# A theory for the high-field current-carrying capacity of one-dimensional semiconductors

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It is shown that current saturation in semiconducting carbon nanotubes is indistinguishable from metallic nanotubes if the carrier density is above a critical value determined by the bandgap and the optical phonon energy. This feature stems from the higher number of current-carrying states in the semiconducting tubes due to the van Hove singularity at the band edge. Above this critical carrier density, the ensemble saturation velocity at high fields is found to be independent of the bandgap, but strongly dependent on the carrier density, explaining recent observations. The results derived are valid in the limit of ultrafast electron-optical phonon interaction and diffusive transport at high electric fields. The analytical results derived are then applied to one-dimensional (1D) semiconducting graphene nanoribbons as well as semiconductor nanowires with parabolic bandgap. A generalized concept of phonon-limited saturation currents in high-field transport in 1D structures emerges from these considerations. © *2009 American Institute of Physics*.
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## I. INTRODUCTION

Carbon nanotubes (CNTs) exhibit exceptional current carrying capability. For example, Yao *et al.*[1] in a seminal work on single-wall metallic CNTs (m-CNT) observed that the current carrying capacity as high as $10^9$ A/cm$^2$ was fundamentally limited by the emission of longitudinal optical (LO) phonons by energetic electrons at high electric fields. The exceptionally high current carrying capacity was attributed by the authors to the fact that each carrier within a energy bandwidth determined by the LO phonon energy $\hbar\omega_{\mathrm{LO}}\sim 160$ meV moves with the Fermi velocity ($v_F \sim 10^8$ cm/s), leading to a fundamental limit of the current determined by $I_0=(4e/L)\Sigma_k f_k v_F=4ef_{\mathrm{LO}}$, where $f_{\mathrm{LO}}=\omega_{\mathrm{LO}}/2\pi$, $L$ is the CNT length, the factor $g=g_s g_v=4$ is the product of the spin and valley degeneracy, and $f_k$ is the occupation probability of state $|k\rangle$. The current evaluates to $\approx 25$ $\mu$A, precisely explaining the experimental saturation current. This result is fundamental for long m-CNTs, where transport is in the diffusive limit; for short m-CNTs, the current can exceed the diffusive limit of 25 $\mu$A due to ultrafast phonon emission leading to nonuniform heating. It has been shown that the increase in the saturation current over this limit can be explained by consideration of nonequilibrium (hot) phonons.[2,3]

There have been reports of similar current saturation in semiconducting CNTs (s-CNT) as well.[4–6] However, the physical mechanism of current saturation is not yet clear. Previous theoretical considerations indicate a velocity saturation[7] and in Ref. 10, a dependence of the ensemble saturation velocity on the carrier density was established by the solution of the Boltzmann transport equation (BTE). The purpose of this paper is fourfold:

(a) to show that for one-dimensional (1D) s-CNTs *current saturation* is as fundamental as in m-CNTs,
(b) as opposed to m-CNTs, the saturation current in a s-CNT is sensitive to the location of the Fermi level $\mathcal{E}_F^0$ *before* the application of a bias,
(c) the net ensemble velocity ("saturation velocity") of carriers in s-CNTs is *not* universal, but strongly dependent on $\mathcal{E}_F^0$ as well, and can range from $0.1-1\times v_F$, and
(d) the saturation velocity of carriers in s-CNTs becomes independent of the bandgap for large carrier densities.

These four facts are proved using analytical arguments based on the band structure, and the ultrafast electron-optical phonon interactions in CNTs. The results derived are valid in the limit of ultrafast electron-optical phonon interaction and diffusive transport at high electric fields. They offer a simple explanation for various recent observations made from experiments and numerical simulations.[7] Furthermore, the results are generalized for 1D graphene nanoribbons, as well as for semiconductor nanowires with parabolic band structures, and a universality of current-carrying capacities of 1D structures emerges from these considerations.

