Modeling of electronic dynamics in swift heavy ion irradiated semiconductors

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Motivation

- The modern particle physics requires the use of extremely large and costly composite detectors. The new generation of high energy experiments at colliders will use semiconductor (silicon) tracking detectors in a heavier way than in the past.

- One of the scientific pillars of FAIR is nuclear-structure physics with radioactive ion beams.

- The semiconductor (silicon) instrumented trackers - detectors should be fully operational for at least *10 years*

- Detector diagnostic and repair comprises a very expensive and labor-consuming procedure.

- At the microscopic level the radiation damage suffered by the detectors can be divided in two different classes: effects which are due to surface damage and those which are due to **bulk damage**.

- The study of interaction of swift heavy ions with semiconductor single crystals is very important both for the fundamental investigations of **radiation effects in condensed matter** and for the creation of **ion tracks in semiconductor materials** – provides detector reliability and hardness insurance.

- To achieve microscopic understanding of the fast ion irradiation of materials used for detectors we restrict ourselves to describing the damage produced in GaAs semiconductor when irradiated with swift heavy ions (coming from a given experimental radiation environment) by

- utilizing a theory developed for GaAs material irradiated with femotosecond laser pulse.

•We consider a bulk GaAs semiconductor doped with electron concentration to form a 3D electron gas.

•We separate the dynamics of a many-electron system into a center-of-mass motion plus a relative motion under both dc and infrared fields-

•X.L. Lei and C.S. Ting, J. Phys. C **18**, 77 (1985), D. Huang, T. Apostolova, P. Alsing, D. A. Cardimona, Phys. Rev. B 69, 075214 (2004)

•The relative motion of electrons is studied by using the Boltzmann scattering equation including anisotropic scattering of electrons with phonons and impurities beyond the relaxation-time approximation.

•The coupling of the center-of-mass and relative motions can be seen from the impurity and phonon parts of the relative Hamiltonian

•The incident electromagnetic field is found to be coupled only to the center-of-mass motion but not to the relative motion of electrons.

•This generates an oscillating drift velocity in the center-of mass motion, but the time-average value of this drift velocity remains zero.

$$\hat{H}_{CM} = \frac{(\hat{\vec{P}}^C)^2}{2N_e m^*} + \frac{N_e e^2 A^2}{2m^*} - \frac{e\vec{A}.\hat{\vec{P}}^C}{m^*}$$

•The oscillating drift velocity, however, affects the electron-phonon and electron-impurity interactions.

•The dynamics of electrons is determined by the relative motion of electrons - scattering of electrons with impurities, phonons, and other electrons.

- The effect of an incident optical field is reflected in the impurity- and phonon-assisted photon absorption through modifying the scattering of electrons with impurities and phonons.

- The distribution of electrons is driven away from the thermal equilibrium distribution to a **non-equilibrium** one.

- The electron average kinetic energy (temperature) **increases** with the strength of the incident electromagnetic field, creating hot electrons.

Previously- Boltzmann scattering equation – impurity and phonon-assisted photon absorption and Coulomb electron scattering for a doped GaAs semiconductor

$$\frac{\partial}{\partial t} n^{e}_{\vec{k}} = W_{k}^{(in)(\alpha)}\left(1 - n^{e}_{\vec{k}}\right) - W_{k}^{(in)(\alpha)} n^{e}_{\vec{k}} \qquad \alpha = (im),(ph),(c)$$

$$W_{k}^{(in)(ph)} = \frac{2\pi}{\hbar} \sum_{\vec{q}\lambda, M} \left|C_{\vec{q}\lambda}\right|^{2} J^{2}_{|M|}\left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right| / \sqrt{2} m^{*} \Omega^{2}_{L}\right)^{2}$$
$$\times [n_{\vec{k}-\vec{q}} N^{ph}_{\vec{q}\lambda} \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} - M\hbar\Omega_{L}\right)$$
$$+ n_{\vec{k}+\vec{q}}\left(N^{ph}_{\vec{q}\lambda} + 1\right)\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} + M\hbar\Omega_{L}\right)]$$

$$\left|C_{q\lambda}\right|^{2} = \left(\frac{\hbar\omega_{LO}}{2V}\right)\left(\frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_{0}}\right)\frac{e^{2}}{\varepsilon_{0}\left(q^{2} + Q_{s}^{2}\right)}$$

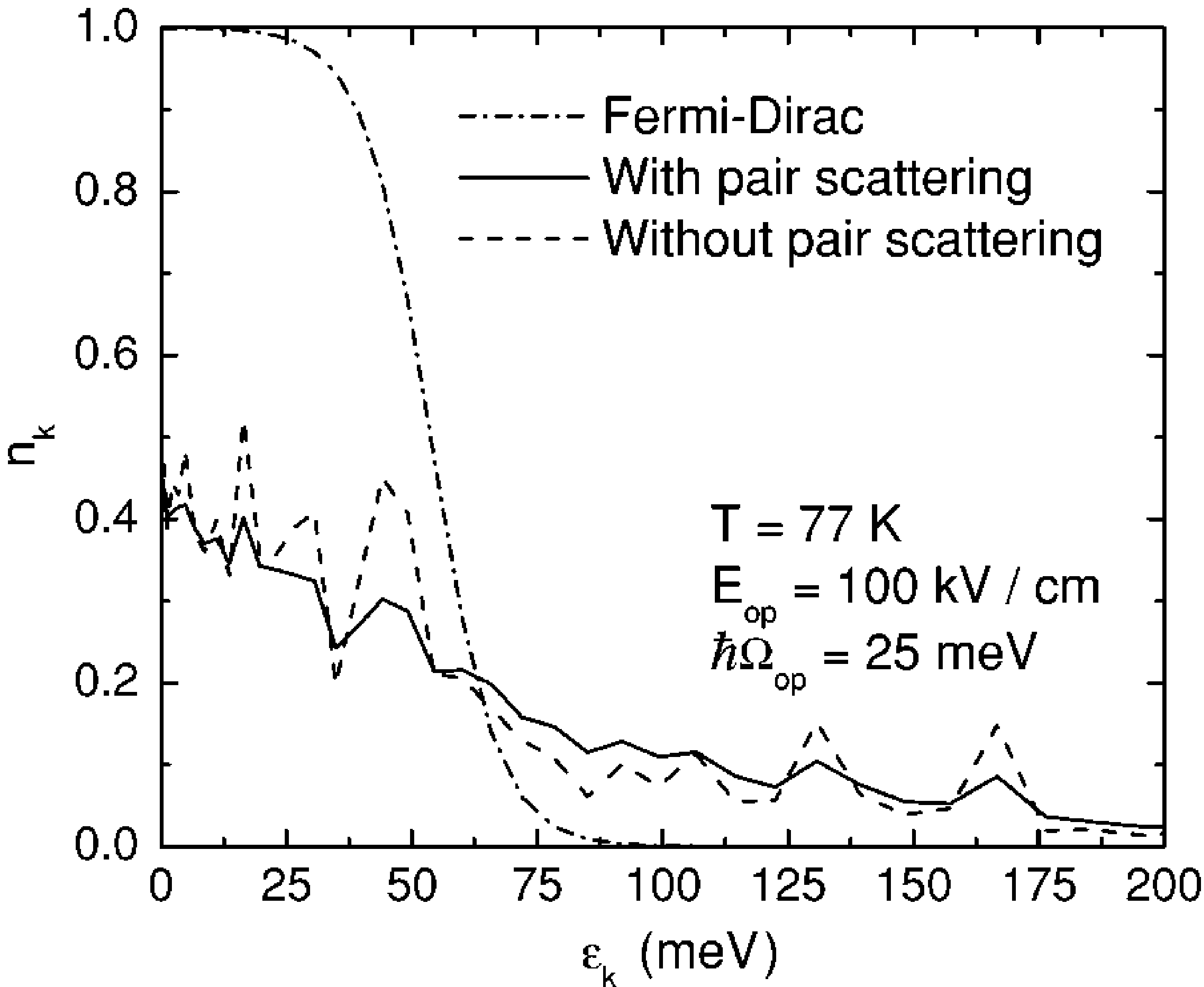
$$W_k^{(in)(im)} = n_I \sum_{\vec{q},M} \left| U^{(im)}(q) \right|^2 J_{|M|}^2 \left(e \left| \vec{q}.\vec{\mathrm{E}}(t) \right| / \sqrt{2} m^* \Omega_L^2 \right)^2$$

