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Field emission from two dimensional materials: a quantum mechanical model and its application to graphene

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Abstract—Electron field emission from two dimensional materials and in particular from graphene is modelled using the Bardeen transfer Hamiltonian formalism. In the case of graphene, a full electronic band model of the material (the tight-binding model) is necessary to obtain reasonable results because emission is not restricted to the vicinity of the Dirac points. The emitted current density is small and follows a modified Fowler-Nordheim law with respect to the applied field, with a prefactor exponent for the field $n \approx 1.5$ intermediate between the values for the 2D ($n = 0$) and 3D ($n = 2$) free electron gases. Our study suggests that emission from graphene results almost exclusively from defects.

I. INTRODUCTION

The original Fowler–Nordheim model (FN) still forms nowadays the dominant paradigm to understand electronic field emission [1]. It provides, in particular, an analytical relation between emitted current density J and applied electric field F :

$$J(F) = \frac{q^3 F^n}{16\pi^2 \hbar W} e^{-\frac{4}{3} \left(\frac{2m}{\hbar^2} \right)^{\frac{1}{2}} \frac{W^2}{qF}} \quad (\text{eq. 1})$$

with $n=2$. \hbar is the reduced Planck constant, q the absolute value of the charge of the electron, m its mass, W the work function of the emitting material. Although used widely and successfully over the years, the FN model relies on a crude description of the emitting electrode with a three dimensional (3D) homogeneous electron gas which is obviously questionable if the electrode is a two dimensional (2D) material such a graphene [2-4]. We present here a new model of field emission which is applicable to both 2D and 3D materials [2].

II. MODEL

The present general model is based on the Bardeen transfer Hamiltonian formalism [5-6] coupled to a detailed description of the electronic structure of the material. We consider a portion of area S (in the (x,y) plane) of an emitting material of thickness L . When subjected to the external electric field F , it emits an averaged current density $J(F)$ which is obtained by integration over the electron momentum \mathbf{k} in the first Brillouin zone of the D-dimensional reciprocal space:

$$J(F) = \frac{L^{D-2}}{2^{D-1} \pi^D} \iint d^D \mathbf{k} I_{\mathbf{k}}(F) \quad (\text{eq. 2})$$

$D = 2$ or 3 refers to the dimensionality of the material. The contribution of the electrons with momentum \mathbf{k} is:

$$I_{\mathbf{k}}(F) = q \frac{2\pi}{\hbar} \left| \iint_{x,y \in S} dx dy M_{\mathbf{k}}(\mathbf{r}, z_0, F) \right|^2 \quad (\text{eq. 3})$$

where $\mathbf{r} = (x, y)$ and z_0 is the height of the electrostatic potential barrier confining the electrons in the material. $M_{\mathbf{k}}$ is given by:

$$M_{\mathbf{k}}(\mathbf{r}, z_0, F) = \frac{\hbar^2}{2m} \left(\Psi_{\mathbf{k}}(\mathbf{r}, z_0, F)^* \frac{d\Phi_{\mathbf{k}}(\mathbf{r}, z_0)}{dz} - \Phi_{\mathbf{k}}(\mathbf{r}, z_0) \frac{d\Psi_{\mathbf{k}}(\mathbf{r}, z_0, F)^*}{dz} \right) \quad (\text{eq. 4})$$

$\Phi_{\mathbf{k}}(\mathbf{r}, z)$ is a material valence electron orbital and $\Psi_{\mathbf{k}}(\mathbf{r}, z, F)$ the continuum state that describes the electron outside the material. In our implementation for graphene [2], $\Phi_{\mathbf{k}}(\mathbf{r}, z)$ is obtained from a tight-binding model [7] and $\Psi_{\mathbf{k}}(\mathbf{r}, z, F)$ is the product of a plane wave in \mathbf{r} and of a properly normalized Airy function in z .

III. RESULTS

In order to validate the proposed formalism, we first apply it to the material of the FN model which is a 3D free-electron gas. We obtain:

$$J(F) = \frac{q^3 F^2}{16\pi^2 \hbar (WW_B)^{\frac{1}{2}}} e^{-\frac{4}{3} \left(\frac{2m}{\hbar^2} \right)^{\frac{1}{2}} \frac{W^2}{qF}} \quad (\text{eq. 5})$$

where W_B is the material valence band width. This result is similar to the FN current density (eq. 1) if we substitute W to $(WW_B)^{\frac{1}{2}}$. In particular, the same field exponent $n=2$ is obtained for the prefactor. As both quantities W and $(WW_B)^{\frac{1}{2}}$ have the same order of magnitude, the present model provides results close to the FN one.

Contrary to the FN model, the present formalism extends naturally and immediately to 2D materials. In the case of a 2D free electron gas : $\Phi_{\mathbf{k}}(\mathbf{r}, z) = \frac{1}{\sqrt{S}} e^{i\mathbf{k}\mathbf{r}} \varphi(z)$ where $\varphi(z)$ is a bound state in z describing the motion of the confined electrons perpendicular to the material plane. Insertion of this expression in eqs. 2-4 provides:

$$J(F) = \frac{q(2m)^{\frac{1}{2}}}{\pi\hbar^2} W_B (W + W_B)^{\frac{1}{2}} |\varphi(z_i)|^2 e^{-\frac{4}{3} \frac{(2m)^{\frac{1}{2}} (W + W_B)^{\frac{3}{2}}}{qF}} \quad (\text{eq. 6})$$

In going from the 3D to the 2D free electron gas, the F^2 pre-factor is lost as the field exponent changes from $n=2$ to $n=0$. $\log J(F)$ is linearly dependent with respect to $1/F$, with a slope controlled by $W+W_B$ in the 2D case, the energy necessary to extract an electron from the band bottom, instead of by W , the work function necessary to extract an electron from the band top, in the 3D case.