### A. CNT band structure and saturation current

For the analysis of transport properties, it suffices to consider expansions of the energy dispersion for small momenta around the $\mathcal{K},\mathcal{K}'$ points of the underlying graphene band structure.[8] Let the band structure of the $n$th subband of a s-CNT be given by the dispersion $\mathcal{E}_n(k_x)=\hbar v_F\sqrt{k_x^2+k_n^2}$, where $\hbar$ is the reduced Planck's constant, $k_x$ is the longitudinal wave vector, and $k_n$ is the transverse wave vector quantized by the diameter of the CNT. All energies are measured with respect to the Dirac point of the underlying graphene band structure. The bandgap of the CNT with this band structure is given by $\mathcal{E}_g=2\hbar v_F k_0$, where $k_0$ is the smallest allowed (non-

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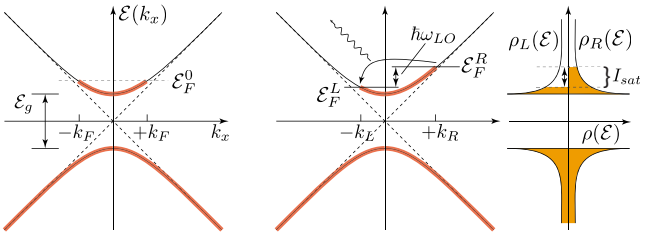


FIG. 1. (Color online) Schematic representation of the mechanism of LO phonon scattering in s-CNTs. If the Fermi level before the application of a bias is high in the conduction band, the ultrafast optical phonon scattering leads to the steady state carrier distribution shown in the middle and right figures; the saturation current is effectively carried by right-moving electrons spread over an energy bandwidth of $\hbar\omega_{\mathrm{LO}}$.

zero) transverse wave vector, fixed by the size quantization ($\mathcal{E}_g \sim 800/d$ meV, where $d$ is the diameter of the s-CNT in nanometers).

An electric field $\mathbf{F}=-F_0\hat{x}$ is applied across the drain-source contacts to the s-CNT, which are assumed to be perfectly transparent to electron flow.[9] To determine the exact shape of the new Fermi surface, one needs to solve the BTE, as has been done in Ref. 10 for $T=300$ K. However, for the $T\to 0$ limit, various analytical results may be derived to illustrate the physics of current saturation in s-CNTs. When the Fermi energy is much larger than $kT$—as is typically the case when CNT transistors are in the on state, the analytical results derived for low temperature remain valid at room temperature (see Ref. 1). The Fermi surface at low temperatures is sharp and the force due to the electric field $(-e)\mathbf{F}=\hbar d\mathbf{k}/dt$ populates $+k_x$ states by emptying out $-k_x$ states near the Fermi surface. Ohmic contacts do not inject carriers into the wire (no space-charge currents), therefore the equilibrium occupation function $f_k^0=\Theta(k_F-|k_x|)$ [where $\Theta(\ldots)$ is the Heaviside unit-step function] shifts to the nonequilibrium position $f_k=1$ for $-k_L\le k_x\le +k_R$, while conserving the particle number inside the wire. Here $k_L, k_R$ are the wave vectors of the highest right-going and the highest left-going electrons in response to the electric field. This is shown schematically in Fig. 1.

The density of states can be split equally into the left-going and right-going states $\rho_{\mathrm{tot}}(\mathcal{E})=\rho_L(\mathcal{E})+\rho_R(\mathcal{E})$, where

$$\rho_{R,L}(\mathcal{E})=\frac{1}{2}\times\frac{g}{\pi\hbar v_F}\times\frac{\mathcal{E}}{\sqrt{\mathcal{E}^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}}, \tag{1}$$

and the resulting right- and left-going charge carrier densities can be then written in the form $n_{R,L}=\int_{\mathcal{E}_g/2}^{\mathcal{E}_F^{R,L}}\rho_{R,L}(\mathcal{E})d\mathcal{E}$ as