$$\times [n_{\vec{k}-\vec{q}} \delta \left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - M\hbar\Omega_L \right) + n_{\vec{k}+\vec{q}} \delta \left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + M\hbar\Omega_L \right)]$$

$$\left| U^{(im)}(q) \right| = \frac{Ze^2}{\varepsilon_0 \varepsilon_r \left(q^2 + Q_s^2 \right)}$$

$$W_k^{(in)(c)} = \frac{2\pi}{\hbar} \sum_{\vec{k}',\vec{q}} \left| V^{(c)}(q) \right|^2 \left(1 - n_{\vec{k}'} \right) n_{\vec{k}-\vec{q}} n_{\vec{k}'+\vec{q}} \times \delta \left(E_{\vec{k}} - E_{\vec{k}'} - E_{\vec{k}-\vec{q}} - E_{\vec{k}'+\vec{q}} \right)$$

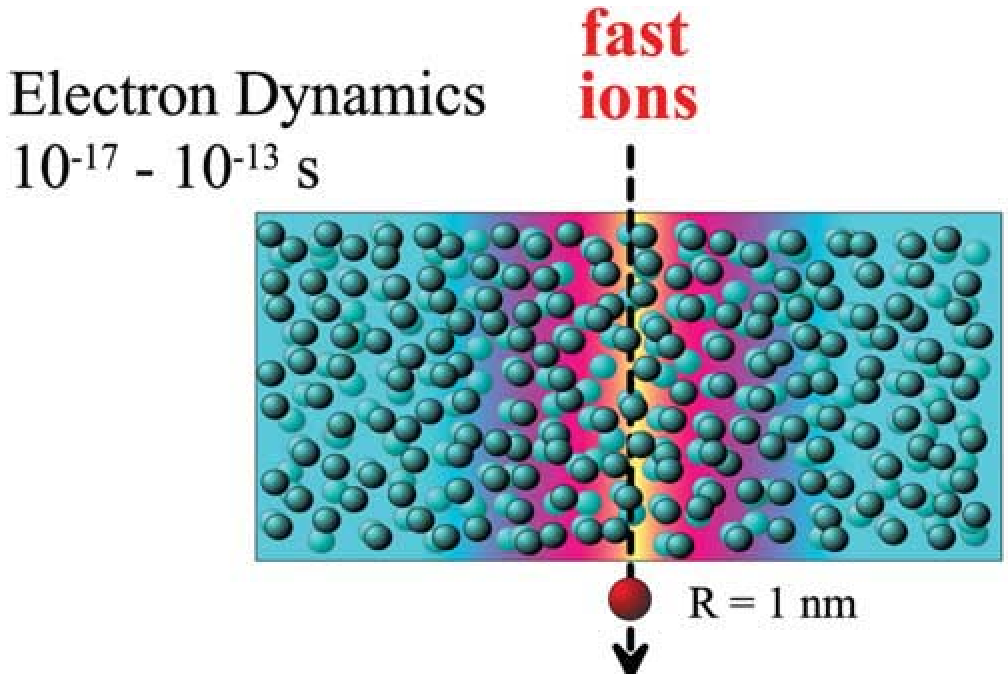
$$\left| V^{(c)}(q) \right| = \frac{e^2}{\varepsilon_0 \varepsilon_r \left(q^2 + Q_s^2 \right) V}$$



D. Huang, P. Alsing, **T. Apostolova** et. al. Phys. Rev. B 71, 195205 (2005)

Electron dynamics in ion-semiconductor interaction

v/c<0.1



•The projectile has reached its equilibrium charge state - there will be only minor fluctuations of its internal state

• It will move with constant velocity along a straight-line trajectory until deep inside the solid.

•Thus, the projectile ion acts as a well defined and virtually instantaneous source of strongly localized electronic excitation.

G. Schiwietz et al. / Nucl. Instr. and Meth. in Phys. Res. B 225 (2004) 4–26

Parallelism

From the fundamental point of view ion damage presents similarities with femtosecond-laser pulse damage.