In the case of graphene, there is no compact analytical form for the emitted current density but a numerical solution to eqs. 2-4 can be found and it can be fitted to an analytical form akin to eq. 1, keeping the field exponent n in the pre-factor and work function W as free fitting parameters. Figure 1 provides current densities obtained for the tight binding model for graphene [2, 7] as well as fit results. The best fit is obtained for $n=1.53$ and $W=12.78$ eV. A power law with $n \approx 1.5$, intermediate between the 2D and 3D free-electron gas cases, is thus found to provide the best model for graphene. A similar $n=3/2$ exponent has already been obtained experimentally [8] as well as in a theoretical study of emission from a graphene nanowall, where the graphene flake is mounted perpendicularly to its substrate [9].

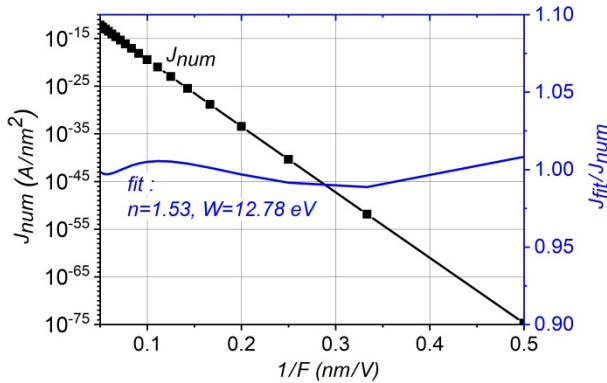


Fig. 1 Full black line connecting symbols (left scale, A/nm^2): emitted current density J_{num} as the function of the applied electric field F (V/nm), obtained by numerical integration [eqs. 2-4]. The parameters of the model are the same as in [2]. Blue line (right scale): ratios between fitted and numerical results $J_{\text{fit}}/J_{\text{num}}$. The fit parameters are: $n=1.53$ and $W=12.78$ eV.

We know which regions of reciprocal space are the main contributors to emission from the dependence of $I_k(F)$ (eq. 3) with respect to \mathbf{k} . Interestingly, emission from the vicinity of the K point - the so called Dirac point at the Fermi level where the valence band touches the conduction one - is negligible. Instead, emission is maximum in an annular region around the Γ point ($\mathbf{k}=0$). In fact, for both 2D and 3D materials, emission is expected to be maximum for \mathbf{k} vectors such that the energy

available to overcome the tunnelling barrier - i.e. the energy associated to the z motion (perpendicular to the potential barrier) - is maximum. This energy is $\Delta e_k = \varepsilon_k - \frac{\hbar^2 k_{xy}^2}{2m}$ where ε_k is the material electron energy and \mathbf{k}_{xy} its momentum component parallel to the surface. Whereas Δe_k maximum is located for 3D materials on the Fermi surface where 2 conditions (ε_k maximum - by definition of the Fermi surface - and $\frac{\hbar^2 k_{xy}^2}{2m}$ minimum - i.e. $\mathbf{k}_{xy}=0$) can be simultaneously satisfied, this is not this case in general for 2D materials where the maximum of ε_k does not correspond necessarily to \mathbf{k} vectors for which $\frac{\hbar^2 k_{xy}^2}{2m}$ is minimum (i.e. $\mathbf{k}_{xy}=0$). In this case, Δe_k maximum is obtained for \mathbf{k} values which do not belong to the Fermi surface. As a consequence, a full band model is necessary to study emission from 2D materials like graphene and linear approximations valid only in the vicinity of the Dirac points are not sufficient.

IV. CONCLUSIONS

We have presented an extension of the Fowler-Nordheim model to 2D materials based on the Bardeen formalism. The model has been applied to free electron gas and to graphene. We have shown that the usual Fowler-Nordheim expression has to be modified to be valid for such materials. Notice finally that the emitted current levels are low because the electron kinetic energy corresponds to a motion parallel to the emitting surface, which is not efficient in promoting emission from the surface. This suggests that the significant emission levels [8, 10-11] measured on graphene result almost exclusively from deviations from the perfect graphene 2D structure considered here.

REFERENCES

- [1] R. Diehl, M. Choueib, S. Choubak, R. Martel, S. Perisanu, A. Ayari, P. Vincent, S. T. Purcell, and P. Poncharal, Phys. Rev. B **102**, 035416 (2020).
- [2] B. Lepetit, J. Appl. Phys. **129**, 144302 (2021).
- [3] Y. S. Ang, S.-J. Liang, and L. K. Ang, MRS Bull. **42**, 505 (2017).
- [4] Y. S. Ang and L. K. Ang, in 31st International Vacuum Nanoelectronics Conference (IVNC), Kyoto (IEEE, 2018), p. 1.
- [5] J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).
- [6] R. Ramprasad, L. R. C. Fonseca, and P. von Allmen, Phys. Rev. B **62**, 5216 (2000).
- [7] A. H. Castro-Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009).
- [8] Z. Xiao, J. She, S. Deng, Z. Tang, Z. Li, J. Lu, and N. Xu, ACS Nano **4**, 6332 (2010).
- [9] X.-Z. Qin, W.-L. Wang, N.-S. Xu, Z.-B. Li, and R. G. Forbes, Proc. R. Soc. A **467**, 1029 (2011).
- [10] L. Chen, H. Yua, J. Zhong, L. Song, J. Wuc, and W. Su, Mater. Sci. Eng. B **220**, 44 (2017).
- [11] F. Giubileo, A. D. Bartolomeo, L. Iemmo, and G. Luongo, Appl. Sci. **8**, 526 (2018).