An essential mechanism of heat dissipation in carbon nanotube electronics

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Excess heat generated in integrated circuits is one of the major problems of modern electronics. Surface phonon-polariton scattering is shown here to be the dominant mechanism for hot charge carrier energy dissipation in a nanotube device fabricated on a polar substrate, such as SiO2. Using microscopic quantum models the Joule losses were calculated for the various energy dissipation channels as a function of the electric field, doping, and temperature. The polariton mechanism must be taken into account to obtain an accurate estimate of the effective thermal coupling of the non-suspended nanotube to the substrate, which was found to be 0.1-0.2 W/m.K even in the absence of the bare phononic thermal coupling.

Introduction

Nowadays the vast majority of human activities are supported by advanced information technology which cannot become a transformative power without progress in semiconductor electronics. Exponentially increasing dissipated power density in integrated electronics circuits is one of the “grand challenges” of modern electronics [1, 2]. Excess heat generated by electric currents in the elements of circuits cannot be completely removed because of the high power density, which leads elevated device operation temperatures, performance reduction, and ultimately results in hardware failures.

Heat dissipation takes place via the transfer of thermal energy that is generated by hot charge carriers, to the cooling units eventually. The three classical mechanisms of heat transfer are convection, conduction, and radiation. The former is inapplicable in existing circuit architecture having no fluid or gas flowing inside. The latter has a total emissive power proportional to $T^4$ according to the Stefan-Boltzmann law, and is not very effective within the acceptable range of temperatures [3, 4]. Thus the major mechanism responsible for the device cooling is the thermal conductance. High thermal conductance can be achieved in bulk solids, but even a small vacuum gap is a quite effective thermal insulator.

This is the case for transistor channels involving a nanostucture, for example a nanowire or a nanotube [5, 6, 7], which is not chemically connected to the substrate, instead it is bound by relatively weaker van der Waals forces. This weak binding has a positive effect on the mobility of the charge carriers, but also has a negative effect on the thermal conductance. In existing nanotube transistors only the contacts have a good thermal exchange rate while the thermal conductance over the van der Waals separation gap is very low, of the order of 0.05–0.2 W/K.m [8, 9, 10, 11, 12]. In addition, the total thermal conductance of the contacts is not too high, being proportional to the cross-sectional area of the nanotube.

In this work we propose that a fourth mechanism of heat dissipation from the hot charge carriers in the nanotube channel into a polar SiO2 substrate should operate and argue that such a mechanism would dominate the thermal transfer especially at large device currents (high bias voltages). Understanding the importance of such a mechanism invokes concepts that are specific to carbon nanotube (NT) field-effect transistors (FET): low thermal conductance due to the van der Waals separation gap (and possible surfactant coating) and the small contact area, high Fermi velocity of the NT charge carriers and the existence of the special electromagnetic (EM) surface modes in the vicinity of the NT channel. Hot electrons, as we will discuss below, can excite surface polariton modes. This mechanism while important for nanoscale channels is ineffective in a macroscopic system because the EM field of the polariton decays exponentially with the distance from the surface plane [13]. This leads to a power low scaling of the scattering rate with the distance from the surface plane [14]. A surface polariton mode would quickly dissipate into bulk substrate modes, thus providing a heat transfer mechanism with an efficiency exceeding the standard thermal conductance or radiation mechanisms.

The existence of surface polariton modes was predicted in 1899 [15] and were later observed at AM radio-wave frequencies. In condensed matter, a metal surface is known to support surface EM modes that is plasmon-polaritons; the focus of recent plasmonics studies [16]. The plasmon-polariton EM mode exists if the real part of the dielectric function $\varepsilon$ of the substrate equals negative one [17]. Similarly, one can observe a surface polariton in a polar insulator where a strong optical phonon provides the required condition: $\varepsilon = -1$. Then the frequency of the surface phonon-polariton (SPP) is close to the frequency of the optical phonon. For exam-
ple, for a SiO$_2$ surface the optical phonon modes that can support SPP are at $\hbar \omega = 50, 62, 100$ and 149 meV \cite{18, 19, 20}. Hot charge carriers in a NT FET with energy exceeding the polariton energy would effectively release energy into the SPP channel.