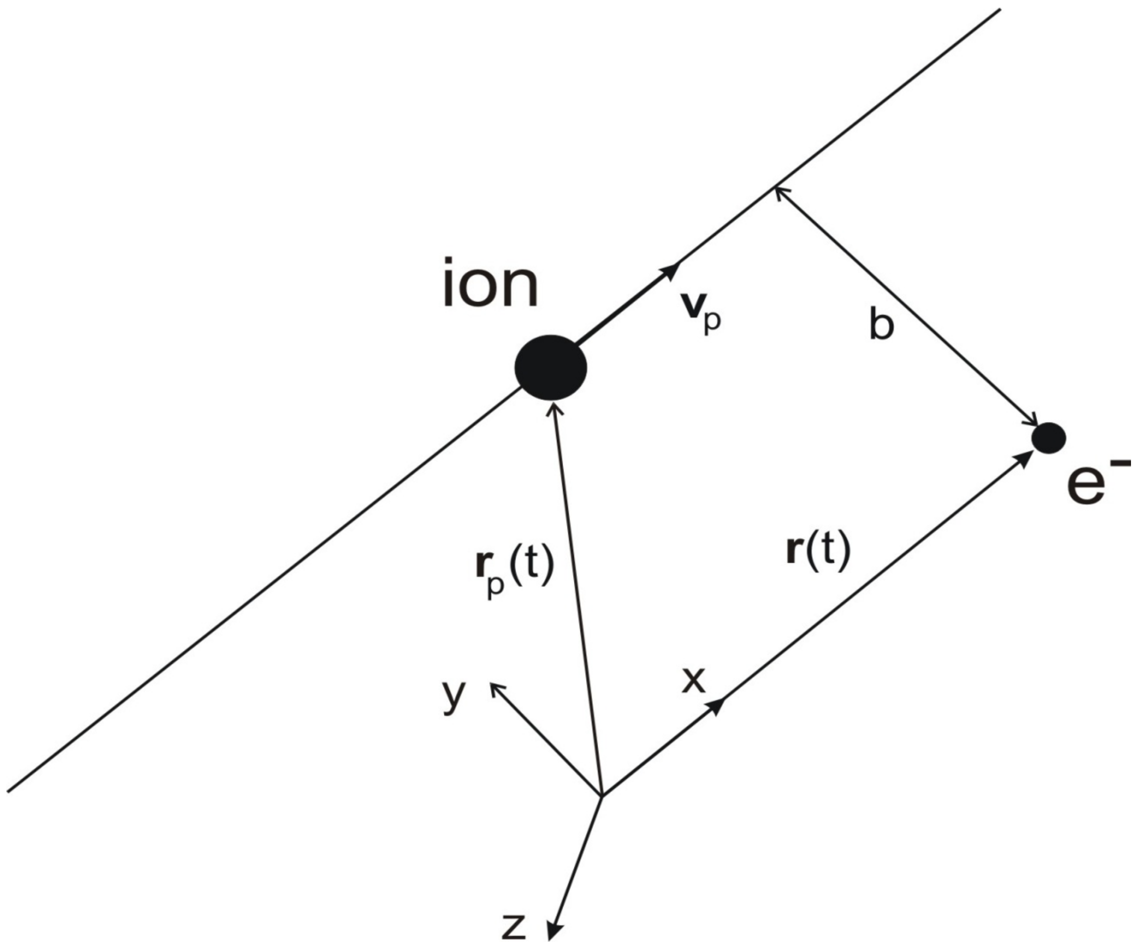
- Deposition of localized high energy densities in solid matter due to very dense electronic excitation by means of either photons or energetic ions leading to the formation of dense electron-hole plasma.

- The interaction occurs roughly in the same time scale and creates highly-localized material excitations $\tau \approx 100\, fs - 1\, ps$

$$\tau = b / v_p - \text{collision time}$$

Electron dynamics in ion-semiconductor interaction

In terms of three-dimensional Cartesian coordinates, we define the reaction to occur in the x-y plane with the beam directed along $\vec{e}_x$ and the impact parameter b along $\vec{e}_y$ defining the straight-line trajectory to be



We establish a Boltzmann scattering equation for the relative scattering motion of electrons interacting with a swift heavy ion by

- considering Coulomb interaction between the ion projectile and the electron system

- including both the impurity- and phonon-assisted photon absorption processes as well as the Coulomb scattering between two electrons.

- We study the dynamics of electrons by calculating the average kinetic energy as a function of impact parameter and charge of the ion.

Use the Hamiltonian

$$H = \frac{1}{2m^*}\sum_i \hat{\vec{p}}_i^{\,2} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r}_i - \vec{r}_j|} - \sum_i \frac{Ze^2}{4\pi\varepsilon_0\varepsilon_r|\vec{r}_p - \vec{r}_i|} + \sum_{i,a} U^{imp}(\vec{r}_i - \vec{R}_{imp})$$

$$\hat{\vec{P}}^C = \sum_{i=1}^{N_e}\hat{\vec{p}}_i \qquad \vec{R}^C = \frac{1}{N_e}\sum_{i=1}^{N_e}\hat{\vec{r}}_{i,} \qquad \hat{\vec{p}}_i' = \hat{\vec{p}}_i - \frac{1}{N_e}\hat{\vec{P}}^C \qquad \vec{r}_i' = \vec{r}_i - \vec{R}^C$$

$$\hat{H}_{CM} = \frac{(\hat{\vec{P}}^C)^2}{2N_e m^*}$$

$$\hat{H}_{rel} = \sum_{\vec{k},\sigma}\varepsilon_k \hat{a}^\dagger_{\vec{k}\sigma}\hat{a}_{\vec{k}\sigma} + \sum_{\vec{q},\lambda}\hbar\omega_{q\lambda}\hat{b}^\dagger_{\vec{q}\lambda}\hat{b}_{\vec{q}\lambda} + \frac{1}{2}\sum_{\vec{k},\vec{k}',\sigma,\sigma'}\sum_{\vec{q}}\frac{e^2}{\varepsilon_0\varepsilon_r q^2 \nu}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}^\dagger_{\vec{k}'-\vec{q}\sigma'}\hat{a}_{\vec{k}'\sigma'}\hat{a}_{\vec{k}\sigma} +$$

$$+ \sum_{\vec{k},\sigma}\sum_{\vec{q},\lambda} C_{q\lambda}(\hat{b}_{\vec{q}\lambda} + \hat{b}^\dagger_{-\vec{q}\lambda})e^{i\vec{q}.\vec{R}^C}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} - \sum_{\vec{k},\sigma}\sum_{\vec{q}}\frac{Ze^2}{\varepsilon_0\varepsilon_r q^2\nu}e^{i\vec{q}.(\vec{R}^C - \vec{r}_p)}\hat{a}^\dagger_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} + \ldots$$

Solve the time-dependent Schrodinger equation

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\vec{p}^{\,2}}{2m^*}\psi(\vec{r},t) + V_p(\vec{r},t)\psi(\vec{r},t)$$

$$V_p(\vec{r},t) = -\frac{Ze^2}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}_p(t)\right|}$$