$$n_{R,L}=\frac{1}{2}\times\frac{g}{\pi\hbar v_F}\times\sqrt{(\mathcal{E}_F^{R,L})^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}, \tag{2}$$

which defines the quasi-Fermi levels $\mathcal{E}_F^R$ and $\mathcal{E}_F^L$. Before the application of a bias $\mathcal{E}_F^R=\mathcal{E}_F^L=\mathcal{E}_F^0$ and the 1D carrier density is given by

$$n_0=n_R+n_L=\frac{g}{\pi\hbar v_F}\times\sqrt{(\mathcal{E}_F^0)^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}. \tag{3}$$

If the contacts to the s-CNT do not inject excess carriers into the tube, then to ensure particle number conservation $n_0=n_R+n_L$ requires that at all bias conditions, the relation

$$2\sqrt{(\mathcal{E}_F^0)^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}=\sqrt{(\mathcal{E}_F^R)^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}+\sqrt{(\mathcal{E}_F^L)^2-\left(\frac{\mathcal{E}_g}{2}\right)^2}, \tag{4}$$

must be satisfied for the quasi-Fermi levels.

At a high field, the distribution function reaches a stage when the difference between the highest filled electronic state (HFES) and the lowest empty electronic state (LEES) equals the LO phonon energy to allow for energy relaxation by the emission of optical phonons. Building upon the theory in Ref. 1 we make a *hypothesis* that if the LO phonon emission process is ultrafast, then the distribution function is locked in this configuration, and is resistant to any further increase in applied bias. Depending on the availability of charge carriers, the LEES may be $\mathcal{E}_F^L$ or the band edge ($\mathcal{E}=\mathcal{E}_g/2$). Before we proceed to calculate the net saturation current, we introduce some critical parameters that serve to highlight this fact.

### B. Critical parameters

A critical Fermi level $\mathcal{E}_{F,\mathrm{cr}}^0$ is the equilibrium Fermi energy such that at a high bias $\mathcal{E}_F^R-\mathcal{E}_F^L=\hbar\omega_{\mathrm{LO}}$ and $\mathcal{E}_F^L=\mathcal{E}_g/2$. From Eq. (4) the critical Fermi energy must be

$$\mathcal{E}_{F,\mathrm{cr}}^0=\frac{1}{2}\times\sqrt{(\hbar\omega_{\mathrm{LO}})^2+\hbar\omega_{\mathrm{LO}}\mathcal{E}_g+\mathcal{E}_g^2}, \tag{5}$$

and is dependent only on the bandgap and the LO phonon energy of the s-CNT, which are fixed by the diameter and the lattice structure. The corresponding equilibrium 1D critical carrier density is

$$n_{\mathrm{cr}}=\frac{g}{2\pi\hbar v_F}\times\sqrt{\hbar\omega_{\mathrm{LO}}(\hbar\omega_{\mathrm{LO}}+\mathcal{E}_g)}, \tag{6}$$

which again is a fundamental quantity for the s-CNT. Physically, if the carrier density is above this, the LEES is a *left*-going state (as depicted in Fig. 1), and if the carrier density is lower, then the LEES is a *right*-going state, as depicted in Fig. 2.

We define two ratios: $\alpha=\mathcal{E}_g/2\mathcal{E}_F^0$ and $\beta=\hbar\omega_{\mathrm{LO}}/2\mathcal{E}_F^0$. In addition, we consider only those semiconducting tubes for which $\mathcal{E}_g>\hbar\omega_{\mathrm{LO}}$ so that no interband optical phonon-assisted transitions are allowed. This condition implies that $\beta<\alpha<1$ when $\mathcal{E}_F^0>\mathcal{E}_g/2$, i.e., when the Fermi level is inside the band and carriers are available for current conduction. If $\mathcal{E}_F<\mathcal{E}_g/2$, no current flows at $T\to 0$ K.

