Electron source in vacuum

$E=E_0+EA+E_f$ for insulator/semiconductor
$E=E_0+E_W+E_f$ for metal
Total reflection is also a possibility

In material

Elastic scattering

E_{kin} < 200 eV (phonon scattering)
Energyloss = fphononloss
Select theta from summed angular differential invMFP
Isotropic phi

Inelastic scattering

200 eV < E_{kin} < 30 keV (Mott); E_{kin} > 30 keV (Rutherford)
Determine the element
Select theta and corresponding energyloss from angular differential invMFP
Isotropic phi

Boundary crossing

Transmission?

$$T(E',\theta') = \begin{cases} \dfrac{4\sqrt{1-U_0/E\cos^2\theta}}{\left(1+\sqrt{1-U_0/E\cos^2\theta}\right)^2} & \text{if } E'\cos^2\theta' > U_0 \\ 0 & \text{otherwise.} \end{cases}$$

If UniformRand<T

Transmission
NewEnergy=OldEnergy-W_{f1}-E_{f1}
The assumption E_{kin}+½mv^2 is made

$$\vec{p}_{\parallel} = \vec{p} - \left(\vec{p}\cdot\vec{N}\right)\vec{N}$$

$$\vec{p}_{\perp} = -\sqrt{\frac{E_{new}}{E_{old}} - \vec{p}_{\parallel}\cdot\vec{p}_{\parallel}}\,\vec{N}$$

$$\vec{p}_{new} = \frac{\vec{p}_{\perp}+\vec{p}_{\parallel}}{\sqrt{\left\|\vec{p}_{\perp}\right\|^2+\left\|\vec{p}_{\parallel}\right\|^2}}$$

If UniformRand>T or
Energy*$\cos^2$(theta)-U_0 < 0 or
Energy*$\cos^2$(theta) < 0

Total internal reflection
NewMomentum = OldMomentum-2*cos(theta)*theFacetNormal
Energy does not change
Aborption if deltaU<0 and
exp(1+frac{oldE}{2*deltaU})>UniformRand

Sample ω':
First get a 'random' cross section from the total cross section at the current energy (calculated in GetMeanFreePath):

$$\omega' cross = CDCS(E)\cdot R$$

Then find the cumulative differential cross section table for the current energy (by interpolating the tabulated values)
And calculate the exact ω' that corresponds to the 'random' cross section we took earlier by linearly interpolating the CDCS.

Find the binding energy of the 'new' electron: If ω'>100 eV, first see if Geant4 can come up with the bindingEnergy. Accept this if it is >50 eV.
Otherwise, get the largest bindingEnergy<ω' from the df file

If ω'<½(E_{kin}+ω'-E_f) and Ebind'>0: sample ω according to the function:

$$F(\omega,\omega') = \begin{cases} \dfrac{1}{\omega(\omega-\omega')} & \omega'+\dfrac{q_-^2}{2} < \omega < \omega'+\dfrac{q_+^2}{2} \\ 0 & \text{otherwise} \end{cases}$$

With:

$$q_{\pm} = \sqrt{2}\left(\sqrt{E} \pm \sqrt{E-\omega}\right)$$

Else sample ω according to the $1/\omega^2$ distribution with ω' and ½(E_{kin}+ω'-E_f) as lower and upper limits:

$$\omega = \frac{Ebind'}{1-R}\left(1-\frac{\omega'}{\frac{1}{2}\left(E_{kin}+\omega'-E_f\right)}\right)$$

Final energy of the primary particle: $E_{kin,final}$=$E_{kin,initial}$-ω

If Ebind==0

For metals:
If 0.1*E_f<ω<1000*E_f:
A normalised cumulative distribution function for the dimensionless variable: y = E'/ω is stored in the vector Psecvalues.
x=E_f/ω, now if >1:
- Find the correct energybin for Psecvalues, psecnr
- P0 is calculated with a log-log interpolation using the first bin where Psecenergies>x-1
- P1 is calculated with a log-log interpolation using the first bin where Psecenergies>x
- P2 = P0 + (P1-P0)*R
- now find the value y that matches P2: If Psecvalues[k+1]>P2:

$$E_{bind} = E_f - \omega\left(P^k_{secenergies}\exp\left(\log(P2)-\frac{\log(P^k_{secvalues})}{\log(P^{k+1}_{secvalues})-\log(P^k_{secvalues})}\left(\log(P^{k+1}_{secenergies})-\log(P^k_{secenergies})\right)\right)\right)$$

Else: Ebind stays 0 (SE is assumed to have kinetic energy equal to the Fermi energy)

