Excessive Phonon Energy in G4DMC Events

Andrew's fork from Rob Agnese's repository

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The Problem

While debugging the track weighting discrepencies, I noticed that even without downsampling, we were getting too much energy out from a simulation.
For an electron recoil we should expect:

$$E_{phonon} = E_{recoil} + 4\text{volt} \times \text{floor}\left(\frac{E_{recoil}}{E_{pair}}\right) \tag{1}$$

For the 1 keV event I tested, that should be $\sim$ 2.4 keV. G4DMC collected a total of $\sim$ 3.1 keV of phonon energy.

Investigation

Some immediate consistency checks:

- Charge drift speeds still match data.
- Energy partitioner creates correct initial tracks (energies sum to E_{recoil}).
- Luke phonon emissions conserve energy on case-by-case basis.

Tests

We have checked several potential sources of error:

- Use uniform electric field instead of COMSOL field - **no change**.
- Turn off inter-valley scattering (known to be non-physical) - **no change**.
- Create only phonons - **Correct energy output**!
- Shoot exactly one charge carrier pair - **Excess still present**.

Places Left to Look

The bug must be in the charge physics. We've ruled out inter-valley scattering and Luke phonon emission. The drift curves also should rule out E-field acceleration bugs. There are three processes left:

- DriftBoundaryProcess - When a charge carrier is absorbed, releases its kinetic energy as phonons.
- DriftRecombinationProcess - When a charge carrier comes to rest in the crystal, it is killed and releases half of the gap energy as phonons.
- EnergyLimiter - When any particle is below its energy threshold, it is simply killed and deposits its kinetic energy as NIEL. This shouldn't be triggering ever for charge carriers as threshold = 0.

Using Columns

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Using Columns

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Pictures

Figure: scaled gator (0.2x)

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Thank You