Case 1: High carrier density: we first consider the situation when $\mathcal{E}_F^0\ge\mathcal{E}_{F,\mathrm{cr}}^0$, and $n\ge n_{\mathrm{cr}}$. Again, by ensuring particle number conservation and the condition $\mathcal{E}_F^R-\mathcal{E}_F^L=\hbar\omega_{\mathrm{LO}}$, the high-bias quasi-Fermi levels for the right and left going states are found to be

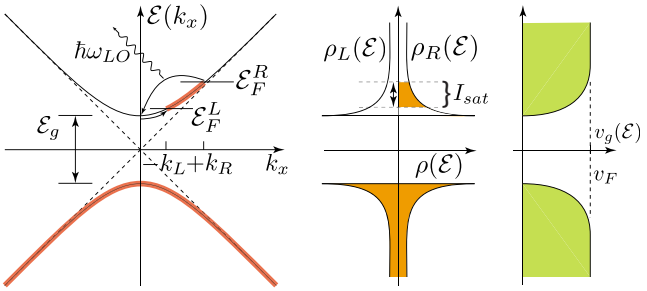


FIG. 2. (Color online) The occupation function of carriers for a s-CNT with $n<n_{cr}$ at high fields. The emission of optical phonons is possible when the highest occupied state and the lowest unoccupied state differ by an energy $\hbar\omega_{LO}$; the lowest unoccupied state here is the band edge. The group velocity of carriers as a function of their energy is also shown.

$$\mathcal{E}_F^R = \mathcal{E}_F^0\sqrt{1+\frac{\alpha^2\beta^2}{1-\alpha^2-\beta^2}}+\frac{\hbar\omega_{\mathrm{LO}}}{2}, \tag{7}$$

and

$$\mathcal{E}_F^L = \mathcal{E}_F^0\sqrt{1+\frac{\alpha^2\beta^2}{1-\alpha^2-\beta^2}}-\frac{\hbar\omega_{\mathrm{LO}}}{2}. \tag{8}$$

Case 2: Low carrier density: if on the other hand the equilibrium Fermi level is such that $\mathcal{E}_F^0<\mathcal{E}_{F,\mathrm{cr}}^0$, and $n<n_{\mathrm{cr}}$, then the condition $\mathcal{E}_F^R-\mathcal{E}_F^L=\hbar\omega_{\mathrm{LO}}$ cannot be satisfied due to insufficient carriers in the conduction band. However, since the LEES is now a right-going state, the condition $\mathcal{E}_F^R-\mathcal{E}_g/2=\hbar\omega_{\mathrm{LO}}$ still allows for the emission of LO phonons. Under this situation, the quasi-Fermi levels are given by

$$\mathcal{E}_F^R = \mathcal{E}_g/2+\hbar\omega_{\mathrm{LO}}, \tag{9}$$

and

$$\mathcal{E}_F^L = \mathcal{E}_F^0\sqrt{4-3\alpha^2+4\beta^2+4\alpha\beta-8\sqrt{\beta}\sqrt{1-\alpha^2}\sqrt{\alpha-\beta}}. \tag{10}$$

In this condition, the HFES $\mathcal{E}_F^R$ gets pinned at the energy $\mathcal{E}_g/2+\hbar\omega_{\mathrm{LO}}$ and the LEES is at the bottom of the conduction band. This case is depicted schematically in Fig. 2.