For insulators/semiconductors:
If ω'>band gap: Ebind=band gap (bandgap excitation)
Else: phononloss

Phononloss:
$E_{kin,final}$=$E_{kin,initial}$-ω'
Energy deposit = ω'
If $E_{kin,final}$<fenergylimit: kill the electron

SE $E_{kin,sec}$ = ω – E_{bind} + E_f (counting from E_f)
theEnergyDeposit += Ebind – E_f
First transform to the shell potential – from both the (initial) primary kinetic energy and the SE kinetic energy first subtract the Fermi energy, then add the binding energy 'twice'. The classical physical picture is that the electric potential near the given (inner shell) orbit is twice the binding energy of that shell. The bound electron has a kintec energy equal to E_{bind} so that its total energy is:
E_{pot} + E_{kin} = -2*E_{bind} + E_{bind} = -E_{bind}.
$E_{kin,delta}$ = ω+E_{bind}=$E_{kin,sec}$-E_f+2*E_{bind}
$E_{kin,prim}$ = E_{kin}-E_f+2*E_{bind}
We assume that the secondary had no net momentum prior to the collision and that both electrons behaved as free electrons.
Sample the scattering angle neglecting atomic motion, RELATIVISTIC (this is default behaviour):
  Mom_{delta} = sqrt($E_{kin,delta}$($E_{kin,delta}$+2*electron_mass_c2))
  Mom_{prim} =sqrt($E_{kin,prim}$($E_{kin,prim}$+2*electron_mass_c2))
  cost=$E_{kin,delta}$($E_{kin,prim}$+2*electron_mass_c2)/(Mom_{delta}*Mom_{prim})
  If (cost > 1) : cost=1
  sint=sqrt(1-cost*cost)
  dirz=cost
  del = sqrt(E_{bind}*(E_{bind}+2*electron_mass_c2)
Else, NON-RELATIVISTIC (non-default behaviour):
  cost2 = $E_{kin,delta}$/$E_{kin,prim}$
  if (cost2 > 1) : cost2=1
  cost1 = sqrt(cost2) **Dit staat fout in de code!!!**
  sint = sqrt(1-cost2)
  dirz = cost1
  del = sqrt(E_{bind}/$E_{kin,delta}$)
Isotropic phi
dirx = sint*cos(phi)
diry = sint*sin(phi) and rotate to align with the incident electron direction
Finally add a component to the SE's momentum that corresponds to its instantaneous momentum:
delcost=2*R-1
sint = sqrt(1-delcost^2)
Isotropic phi
if (E_{bind}<0) abort() **!!Waarom hier?**
dirx += del*sint*cos(phi)
diry += del*sint*sin(phi)
dirz += del*delcost
newdir = (dirx, diry, dirz)

If: Generate secondaries
First: GenerateParticles() from CADPhysicsAtomicDeexcitation for X-ray fluorescence and Auger electrons
Second: Add the normal SE to the secondary particle vector

Else: deposit the lost energy:
theEnergyDeposit += $E_{kin,sec}$

Loop over all secondary particles:
If: electron:
Add the Fermi energy to the kinetic energies of all Auger electrons
If: electron energy large enough: totalNumber++
else: kill electron
If: gamma:
If: energy>250eV:
totalNumber++
else: kill gamma

Register all secondary particles left
Filter the primary electron for too low energies
Update the primary electron momentum assuming momentum conservation

AtomicDeexcitation
GenerateParticles:
provShellId = SelectTypeOfTransition(shellID):
refShell=highest shell that can still serve as a final state for a fluorescent transition (according to G4)
provShellId=-1
if (shellId < = refShell):
loop over the shells that can provide an electron for a radiative transition to shellId
draw a random number R for every 'origin' shell and check whether this shell will be providing an electron.
If yes: provShellId = 'origin' shell
If no 'origin' shell is found, provShellId stays -1

provShellId == -1

GenerateFluorescence:
Isotropic angular distribution for the photon
Energy = provShellId – shellId
The originating shell is added to the vacancies vector again to test for a second atomic deexcitation.

provShellId > 0

GenerateAuger:
Find if the shellId can be the final state for an Auger transition.
If yes, find all possible Auger transitions that have shellId as the lower shell
Loop over all possible Auger transitions:
draw a random number R for every possible Auger transition and check whether this transition will be executed.
if no Auger transition is selected (this should not happen) the vacancy is simply added to the vacancies vector again.
if an Auger transition is selected:
Define new electron:
Isotropic angular distribution
Energy = transitionEnergy
Because of the Auger transition we now have two new vacancies that are added to the vacancies vector.