Chapt8Fig14a.m

Total Elastic Ionized Impurity Scattering Rate

Thomas-Fermi Screening with Angular Integration

Semiconductor Physics Documentation

Abstract

This document provides complete theoretical background and code analysis for `Chapt8Fig14a.m`, which calculates the total elastic scattering rate due to ionized impurities as a function of electron energy. The code employs Thomas-Fermi screening and numerical angular integration using the trapezoidal rule.

Contents

1 Theoretical Foundation

1.1 Ionized Impurity Scattering Theory

Axiom 1 (Fermi's Golden Rule for Scattering)**.** *The scattering rate from state* $\mathbf{k}$ *to state* $\mathbf{k}'$ *is:*

$$W_{\mathbf{k}\to\mathbf{k}'} = \frac{2\pi}{\hbar}|V_{\mathbf{k}\mathbf{k}'}|^2\delta(E_{\mathbf{k}'} - E_{\mathbf{k}}) \tag{1}$$

Definition 1 (Screened Coulomb Matrix Element)**.** *For ionized impurity scattering with Thomas-Fermi screening:*

$$V_{\mathbf{k}\mathbf{k}'} = \frac{e^2}{\varepsilon_0\varepsilon_r}\cdot\frac{1}{q^2 + q_{TF}^2} \tag{2}$$

where $q = |\mathbf{k}' - \mathbf{k}|$ *is the momentum transfer.*

1.2 Total Scattering Rate

Theorem 1 (Total Elastic Scattering Rate)**.** *The total scattering rate is obtained by integrating over all final states:*

$$\frac{1}{\tau(E)} = \sum_{\mathbf{k}'} W_{\mathbf{k}\to\mathbf{k}'} = n_i \int |V(q)|^2 g(\mathbf{k}')\delta(E' - E)\, d^3k' \tag{3}$$

where n_i *is the impurity concentration.*

Theorem 2 (Angular Integration Form)**.** *For elastic scattering on a spherical Fermi surface:*

$$\frac{1}{\tau(E)} = \frac{\pi n_i m^*}{\hbar^3 k^3}\left(\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\right)^2 \int_0^\pi \frac{\sin\theta}{(q^2 + q_{TF}^2)^2}\, d\theta \tag{4}$$

where $q = 2k\sin(\theta/2)$*.*

1.3 Change of Variables

Lemma 1 (Substitution to η)**.** *With* $\eta = \sin(\theta/2)$*:*

- $q = 2k\eta$
- $d\eta = \frac{1}{2}\cos(\theta/2)\, d\theta$
- $\sin\theta = 2\sin(\theta/2)\cos(\theta/2) = 2\eta\sqrt{1-\eta^2}$

The integral becomes:

$$\int_0^\pi \frac{\sin\theta}{(q^2 + q_{\mathrm{TF}}^2)^2}\, d\theta = \int_0^1 \frac{4\eta\sqrt{1-\eta^2}}{(4k^2\eta^2 + q_{\mathrm{TF}}^2)^2}\cdot\frac{2d\eta}{\sqrt{1-\eta^2}} \tag{5}$$

1.4 Thomas-Fermi Screening

Definition 2 (Thomas-Fermi Wavevector)**.**

$$q_{TF}^2 = \frac{k_F m^* e^2}{\pi^2\hbar^2\varepsilon_0\varepsilon_r} \tag{6}$$

where $k_F = (3\pi^2 n)^{1/3}$ *is the Fermi wavevector.*

2 Numerical Method: Trapezoidal Integration

2.1 The Trapezoidal Rule

Theorem 3 (Trapezoidal Rule)**.** *For a function $f(x)$ on interval $[a, b]$ with N subintervals of width $h = (b - a)/N$:*

$$\int_a^b f(x)\,dx \approx h\left[\frac{f(a) + f(b)}{2} + \sum_{i=1}^{N-1} f(a + ih)\right] \tag{7}$$

Theorem 4 (Error Estimate)**.** *The error in the trapezoidal rule is:*

$$E_T = -\frac{(b-a)^3}{12N^2} f''(\xi) \tag{8}$$

for some $\xi \in [a, b]$. The method is second-order accurate: $E_T = O(h^2)$.

2.2 Application to Angular Integration

The code uses a simplified form where the step size equals the increment:

$$\int_0^{\pi} f(\theta)\,d\theta \approx \sum_{j=1}^{180} f(\theta_j) \cdot \Delta\theta \tag{9}$$

where $\Delta\theta = \pi/180$ radians (1° steps).

3 Line-by-Line Code Analysis

3.1 Function Declaration

```
function TFelasticScattering
clear;clf;
```

Declares as a function and clears workspace.

3.2 Physical Constants

```
  m0=9.109382e-31;
echarge=1.6021764e-19;
hbar=1.05457159e-34;
epsilon0=8.8541878e-12;
```

$$m_0, e, \hbar, \varepsilon_0 \tag{10}$$

Fundamental physical constants in SI units.

```
ezero=13.2;
m1=0.070;
```

$$\varepsilon_r = 13.2, \quad m^* = 0.07 m_0 \tag{11}$$

GaAs material parameters.

```
emax=300.0d-3;
n=1.0d16;
npoints = 200;
```

$$E_{\max} = 300 \text{ meV}, \quad n_{\text{initial}} = 10^{16} \text{ cm}^{-3} \tag{12}$$

Maximum energy for plot and starting carrier density.