### C. Saturation current

The current flowing through the s-CNT is given in the $T\to 0$ K limit by the relation

$$I_{\mathrm{sat}} = eg\frac{1}{L}\sum_k f_k v_k = e\frac{g}{2\pi}\int_{k_L}^{k_R} dk v_g(k), \tag{11}$$

where $L$ is the length of the CNT, and $v_g(k)=\hbar^{-1}\nabla_k\mathcal{E}(k)=v_F k_x/\sqrt{k_x^2+k_n^2}$ is the projection of the group velocity of the carriers in the direction of the electric field. The saturation current for the CNT evaluates to

$$I_{\mathrm{sat}}(k_n,k_F) = e\times\frac{g}{2\pi}\times v_F\times[\sqrt{k_R^2+k_n^2}-\sqrt{k_L^2+k_n^2}], \tag{12}$$

which may be reduced the simpler form

$$I_{\mathrm{sat}} = e\times\frac{g}{2\pi}\times\frac{(\mathcal{E}_F^R-\mathcal{E}_F^L)}{\hbar}. \tag{13}$$

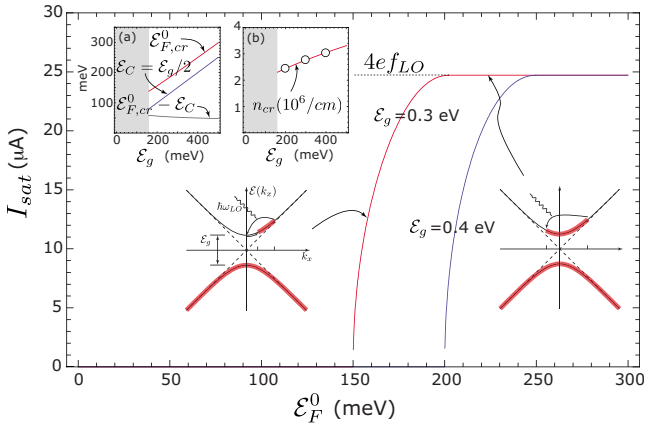


FIG. 3. (Color online) Saturation current of s-CNTs ($\mathcal{E}_g$=0.3 and 0.4 eV as a function of $\mathcal{E}_F^0$. The insets show (a) the critical Fermi level $\mathcal{E}_{F,\mathrm{cr}}^0$ and (b) the critical carrier concentration $n_{\mathrm{cr}}$ as a function of the bandgap of the s-CNT.

This is no different from what has been shown in Ref. 1 for m-CNTs, but it also holds for s-CNTs. The key point here is that for low fields, corresponding to $eV_{\mathrm{DS}}<\hbar\omega_{\mathrm{LO}}$, $\mathcal{E}_F^R-\mathcal{E}_F^L=eV_{\mathrm{DS}}$, and one recovers the Landauer relation $I=g(e^2/h)V_{\mathrm{DS}}$. However, the same relation may be used to understand saturation currents at high bias conditions as well. Since the respective quasi-Fermi levels were shown earlier to depend on the equilibrium Fermi level (or, indirectly, the carrier density), the saturation current in a s-CNT depends on $\mathcal{E}_F^0$. This is in stark contrast to m-CNTs, for which the quasi-Fermi level separation is $\hbar\omega_{\mathrm{LO}}$ leading to a saturation current of $I_{\mathrm{sat}}=4ef_{\mathrm{LO}}\sim 25$ $\mu$A, no matter where the equilibrium Fermi level $\mathcal{E}_F^0$.

In a s-CNT, the group velocity of a fraction of carriers near the band edge is less than or equal to $v_F$, whereas for a m-CNT is it *always* equal to $v_F$. Thus, the single subband saturation current in a s-CNT can *never exceed* the current in a m-CNT for the same carrier density. For high 1D carrier densities in s-CNTs [corresponding to $n>n_{\mathrm{cr}}$ or equivalently $\mathcal{E}_F^0>\mathcal{E}_{F,\mathrm{cr}}^0$ derived in Eqs. (5) and (6)], the saturation current is identical to that in a m-CNT, i.e., $I_{\mathrm{sat}}=4ef_{\mathrm{LO}}$ since the condition $\mathcal{E}_F^R-\mathcal{E}_F^L=\hbar\omega_{\mathrm{LO}}$ holds. This similarity can be understood by noting that there is a van Hove singularity at the band edge of s-CNTs. This implies that there are many more carriers that contribute to the saturation current in a s-CNT than in a m-CNT, though a fraction of those carriers move with velocities less than the Fermi velocity. Since the DOS for a m-CNT is $\rho_M(\mathcal{E})=g/\pi\hbar v_F$, the number of right-going carriers over a energy bandwidth $\hbar\omega_{\mathrm{LO}}$ is $n_M=4f_{\mathrm{LO}}/v_F$. The ratio of effective current-carrying states at saturation in a high-density s-CNT to that in a m-CNT is therefore greater than $n_{\mathrm{cr}}/n_M=\sqrt{1+(\mathcal{E}_g/\hbar\omega_{\mathrm{LO}})}$.