L.Plagne et. al. Phys. Rev. B 61, (2000),

J.C.Wells, et. al. Phys. Rev. B 54, (1996)

$$\vec{r}_p(t) = (v_p t, b, 0)$$

with velocity of projectile v_p

$$\psi(\vec{r},t) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} f(t)$$

$$f(t) = f(0)e^{\frac{i}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0 v_p}\ln(t+\sqrt{t^2+a^2})} e^{-\frac{i}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0 v_p}\ln(a)}$$

$$a = \frac{b}{v_p};\ c = \frac{Ze^2}{4\pi\varepsilon_0 v_p}$$

$$f(t) = f(0)e^{\frac{i}{\hbar}c\ln(t+\sqrt{t^2+a^2})} e^{-\frac{i}{\hbar}c\ln(a)}$$

$$c\ln(t+\sqrt{t^2+a^2}) = c\ln a + c\frac{t}{a} - c\frac{t^3}{6a^3} + c\frac{3t^5}{40a^5} - \ldots\ldots$$

$$c\ln(t+\sqrt{t^2+a^2}) \approx c\ln a + c\frac{t}{a}$$

Looking closely at the problem parameters for justification of the approx.

The electron annihilation operator in the ion potential is given by:

$$\hat{c}_{\vec{k}}(t) = \hat{a}_{\vec{k}}(t)\exp\left[\frac{i}{\hbar}c\ln\left(t+\sqrt{t^2+a^2}\right)\right]\exp\left[-\frac{i}{\hbar}c\ln(a)\right]$$

Boltzmann type scattering equation

$$\frac{\partial}{\partial t}n_{\vec{k}}^{e} = W_k^{(in)(\alpha)}\left(1-n_{\vec{k}}^{e}\right) - W_k^{(in)(\alpha)}n_{\vec{k}}^{e} \qquad \alpha = (im),(ph),(c)$$

$$W_k^{(in)(ph)} = \frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2$$
$$\times[n_{\vec{k}-\vec{q}}N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}}-E_{\vec{k}-\vec{q}}-\hbar\omega_{\vec{q}\lambda}+Ze^2/b4\pi\varepsilon_0\right)$$
$$+n_{\vec{k}+\vec{q}}\left(N_{\vec{q}\lambda}^{ph}+1\right)\delta\left(E_{\vec{k}}-E_{\vec{k}+\vec{q}}+\hbar\omega_{\vec{q}\lambda}+Ze^2/b4\pi\varepsilon_0\right)]$$

$$W_k^{(in)(im)} = n_I \sum_{\vec{q}} \left| U^{(im)}(q) \right|^2$$

$$\times [n_{\vec{k}-\vec{q}} \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} + Ze^2/b4\pi\varepsilon_0\right) +$$

$$+ n_{\vec{k}+\vec{q}} \delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + Ze^2/b4\pi\varepsilon_0\right)]$$

$$W_k^{(in)(c)} = \frac{2\pi}{\hbar} \sum_{\vec{k}',\vec{q}} \left| V^{(c)}(q) \right|^2 \left(1 - n_{\vec{k}'}\right) n_{\vec{k}-\vec{q}} n_{\vec{k}'+\vec{q}} \times \delta\left(E_{\vec{k}} - E_{\vec{k}'} - E_{\vec{k}-\vec{q}} - E_{\vec{k}'+\vec{q}}\right)$$

Numerical results

TABLE I. Parameters of the ion irradiations.

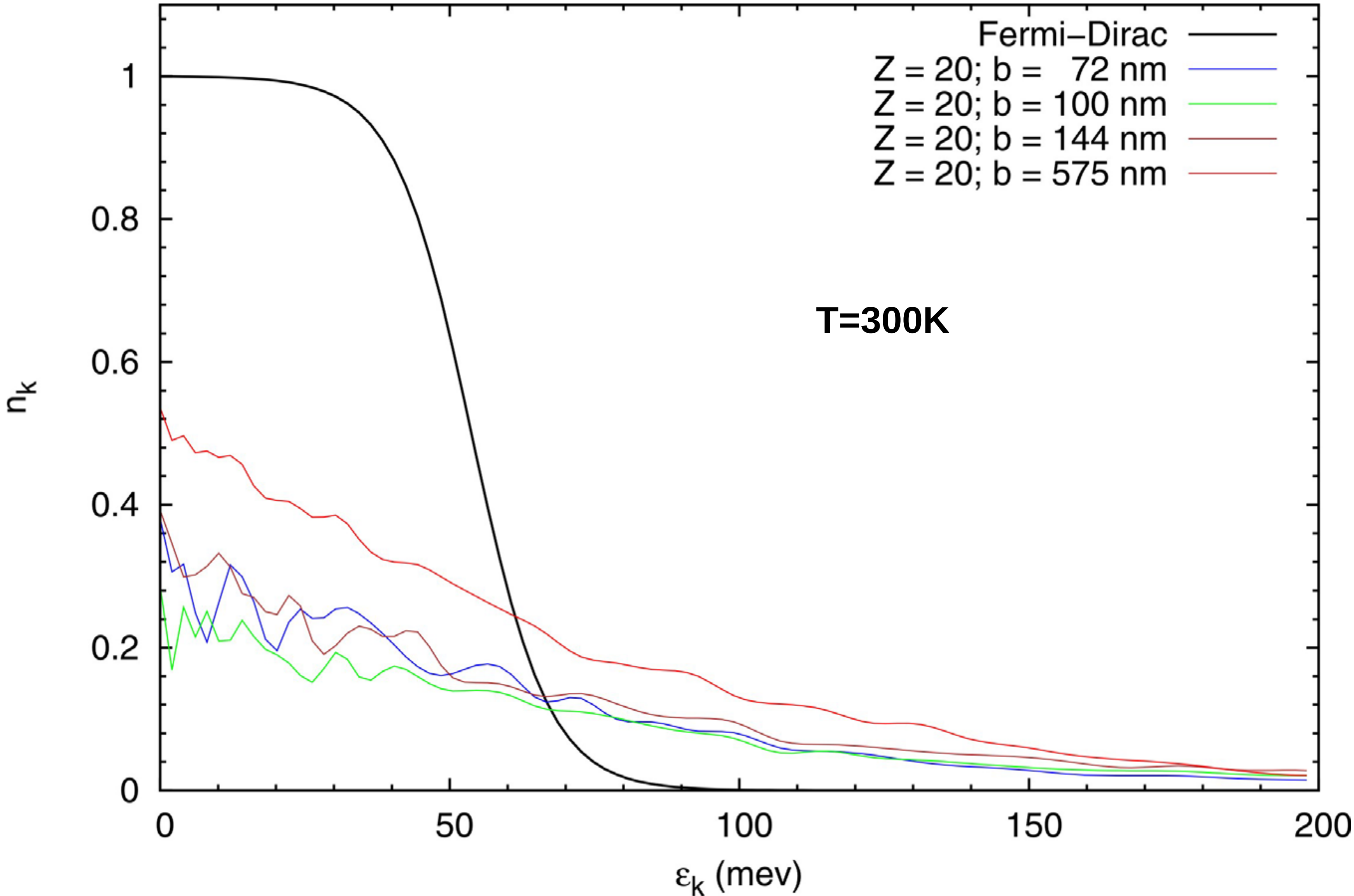
Ion	Energy (MeV/u)	Range (μm)	$(dE/dx)_i$ (keV/nm)	Mean (dE/dx) (keV/nm)
^{58}Ni	11.4	96	5.4	6.9
^{68}Zn	11.4	96	6.0	8.1
^{82}Se	11.4	104	7.4	9.0
^{84}Kr	11.4	98	8.0	9.8
^{130}Xe	11.4	91	14.3	16.3
^{197}Au	11.4	96	24.0	23.4
	5.4	49	27.0	21.7
^{208}Pb	11.4	96	24.9	24.7
	5.4	49	27.9	22.9
	4.0	38	27.9	21.9
^{209}Bi	11.4	95	25.4	25.1
	10.9	91	25.7	25.0
^{238}U	11.4	100	28.8	27.1