We stress that despite the fact that this mechanism is similar to a classical one for hot charge carrier energy relaxation whereby the energy dissipates into optical phonons of the NT \cite{21, 22, 23, 24}, the SPP mechanism transfers the thermal energy directly into a bulk substrate, while the classical one only redistributes it between the NT electrons and the NT lattice, to be followed by thermal conduction into the leads and/or the substrate. The SPP mechanism also differs from the classical radiation since the charge carriers in the channel couple to the evanescent EM modes only. The greatly enhanced surface electric field of such modes has much larger overlap with the NT channel than it would be in the case of the free vacuum EM modes\cite{1}.  

Simulation approach

We have adopted the model described in detail in the previous works \cite{14, 21, 28}. In brief, a standard tight-binding Hamiltonian for the NT charge carriers, $H_e = \sum_{i,j} t_{ij} a_i^\dagger a_j$, is supplemented with Su-Schrieffer-Heeger terms for the electron-NT-lattice-phonon coupling (Eq.(1) of Ref.\cite{24}):

$$H_{NT} = \sum_{k,q,\mu} M_{kq}^\mu (a_{-q}^\dagger + a_{q}) \left( c_{\nu,k+q}^\dagger c_{\nu,k} + c_{\nu,k+q}^\dagger c_{\nu,k} \right)$$ (1)

here the matrix element of the interaction is $M_{kq}^\mu \propto \Xi = 5.3$ eV/Å. The coupling constant is $\Xi \propto t - t_o$, where $t_o = 3$ eV is the bare tight-binding hopping integral being modulated by the phonon modes. $a_{q}$ and $c_{\nu,k}$ are annihilation operators for NT phonons ($\mu$ is a phonon branch index) and charge carriers in conduction and valence bands, respectively, that are labeled with the one-dimensional axial momentum $q$ or $k$. In addition to the NT lattice phonons we include the operator of the interaction with the SPP mode (cf. Eq.(2) in Ref.\cite{24}):

$$H_{SPP} = \sum_{k,q,\nu} V_{k,q,\nu} \left( a_{-q,k,\nu}^\dagger + a_{q,k,\nu} \right) c_{k+q}^\dagger c_k$$ (2)

where $a_{q,k,\nu}$ is the annihilation operator for the $\nu$-th surface phonon mode (not to be confused with the NT lattice phonons), and an explicit form of $V_{k,q,\nu}$ was derived in Ref.\cite{27}:

$$V_{k,q,\nu} = \frac{2i\pi e F_\nu (-q) m e^{-h \sqrt{q^2 + q_\perp^2} I_m(qR)}}{\sqrt{q^2 + q_\perp^2} \left( \sqrt{q^2 + q_\perp^2} - q_\perp \right)^m}$$ (3)

where $q$ and $q_\perp$ are the components of the SPP momentum that are parallel and normal to the NT axis respectively (see Fig.\[1\]), $m$ is the angular momentum transfer to the SPP mode (equals 0 in case of the NT intra-subband scattering which is the strongest scattering channel), $R$ is the NT radius, $h \approx R + 4$ Å is the distance from the NT axis to the surface, $I_m(x)$ is the Bessel function of imaginary argument $\frac{1}{2}$. $c$ is the elementary charge and $F_\nu$ characterizes the strength the electric field of the SPP mode \cite{17}:

$$F_\nu^2 = \frac{\hbar \nu_{LO}^\nu}{2\pi S} \sqrt{1 + \frac{\epsilon_\infty^2}{\epsilon_\infty^1} \left( \frac{1}{\epsilon_\infty^1 + 1} - \frac{1}{\epsilon_0 + 1} \right)}$$ (4)

where $S$ is the normalization surface area, $\omega_{LO}^\nu$ is the frequency of the longitudinal optical phonon of the polar substrate with the static permittivity $\epsilon_0$ and the low-frequency dielectric function $\epsilon_\infty$. We should emphasize that while there are four surface modes present (the highest energy one being doubly degenerate), only two of them have strong coupling strength \cite{13, 27}: $S F_\nu^2 |_{\nu = 1, 5} = 0.042, 0.38, 0.069, 1.08, 1.08$. The characteristic distribution of the electric field of the SPP mode above the substrate surface is shown in Fig.\[1\]. The field oscillates along the surface (along $q$) and decays exponentially in the space (along $q_\perp$). The transverse component of the SPP momentum, $q_\perp$, is not conserved and has to be integrated for the final result.

