These instructions are valid for materials files having beta5 in the first line.

To modify the materials file directly, first open the materials file with a text editor. If you use MS Word, be sure that you save the file as text file when you are finished. Materials are of two types, binary or ternary. I suggest that you copy the information for either type (depending on what you want to add) and then change the numbers. The units are cm for length, an C/cm^2 for polarization.

If a binary, the information is given on three lines:

Line 1: Semiconductor name, "binary", semiconductor family, comment

Line 2: Energy gap, Band offset, rel. dielectric constant, electron eff. mass, cond band valley degeneracy, heavy hole eff mass, light hole eff mass, donor ionization energy, acceptor ionization, deep donor ionization, deep acceptor ionization. (Some materials files will have a barrier height at the end of this line. It is not necessary, and is ignored).

Line 3: Donor concentration, acceptor conc., deep donor conc., deep acceptor conc., electron mobility, hole mobility, electron lifetime, hole lifetime, polarization, absorption coefficient

If you want a new ternary, things are more complicated. There are 20 lines for a ternary.

Line 1: Semiconductor name, "ternary", semiconductor family, comment

Line 2: Donor concentration, acceptor conc., deep donor conc., deep acceptor conc., dummy number(optional, not used)

Lines 3-19 are one line for each parameter. On each line is a 2-3 letter descriptor, followed by 1 to 3 groups of 5 numbers defining the coefficients of the 2nd order polynomial describing the parameter, and defining the x interval over which it is valid. The order is as follows:
xmin, xmax, constant, linear, quadratic.

The parameter lines are in the order: Energy gap, Band offset, rel. dielectric constant, donor ionization energy, acceptor ionization, deep donor ionization, deep acceptor ionization, electron eff. mass, cond band valley degeneracy, heavy hole eff mass, light hole eff mass, electron mobility, hole mobility, electron lifetime, hole lifetime, absorption coefficient. Use the example of an existing ternary material to get the correct descriptors and ordering.

Line 20: end"your material name"

Good luck.