K. Schwartz, C. Trautmann, T. Steckenreiter, O. Geiß, and M. Krämer, Phys. Rev. B 58, 11232–11240 (1998)

hydrogen 1 H 1.0079																		helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122												boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305												aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

*Lanthanide series	lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
**Actinide series	actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Calculated electron distribution function for bulk GaAs as a function of electron kinetic energy



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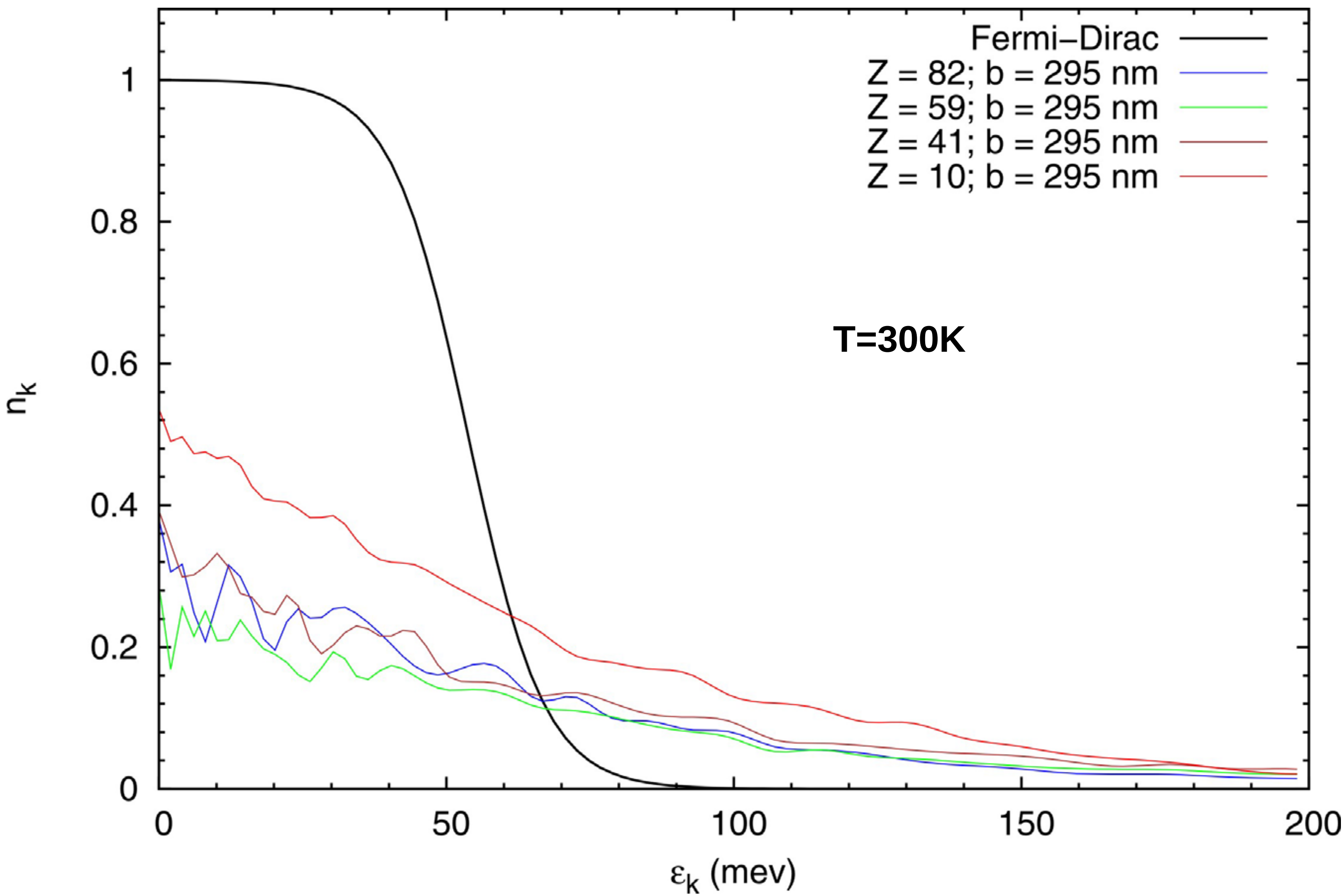