To simulate the current-voltage curves we solved numerically the steady-state Boltzmann equation for the NT in a constant electric field (including as many subbands as needed for given temperature and drain field values). One can assume that in the bulk of the FET channel the drain voltage $V_d$ is related to the applied electric field via the effective channel length $L$: $F = V_d/L$. The scattering rates for the Boltzmann equation are as follows (see Refs.\cite{11} and \cite{24} for further details):

$$W_{kq} = \frac{S}{\hbar L} \sum_\nu \int_0^\infty dq_\perp |V_{k,q,\nu}^\nu|^2 \times$$

$$\times \left( n_{q_\perp} \delta (E_f(k) + \hbar \omega_{SO}^\nu - E_i(k + q)) + (n_{q_\perp} + 1) \delta (E_f(k) - E_i(k + q) - \hbar \omega_{SO}^\nu) \right)$$ (5)

where $\hbar \omega_{SO}^\nu$ is the frequency of the SPP mode \cite{17}: $n_{q_\perp}$ its phonon occupation number, $E_f(i/k)$ is the energy of the final/initial state as obtained from the Hamiltonian $H_e$. Non-equilibrium distribution function $g_k$ has been calculated numerically for every given value of the temperature, field and charge density and then it was used to compute the total electron current, $I_d$, as well as to determine the partial phonon emission rates for the heat dissipated in the NT lattice $P_J$ and that dissipated directly into the substrate via the SPP mode $P - P_J$, ac-
SPP Scattering and NT-FET High Bias Regime

The role of the SPP modes with respect to charge carrier scattering (so-called Remote Interface Phonon scattering) for Si devices has been first studied by Hess and Vogl [25], though this mechanism was not found to dominate the transport [26]. As we show in this work, for nanotube devices the SPP scattering mechanism is very fast, as been indicated already in our earlier paper [27] and cannot be neglected even for the low-field transport [14].

The SPP energy relaxation rate exceeds the intrinsic NT phonon relaxation rates (for both optical and acoustic modes) for the whole range of the charge densities and applied electric fields (gate and drain biases) studied here as shown by the results in Fig. 1b.

Recently SPP scattering was demonstrated to determine the mobility in graphene on a polar substrate and to limit the ultimate performance of graphene devices [29][30][31]. Fig 1 shows typical current-electric field curves calculated with and without the SPP mechanism taken into account. Neglecting the SPP channel significantly overestimates the low-field current. Two important conclusions are drawn from these data: firstly, the negative differential resistance region of the current-voltage characteristic is totally removed when the SPP channel included, because the very effective SPP energy relaxation prevents the hot electron run-away as we further discuss in Ref. [14]. Secondly, the SPP mechanism dominates over the NT phonon scattering for both low- and high-field regimes but the remnants of the non-SPP behavior can be seen at low applied field especially at low temperature.

Results on the relative importance of the SPP and NT-phonon scattering channels for the energy relaxation of the hot charge carriers are shown in Fig 2a. In Fig 2a we plot, in a logarithmic scale, the partial specific energy losses due to the SPP channel (full curves) and only the NT phonon channel (broken curves), calculated for [17,0] NT at the doping level $\rho = 0.1$ e/nm at various temperatures. The SPP losses are up to two orders of magnitude larger than the NT phonon losses. Fig 2b presents the ratio of the SPP partial losses to the NT phonon partial losses calculated for the same NT. The high frequency NT optical phonons increase the NT partial losses at higher fields and higher $T$ (Fig 2b). Even in that limit their ratio $\xi$ is always greater than one.

We also studied the dependence of the loss ratio on the doping level $\rho$ (Fig 2a, inset) at the fixed applied electric field $F = 5$ V/µm. The relative decrease of the SPP contribution at higher electron density (higher gate bias) is shown in Fig 2c as a percentage of the total losses and is due to the SPP and NT phonon losses having a different functional dependence on $\rho$. The non-equilibrium distribution function (obtained as a numerical solution

$$P - P_f = \frac{2}{hL} \sum_{k,q} W_{k,q} g_k (1 - g_{k+q}) (E(k) - E(k + q))$$

where $P = I_dF$ are the total Joule losses. A similar equation holds for NT losses $P_f$ with the scattering rate obtained from Eq. (1). In the following we study dependencies of the SPP to the NT channel loss ratio, defined as $\xi = P/P_f - 1$, on the bias, density, and temperature.