3.3 Carrier Density Loop

```
for k=1:2
 n=n*10;
```

$$n \in \{10^{17}, 10^{18}\} \text{ cm}^{-3} \tag{13}$$

Loop over two carrier densities (plotted as two curves).

```
kF1=(3*(pi^2)*n)^(1/3);
kF1=kF1*1.e2;
```

$$k_F = (3\pi^2 n)^{1/3} \times 10^2 \text{ (convert cm}^{-1} \to \text{m}^{-1}) \tag{14}$$

Fermi wavevector calculation and unit conversion.

```
   kF2=kF1^2;
   kF3=kF1^3;
```

$$k_F^2, k_F^3 \tag{15}$$

Powers of Fermi wavevector for later use.

3.4 Thomas-Fermi Screening Wavevector

```
qTF2=kF1*m0*m1*(echarge^2)/(epsilon0*ezero*(pi^2)*(hbar^2));
```

$$q_{\text{TF}}^2 = \frac{k_F m_0 m_1 e^2}{\varepsilon_0 \varepsilon_r \pi^2 \hbar^2} \tag{16}$$

Thomas-Fermi wavevector squared.

3.5 Fermi Energy

```
eF=((hbar*kF1)^2)/(2.0*m0*m1*echarge);
```

$$E_F = \frac{(\hbar k_F)^2}{2m^*} \cdot \frac{1}{e} \text{ [eV]} \tag{17}$$

Fermi energy in eV (division by e converts from J to eV).

3.6 Constant Prefactor

```
const=(pi*n*1.0e6*(echarge^4)*m0*m1);
const=const/(((4.*pi*epsilon0)^2)*(ezero^2)*(hbar^3));
```

$$C = \frac{\pi n \cdot 10^6 \cdot e^4 \cdot m_0 m_1}{(4\pi\varepsilon_0)^2 \varepsilon_r^2 \hbar^3} \tag{18}$$

Prefactor for scattering rate (includes unit conversion).

3.7 Energy Grid Setup

```
emin=eF;
demax=(emax-emin)/200.0;
dth=pi/180.0;
```

$$E_{\min} = E_F, \quad \Delta E = \frac{E_{\max} - E_F}{200}, \quad \Delta\theta = \frac{\pi}{180} \tag{19}$$

Energy step and angular step (1° increments).

3.8 Main Energy Loop

```
ei=emin;
for i=1:npoints
  ei=ei+demax;
  ak=(sqrt(2.*m0*m1*ei*echarge))/hbar;
  ak3=ak^3;
```

$$k = \frac{\sqrt{2m^* E \cdot e}}{\hbar}, \quad k^3 \tag{20}$$

Electron wavevector at each energy.

3.9 Angular Integration Loop

```
  aint1=0.0;
  theta=0.0;
 for j=1:180
    theta=theta+dth;
    aint1=aint1+(dth*gchi1(theta,ak,qTF2));
 end
```

$$I = \sum_{j=1}^{180} g(\theta_j) \cdot \Delta\theta \tag{21}$$

Trapezoidal integration over angle (calls helper function gchi1).

3.10 Store Results

```
        y1(i)=const*aint1/ak3;
  x1(i)=ei*1.d3;
```

$$\frac{1}{\tau(E)} = \frac{C \cdot I}{k^3}, \quad E \text{ [meV]} \tag{22}$$

Scattering rate calculation and energy in meV.

3.11 Helper Function: gchi1

```
function gchi1 = gchi1(theta,k,qTF2)
 x=2.0*k*sin(theta/2.0);
 x2=x^2;
 g=(tan(theta/2.0))*((sin(theta/2.))^2)*((1.0+(qTF2/x2))^2);
 gchi1=1.0/g;
return
```

$$g(\theta) = \frac{1}{\tan(\theta/2) \cdot \sin^2(\theta/2) \cdot (1 + q_{\text{TF}}^2/q^2)^2} \tag{23}$$

where $q = 2k\sin(\theta/2)$.

This computes the integrand for the angular integration.

3.12 Plotting

```
figure(1);hold on;plot(x1,y1,'r');axis([0,emax*1.d3,0,16e12]);
```

Plot scattering rate vs energy with axis limits.

4 Physical Interpretation

4.1 Energy Dependence

The scattering rate $1/\tau(E)$ typically:

- Decreases with increasing energy (faster electrons harder to scatter)
- Scales approximately as $E^{-3/2}$ at high energy
- Has a plateau or peak near E_F

4.2 Density Dependence

Higher carrier density leads to:

- Stronger screening (larger q_{TF})
- Lower scattering rate at small angles
- But higher overall scattering due to more impurities (if $n_i = n$)

5 Summary

This code calculates the total elastic scattering rate by numerically integrating over all scattering angles using the trapezoidal rule. The helper function `gchi1` encodes the screened Coulomb scattering matrix element with Thomas-Fermi screening. Results show how scattering rate varies with electron energy and carrier density.