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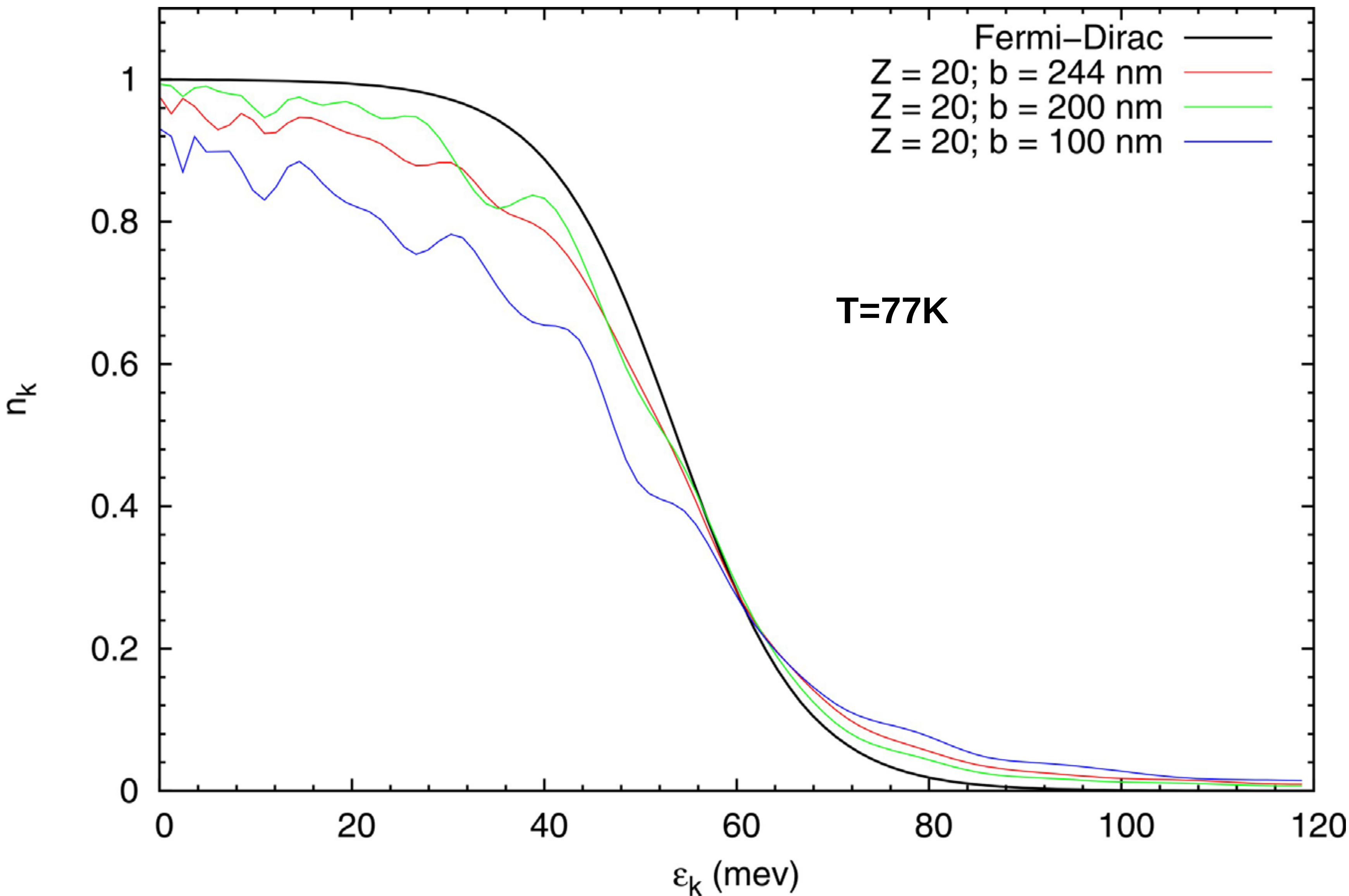
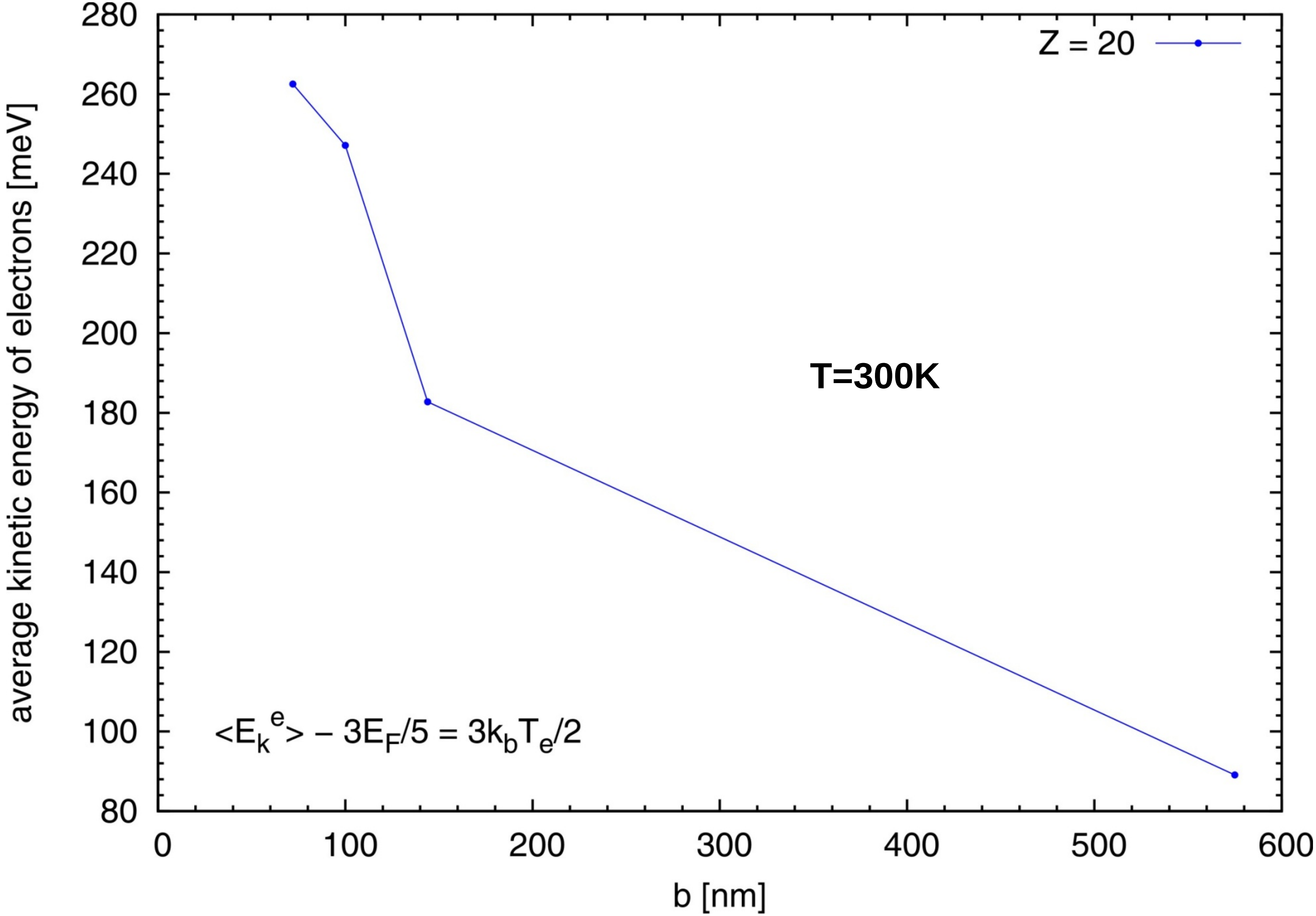
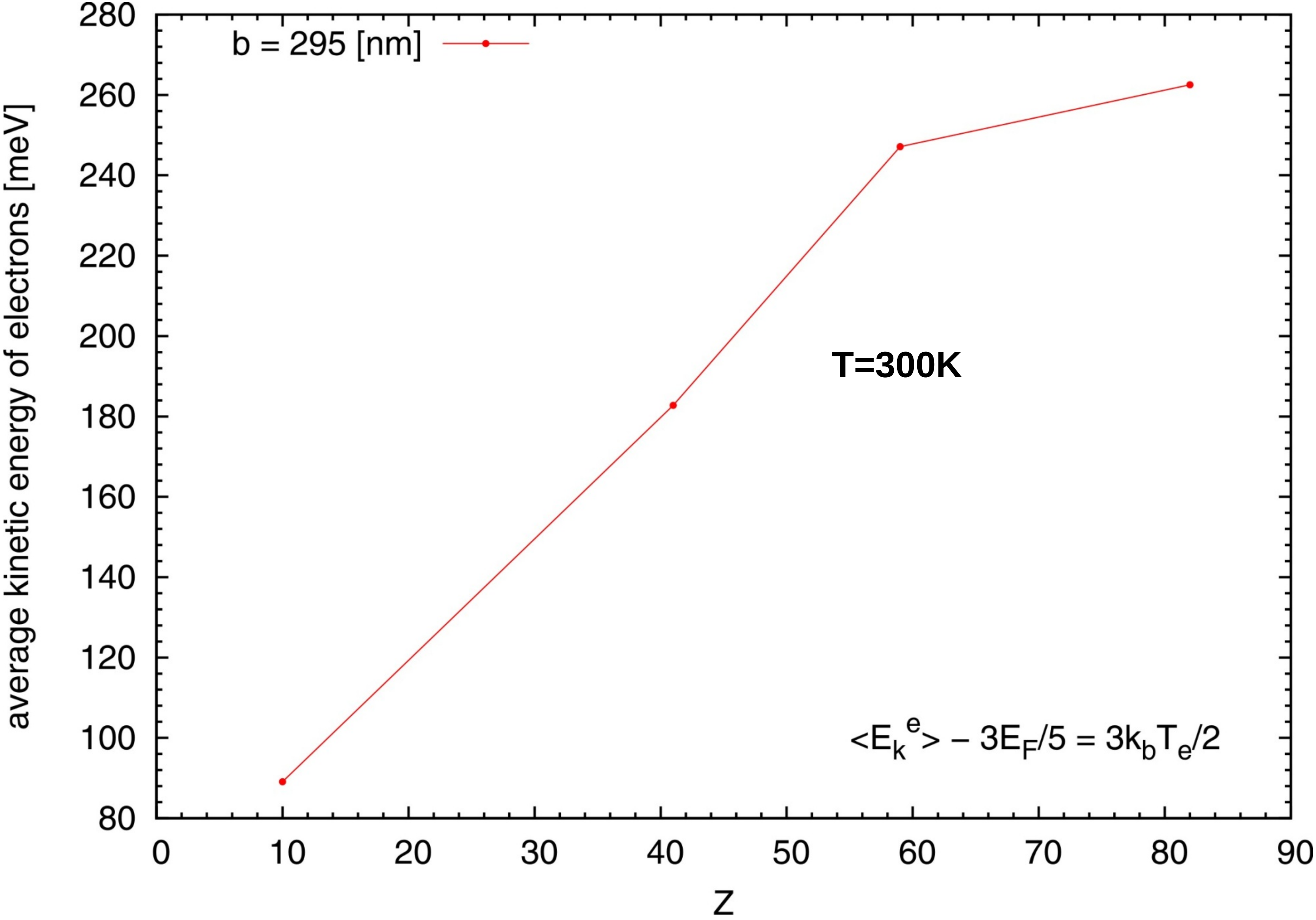