**FIG. 1:** Role of SPP inelastic scattering mechanism for NT FET transport. (a) Current-electric field curves for [17,0] NT at the doping level $\rho = 0.1$ e/nm, $T = 77, 150, 210, 300, 370, 450$ K as indicated by the color code. Full line corresponds to the room temperature characteristic with both SPP and NT phonon scattering mechanisms included, as compared to the SPP scattering only (red dotted curve slightly above) and NT phonon scattering only (light blue dotted curve at the top). Insets in (a) shows the drift velocity vs. the doping level at $F = 5$ V/µm and $T = 300$ K. (b) The energy relaxation time vs. applied electric field using both SPP and NT scattering for the same NT and same temperatures. Inset in (b) shows dependence of the energy relaxation time on the doping level at $F = 5$ V/µm and $T = 300$ K. (c) Schematics of the NT channel on a SiO$_2$ substrate (3D image is generated using Molecular Dynamics in NAMD/VMD). Accepted convention for the components of the in-plane wave-vector of the SPP mode and the coordinate system are shown. (d) Distribution of the electric potential and its gradient for a Surface Phonon Polariton (SPP) mode.
of the Boltzmann equation) varies with the doping level. The SPP losses, correlated with the non-equilibrium distribution function, scale similar to the total losses (proportional to the current) and are approximately a linear function of the doping level (total number of electrons). The NT phonon losses are superlinear in $\rho$ and grow faster, thus their ratio $\xi$ decreases with $\rho$.

To understand the dependencies of the NT and SPP losses on field strength and temperature, we show the scattering rate of electrons via these two channels in different bands as a function of energy (see Supplemental Information Fig. 3). In the first two energy bands the SPP scattering dominates over the NT scattering, while in the higher energy bands the NT scattering becomes comparable to that of the SPP scattering. This is because in the SPP scattering the angular momentum is conserved $\Delta m = 0$, so that only intra-band scattering takes place, while NT optical phonons can lead to both intra and inter-band scattering and the phase space for such scattering grows with the band index. Therefore, as the electronic distribution becomes hotter either due to the field or temperature the relative role of the NT phonons increases and the loss ratio $\xi$ decreases. Fig. 4S (Supplemental Information) further supports that the electronic distribution function rather than the scattering rate (see Eq. (6)) is primarily responsible for the value of the loss ratio at the high bias regime. Therefore the NT and SPP losses scale in exactly the opposite way with temperature.

Near-Field Thermal Conductance and Self-Heating of NT-FET Channel

Next we discuss another aspect of SPP scattering, namely we address how the heat generation is controlled by the fast SPP energy relaxation rates.

So far we set the NT temperature equal the substrate temperature. That is we assumed an ideal thermal coupling to the substrate which is a condition not confirmed experimentally. As a next level of approximation we use thermal coupling values (per NT length) from the literature [8, 9, 10, 11, 12] ranging from $g_o = 0.05$ to $0.2 \text{ W/K.m}$ and estimate the FET channel heating. The lower bound of the thermal coupling, as it will be shown below, gives so small a thermal exchange to the substrate that it is almost equivalent to assuming no thermal coupling at all (see Supplementary Figure 1). Thus we analyze first the temperature of the NT FET channel for the high value of the thermal coupling to the substrate $g_o = 0.19 \text{ W/(K.m)}$.

All energy loss of the hot electrons, same as the total dissipated power, is distributed between two channels: the SPP losses which are to be subtracted from the total heat flux in the NT, and the NT losses which have to be partially transmitted to the substrate via the coupling $g_o$. Fig. 2(c) presents an effective channel temperature (the Joule overheating) as a function of the applied electric field calculated for NT phonons only (upper curves’ family) and for both NT and SPP channels (lower curves’ family). The SPP scattering channel couples to the substrate phonons and thus transfers most of the excess thermal energy of the hot electron directly into the substrate. In contrast, the NT phonon scattering transfers the energy to the NT lattice. As a result the steady-state temperature of the NT lattice increases from the ambient temperature, $T_{sub}$. For a very long NT FET channel all edge effects due to the electron and phonon thermal conductivity can be neglected, as well as a heat flux due to