For carrier densities in s-CNTs less than $n_{\mathrm{cr}}$, the saturation current is given by Eq. (13), with $\mathcal{E}_F^R,\mathcal{E}_F^L$ from Eqs. (9) and (10). This dependence exemplifies how a s-CNT under a high source-drain bias "switches-off" when the Fermi level is pulled down toward the band edge and then into the gap, for example, by electrostatic gating. The dependence of the saturation current on $\mathcal{E}_F^0$ is plotted in Fig. 3 for s-CNTs for two representative bandgaps. The insets show the critical Fermi level [Fig. 3(a)] and the critical 1D carrier concentration

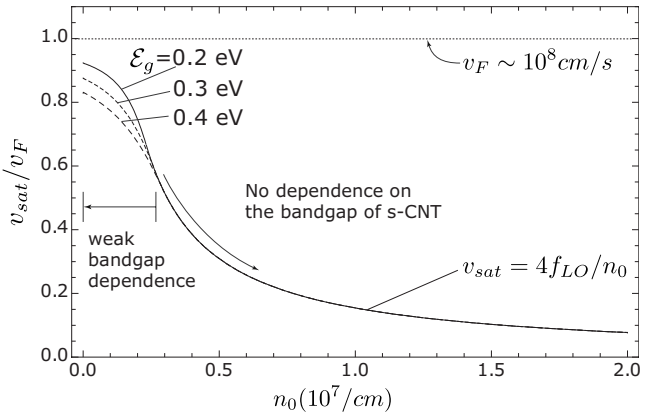


FIG. 4. Saturation velocity of carriers in s-CNTs with $\mathcal{E}_g$=0.2, 0.3, and 0.4 eV as a function of the 1D carrier density. For carrier densities $n_0 > n_{cr}$, $v_{sat}=4f_{LO}/n_0$, and has no dependence on the bandgap of the s-CNT; for $n_0 < n_{cr}$, the saturation velocity has a weak dependence on $\mathcal{E}_g$.

[Fig. 3(b)] above which the saturation properties of the s-CNT become indistinguishable from that of a m-CNT.

### D. Saturation velocity

Under the assumption that all carriers in the conducting band contribute to the saturation current equally, the saturation velocity of carriers may be written as $v_{sat}=I_{sat}/en_0$, which evaluates to

$$v_{sat} = v_F \times \frac{\frac{1}{2}(\mathcal{E}_F^R - \mathcal{E}_F^L)}{\sqrt{(\mathcal{E}_F^0)^2 - \left(\frac{\mathcal{E}_g}{2}\right)^2}} = \frac{g}{2\pi\hbar n_0} \times (\mathcal{E}_F^R - \mathcal{E}_F^L), \qquad (14)$$

and is strongly dependent on the 1D carrier density in the band. Figure 4 shows the dependence of the saturation velocity on the density as well as the corresponding equilibrium Fermi level for s-CNTs of varying bandgaps. For carrier densities $n < n_{cr}$, it increases and approaches $v_F$ as $n \to 0$ and $\mathcal{E}_g$ decreases. However, from Eq. (14), the saturation velocity at carrier densities $n > n_{cr}$ is given by $v_{sat}=4f_{LO}/n_0$, and is inversely proportional to the 1D carrier density. The theory is able to explain why the saturation velocity becomes *independent* of the bandgap of the s-CNT, as was found in numerical simulations of the BTE in Ref. 7.