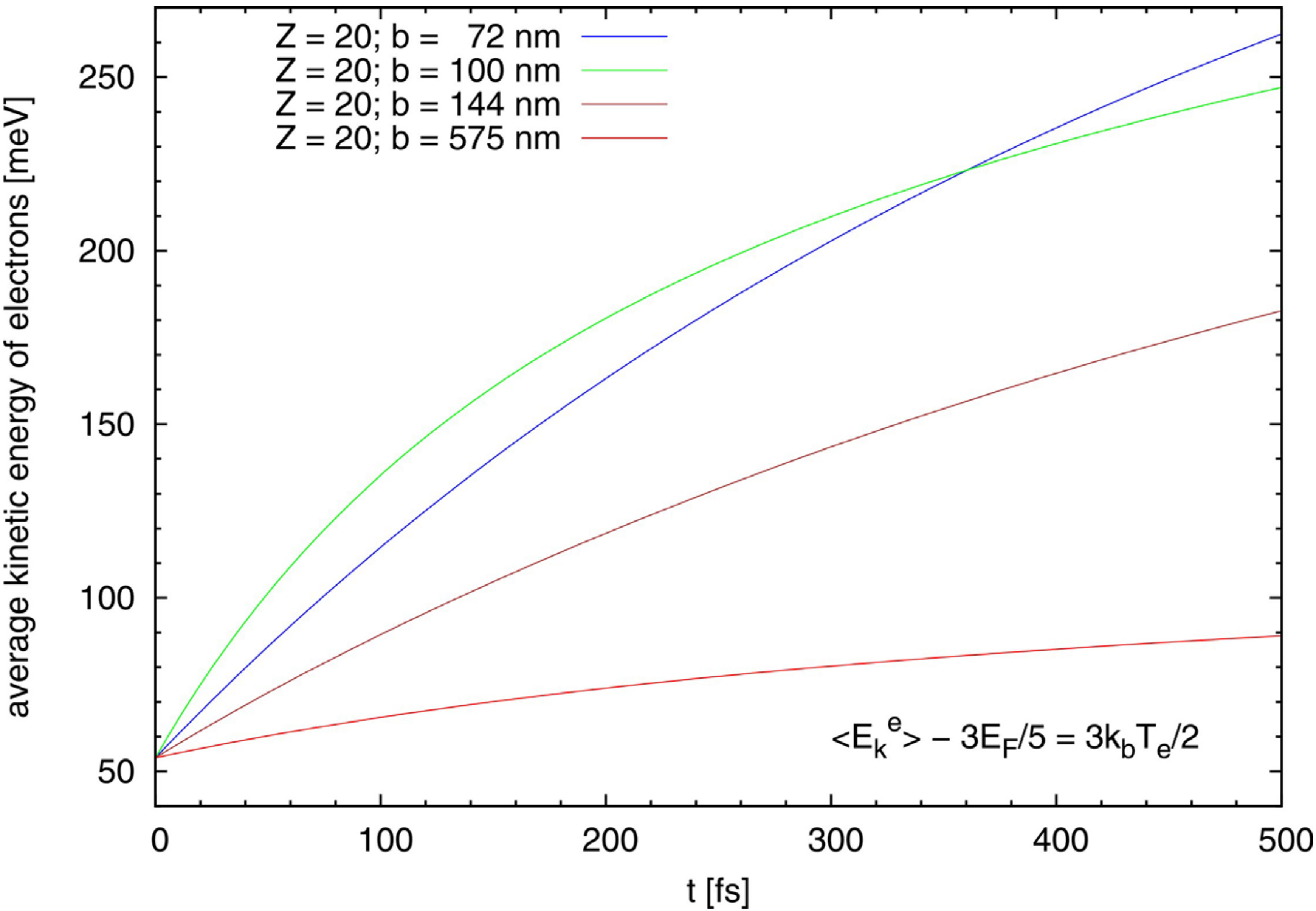
Average electron kinetic energy as a function of impact parameter