$$T = T_{sub} + \Delta T = T_{sub} + \frac{P_J}{g_o} \quad (7)$$

where $P_J$ is the dissipated power per NT length due to the NT phonon scattering. The Joule overheating $\Delta T$ is found to be orders of magnitude smaller compared to the case when SPP channel is neglected and all the measured Joule losses are attributed to the NT phonons, i.e. $P_J = P = I_d F$ (see Fig. 2c). The ratio of the SPP losses to NT losses, $\xi$, as a function of the applied field and doping level is given in Fig. 2c and in the inset (e). The temperature rise $\Delta T$ is inversely proportional to $g_o$ according to Eq. (7). Even though the loss ratio depends on $g_o$ (see below), which is not precisely known, it is safe to conclude that the temperature of non-suspended NT channel will be much lower for the same total power density $P$.

Within this non-self-consistent scheme one overestimates the overheating because one neglects $\Delta T$ when calculating the current, the SPP and Joule heat (NT) losses. Next we part this approximation and provide fully self-consistent analysis of the channel temperature.

Given the expected temperature rise of the NT FET channel (for a given value of the bare thermal coupling) we recalculate the electron and phonon distribution and obtain the self-consistent NT temperature by iteration. At $n$-th step we solve the Boltzmann equation using the NT-lattice temperature $T_{n-1}$, calculated at the previous step according to Eq. (7), and then compute the total energy released in the NT-phonon subsystem. Next, using Eq. (7) we calculate the new lattice temperature $T_n$. The process is iterated until convergence.
In a real device the non-zero bare thermal coupling \( g_o > 0 \) results in even higher values of the total thermal coupling. Effective thermal coupling \( g \) and the ratio \( g/g_o \) are presented in Fig. 3 panels (c-f) vs. the doping level at fixed electric field \( F = 5 \, \text{V/µm} \) and also vs. the field for \( \rho = 0.1 \, \text{e/µm} \) and various bare couplings \( g_o = 0.05, 0.10, 0.15 \) and 0.19 \( \frac{W}{K \, m} \) (from red to blue). We conclude that the SPP, near-field, thermal conductance is always larger than the bare thermal coupling by at least an order of magnitude.

We note that in the presence of dissipation mechanisms to both SPP and NT channels, the total thermal conductivity of the NT FET becomes a function of bias and density and the analysis of the electric heating through Joule’s, Fourier’s and Ohm’s laws, often used in literature \([33, 34]\), must account for these dependencies. In such a case, one has to calculate a self-consistent non-equilibrium distribution function first and find the lattice (phonon) temperature. The total thermal flux has two components: the SPP channel flux and the NT-substrate flux. We predict that for supported (non-suspended) NT device on a polar substrate the SPP dissipation channel is major and dominates over the NT-substrate thermal dissipation. Therefore, an effective thermal coupling through the NT-substrate interface appears to be significantly larger as compared to the bare thermal coupling on a non-polar substrate.

**Conclusions**

In this paper we presented a microscopic quantum modeling of a novel heat dissipation mechanism for nanotube electronic devices. This mechanism is specific for NT devices fabricated on polar substrates, such as SiO₂, due to (i) existence of surface EM modes at the frequencies of the surface photon-polaritons, (ii) strong coupling of such modes to the charge carriers in the NT lying on the substrate. We note that a similar SPP thermal coupling should exist in other 1D and 2D systems fabricated with other channel materials on polar insulator substrates. In particular, high-k oxides are expected to produce strong SPP scattering due to their large Fröhlich constants and their low optical phonon frequencies.