### E. Graphene nanoribbons and semiconductor nanowires

The results derived here are applicable to gapped 1D graphene nanoribbons, but with a valley degeneracy of $g_v=1$, leading to half the saturation current compared to s-CNTs. Furthermore, the same theory may be applied to 1D quantum wires with parabolic band structures characterized by the effective mass $m^\star$. For the DOS defined by $\rho(\mathcal{E})=(g/2\pi)(2m^\star/\hbar^2)^{1/2}(\mathcal{E}-\mathcal{E}_c)^{-1/2}$ ($\mathcal{E}_c$ is the conduction band edge), the critical Fermi level is $\mathcal{E}_{F,cr}^0=\mathcal{E}_c+\hbar\omega_{LO}/4$, and the 1D critical carrier density is $n_0=(g/2\pi)[2m^\star(\hbar\omega_{LO})/\hbar^2]^{1/2}$. If the equilibrium Fermi level is located higher than the critical value, the saturation current in the nanowire is $I_{sat}=egf_{LO}$, and the ensemble saturation velocity of carriers is given by $v_{sat}=gf_{LO}/n_0$, where $n_0=(g/\pi)(2m^\star/\hbar^2)^{1/2}(\mathcal{E}_F^0-\mathcal{E}_c)^{1/2}$ is the 1D carrier density. Thus, in semiconductor nanowires in ideal 1D conditions, if the electron-LO phonon interaction is very strong and higher satellite valleys in the band structures are located at energies larger than $\hbar\omega_{LO}$ above the first subband minimum, the same phonon-limited saturation current limit should apply.

### F. Deviations from the theory

Within the limits of the theory presented, the saturation current in a s-CNT due to single subband conduction in the diffusive limit can never exceed $I_0=4ef_{LO}$. Any experimental observation of higher saturation currents in s-CNTs *must* be therefore attributed to effects that have not been considered. Five possible factors are listed: (a) nonuniform heating due to ultrafast LO phonon emission[2] and/or hot-phonon effects,[11] (b) ballistic effects (i.e., if the length of the CNT is shorter than the mean-free path for LO-phonon emission $L < \mathcal{L}_{LO}$),[12] (c) occupation of multiple subbands, (d) contribution from band-to-band Zener tunneling[13] and/or electron avalanching,[14] and (e) space-charge injection into the s-CNT by the contacts. These factors can be incorporated into the analytical framework presented here, but are not specifically considered in this work. Among the five factors, hot-phonon effects reduce the current drive, whereas ballistic transport is possible when electrons traverse the CNT without the emission of a single phonon. This implies a higher nonsaturating current—this is experimentally observed for short CNTs. Zener tunneling and avalanche processes add to the current carrying capacity above what is derived in this work, and typically precede catastrophic breakdown behavior.

## II. CONCLUSIONS

In conclusion, a simple analytical theory is presented that shows that current saturation in s-CNTs and m-CNTs are indistinguishable if the carrier density in the s-CNT is above a critical value determined by the bandgap and the LO phonon energy of the s-CNT. The ensemble saturation velocity is found to be independent of the bandgap of the s-CNT for such carrier densities. It is found that the same theory for the current-carrying capacity applies to graphene nanoribbons and semiconducting nanowires. The results derived are valid in the limit of ultrafast electron-optical phonon interaction and diffusive transport at high electric fields. Similar results can be derived for bulk semiconductors and two-dimensional electron systems such as in heterostructures and graphene. and be used to quantify the current carrying capacity of semiconductors of different dimensionality, and is a subject of future work.

## ACKNOWLEDGMENTS

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