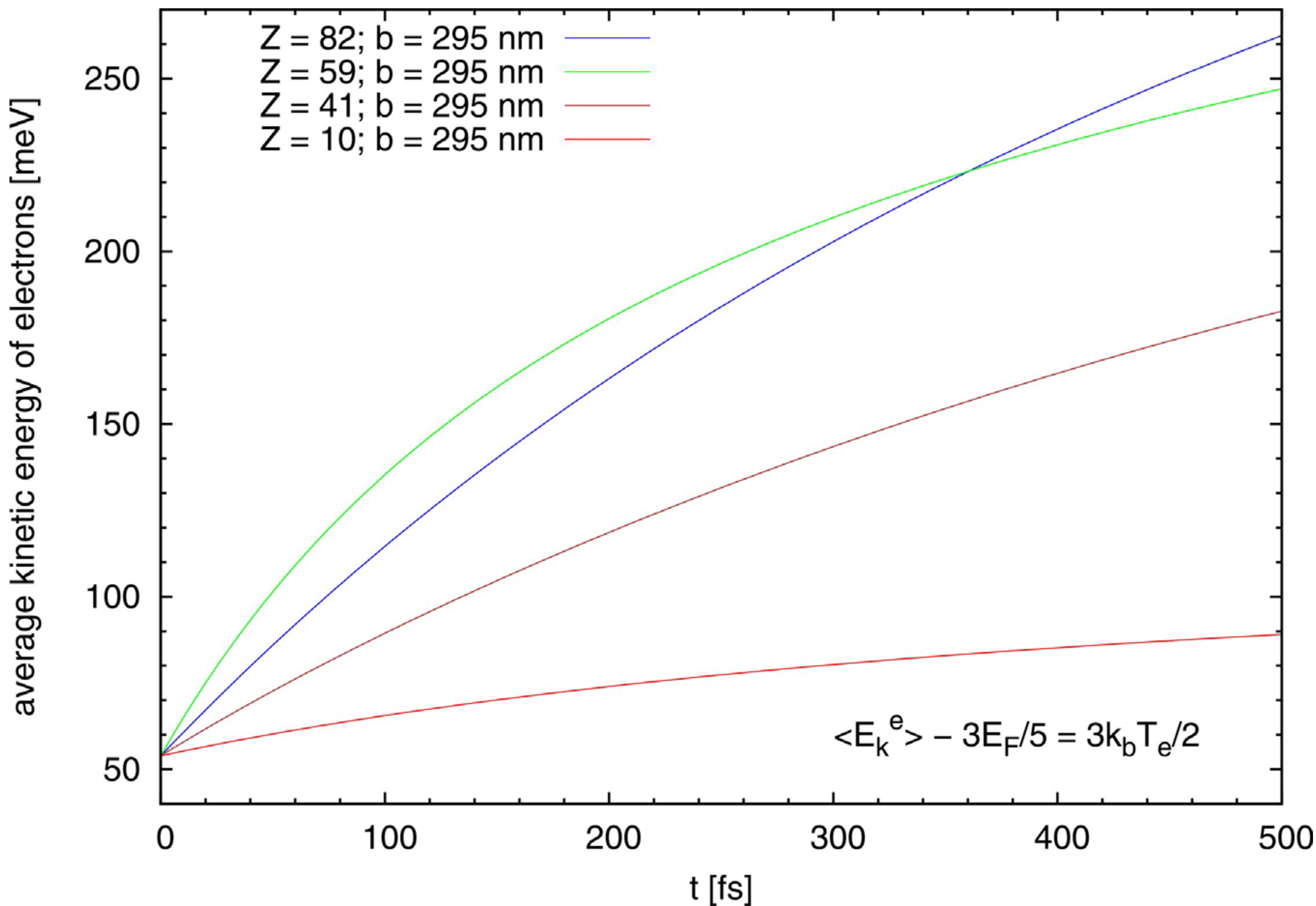
Average electron kinetic energy as a function of ion charge Z



Calculated average kinetic energy of electrons for bulk GaAs as a function of time



Calculated average kinetic energy of electrons for bulk GaAs as a function of time



Conclusions

- The effect of the potential of the incident ion is reflected in the phonon and impurity assisted electron transitions through modifying (“renormalizing”) the scattering of electrons with phonons and impurities via the time dependent potential of the ion projectile

- This method can offer unique ability to study the change in the electron dynamics when a single projectile characteristic is modified.

- The same numerical code as with the excitation with a laser field is used.

Thank you for your attention!