Using a semiempirical quantum approach we have calculated current-voltage curves with and without SPP scattering and concluded that the SPP mechanism dominates the scattering and determines the drain current in the whole range of drain voltages, and for all studied doping levels and temperatures. The current (charge density) and temperature scaling of the SPP and NT scattering mechanisms are different, thus allowing verification of our predictions experimentally. In this work we focused on the FET high bias regime and demonstrated that the SPP mechanism, being much more efficient than the scattering by NT lattice modes, results in the elimination of the negative differential resistance part of the current-voltage curve. We analyzed the relative impor-

**FIG. 2:** Comparison of the hot electron temperature relaxation via SPP and other inelastic scattering channels. (a) Logarithm of the partial specific energy losses due to the SPP channel (full lines) and the NT phonon channel (broken curves) for \([17,0]\) NT at the doping level \( \rho = 0.1 \, \text{e/µm} \) (the temperature range is indicated by the color code \( T = 77, 150, 210, 300, 370, 450 \, \text{K} \) arrows point to increasing temperatures). (b) The ratio of the SPP partial losses to the NT partial losses, \( \xi = P/P_j \) – 1, vs. applied electric field for the same NT. (c) Estimated effective NT FET channel temperature vs. applied electric field calculated for \([17,0]\) NT on SiO₂ substrate. NT phonon contribution (upper curves’ family) is compared with both NT and SPP channels (lower curves’ family) for the bare thermal coupling to the substrate \( g_o = 0.19 \, \frac{W}{K \, m} \), \( \rho = 0.1 \, \text{e/µm} \). (d) The loss ratio \( \xi \), calculated including self-consistent NT heating, is shown as a function of the doping level and the applied electric field. Here \( g_o = 0.19 \, \frac{W}{K \, m} \), \( T_{\text{sub}} = 300 \, \text{K} \). (e) Relative contributions of the SPP (red curve) and NT (blue curve) channels to the total energy losses (black curve) vs. the doping level at \( F = 5 \, \text{V/µm} \); the inset shows their ratio.

At zero bare thermal coupling \( g_o = 0 \), SPP channel controls the Joule heating. The field and concentration dependence of the FET temperature at \( g_o = 0 \) is presented in Fig. 3a. The upper (purple) curve corresponds to \([17,0]\) NT on SiO₂ substrate at \( T_{\text{sub}} = 300 \, \text{K} \), \( \rho = 0.4 \, \text{e/µm} \). A temperature rise higher than 600 K can be expected at such conditions \([22]\). By decreasing the doping level 4 times (red curve) we decrease the steady-state temperature due to a smaller value of the Joule losses, proportional to the current \( \sim I_d \sim \rho \). Additional decrease is associated with a gradual dependence of the loss ratio \( \xi \) on the density (Fig. 2 inset). To further explore the nature of this cooling down of the NT FET channel we compute the effective thermal coupling to the SiO₂ substrate, defined as \( g = (I_d F)/\Delta T \). We extract it from the self-consistent temperatures data (as in Fig. 2a) and plot it vs. the applied field, \( F \), and vs. the total dissipated power per NT length, \( P \), in Fig. 3b.
Bare thermal coupling is set to \( g_0 = 0 \) by an order of magnitude. The dependence of the effective thermal conductivity via the NT-SiO\(_2\) interface for the same NT as in (a) due to the SPP coupling, as extracted from the self-consistent temperatures data, vs. applied electric field. Inset shows the same data vs. dissipated power per NT length. (c-f) Effective thermal coupling \( g \) and \( g/g_0 \) ratio vs. the doping level at \( F = 5 \) \( V/\mu m \). The same vs. applied electric field at \( \rho = 0.1 \) \( e/\text{nm} \). Bare thermal coupling is \( g_0 = 0.01, 0.05, 0.19 \) \( W/\text{K.m} \) in (c) and (d) and \( g_0 = 0.01, 0.05, 0.10, 0.15 \) and \( 0.19 \) \( W/\text{K.m} \) (from blue to red) in (d) and (f).

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\[ g_{SB} = \frac{S/L}{\pi^2 k_B^4 / (60 \pi h^2 c^2)} (T_1^4 - T_2^4) / (T_1 - T_2), \]

where \( T_{1,2} \) are the NT and substrate temperatures (giving two fluxes in the opposite directions), the channel area per unit length can be estimated as \( S/L = 2 \pi r \), where \( R \) is a tube radius. In case of a near room temperature environment \( (T_1 = 400 \text{ K} \) and \( T_2 = 300 \text{ K} \) we obtain: \( g_{SB} \sim 10^{-7} \text{ W/(K.m)} \), which is much smaller than the bare phonon thermal conductivity in the range of \( g_o \sim 0.05 - 0.2 \text{ W/(K.m)} \).
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