(\mathrm{Ar}) \approx 20^\circ(\mathrm{keV}/E)^{1/2}$ [14]. Interestingly, our formula approximates the MD-simulated one.

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Lindhard proposed his classical (2.3) for the critical angles from consideration of conservation of transverse energy, so that (2.3) applies for special cases, such as low-energy proton and deuterium channeling in compact crystals. We generalized those ideas via consideration of conservation of transverse momentum, and proposed the improved (2.4), which applies to other special cases, such as low-energy He and Ar ion channeling in carbon nanotubes. Of course, there are the intermediate cases, such as low-energy B, P and As ion channeling in compact crystals, between the two special cases above. The new equation for the intermediate cases takes account of conservation of both transverse energy and transverse momentum. Our (2.3) for some special cases, and (2.4) for others, are recovered from (2.5) via the choices of our vector $\boldsymbol{k} = (1, 1,-1,-1,0,0)$ and $(1,1,-1,-1,1,-1)$, respectively. Thus, $-1 \leq k_j \leq 1$ in the new equation for intermediate cases. It is not possible to reliably determine certain values of k_j in the new equation if there are no relevant experimental data.

Conclusion

The phenomena of channeling critical angles for carbon nanotubes are the new phenomena that are not explained by Lindhard's (2.3), and we proposed an improvement (2.4) to explain such new phenomena. Our (2.5) is generally valid, but (2.3) and (2.4) are of limited validity.

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References

[1] V.V. Klimov, V.S. Letokhov, Phys. Lett. A222 (1996) 424.
[2] L.A. Gevorgian, K.A. Ispirian, R.K. Ispirian, Nucl. Instr. Meth. B145 (1998) 155.
[3] G.V. Dedkov, Nucl. Instr. Meth. B143 (1998) 584.
[4] N.K. Zhevago, V.I. Glebov, Phys. Lett. A250 (1998) 360.
[5] N.K. Zhevago, V.I. Glebov, Phys. Lett. A282 (2001) 97.
[6] A.A. Greenenko, N.F. Shul'ga, Nucl. Instr. Meth. B205 (2003) 767.
[7] S. Petrović, D. Borka, N. Nešković, Eur. Phys. J. B44 (2005) 41.
[8] N. Nešković, S. Petrović, D. Borka, Nucl. Instr. Meth. B230 (2005) 106.
[9] L.P. Zheng, Z.Y. Zhu, Y. Li, F.O. Goodman, Nucl. Instr. Meth. B268 (2010) 120.
[10] J. Lindhard, Phys. Lett. 12 (1964) 126.
[11] J. Lindhard, Mat. Fys. Medd. Dan. Vidensk. Selsk. 34 (1965) 14.
[12] G. Hobler, Radiat. Eff. Defects Solids 139 (1996) 21.
[13] Zhu Zhiyuan, Zhu Dezhang, Lu Rongrong, Xu Zijian, Zhang Wei and Xia Huihao. in: Proceedings of the International Workshop Channeling 2004" – Charged and Neutral Particles Channeling Phenomena, Proceedings of SPIE, vol. 5974, 597413-1 (2005).
[14] A.V. Krasheninnikov, K. Nordlund, Phys. Rev. B71 (2005) 245408.
[15] L.P. Zheng, Z.Y. Zhu, Y. Li, D.Z. Zhu, H.H. Xia, J. Phys. Chem. C112 (2008) 15204.
[16] L.P. Zheng, C.B. Wang, Z.J. Xu, Z.Y. Zhu, D.Z. Zhu, H.H. Xia, Nucl. Instr. Meth. B260 (2007) 513.
[17] L.P. Zheng, Z.Y. Zhu, Y. Li, D.Z. Zhu, H.H. Xia, Nucl. Instr. Meth. B266 (2008) 849.
[18] M.T. Robinson, O.S. Oen, Phys. Rev. 5 (1963) 113.
[19] W.K. Chu, J.W. Mayer, A. Nicolet, Backscattering spectrometry, Academic Press, New York, 1978. p. 233.
[20] C.J. Andreen, R.L. Hines, Phys. Rev. 159 (1967) 285.
[21] G. Foti, F. Grasso, R. Quattrocchi, I.F. Quercia, E. Rimini, Phys. Lett. A31 (1970) 214.
[22] F. Grasso, M. Lo Savio, E. Rimini, Radiat. Eff. Defects Solids 12 (1972) 149.