Should I always start from n-type layers in ‘Heterostructure’ list?

Yes, the ‘Heterostruture’ list has a fixed direction, from n-side to p-side, no matter what is the actual growth direction. Besides, in all graphs representing the heterostructure (band diagram, waveguide modes, etc) direction from left to right corresponds to the direction from n-side to p-side.

What should be the first heterostructure layer?

If you are simulating an LED with planar current spreading, the first heterostructure layer to be thick n-type contact layer responsible for the lateral current spreading. You need not input nucleation buffer layers. For instance, if your real structure looks as

sapphire substrate / nucleation layer / buffer layers / undoped GaN / 3 um n-GaN / LED structure

your input in SiLENSe should be only

200 nm n-GaN / LED structure

The reason is that SiLENSe assumes that the current flows through all the layers specified in 'Heterostructure' tab of SiLENSe. Also, you can reduce the thickness of the first layer down to 200-300 nm (far away from the active region the current is governed just by the Ohm law).

‘Strain in the first layer’ section in ‘Heterostructure’ tab (version 4.0 and higher)

'First layer' means the first layer in the 'Heterostructure' tab. Note than in that list the layers are listed from n-side to p-side. The first layer must be the thick n-type contact layer responsible for the lateral current spreading. You need not input nucleation buffer layers. In 99% of cases, first layer is relaxed, i.e. it has its natural lattice constants. In some very rare cases, first layer is strained (for instance, n-AlGaN layer grown without relaxation on top of thick GaN layer we ignore in SiLENSe). If the first layer is strained, the user needs to specify its lattice constant. All next layers are assumed to have the same lattice constant as the first layer, until partial strain relaxation is not explicitly specified by the user (see 'Degree of relaxation' layer property).

‘Substrate’ section in ‘Heterostructure’ tab (version 3.6 and lower)

The 'Substrate' section of the 'Heterostructure' tab is designed to provide users a way to specify lattice constant of the first heterostructure layer. By default, all next layer are assumed to have the same lattice constant, until partial strain relaxation is not explicitly specified by the user (see 'Degree of relaxation' layer property).

However, heterostructures are usually includes nucleation and buffer layers, where strain relaxation occurs. These layers do no effect the current injection and should not be specified in SiLENSe. But their effect on the heterostructure strain can be considered by specification of the lattice constant.

Thus, in the 'Substarte' section users should specify not the sapphire lattice constant, but that of the thick semiconductor layer underlying the light-emitting heterostructure. Usually it is GaN, but may be AlGaN for UV applications.

Some materials (sapphire, SiC) have a lack of properties

As for sapphire and SiC materials, they was included to database only for their optical properties, since they are important for computation of the waveguide modes in laser diodes (see substrate specification in the 'Laser parameters' tab). We do not expect their use in the 'Heterostructure' tab, so we do not care about their properties except to the optical ones.

Non-radiative recombination parameters

The non-radiative recombination is calculated as a sum of contributions of dislocations, point defects, and Auger recombination (Eq. 6.1 of SiLENSe Physics Summary). Both dislocations and point defects are described within the Shockley-Read-Hall approach. We have developed a special model which relates the dislocation density to the carrier non-radiative lifetimes. Direct input of the lifetimes is also possible in respective text fields. Blank value for both electron and hole non-radiative lifetimes results in zero recombination. If one value is blank, while other is filled, the only filled field is taken into account. For instance, if tau_e =1ns and tau_h = "blank", R = n/tau_e .

Thus, the user can use the model and input dislocation density (with blank recombination lifetimes because of point defects) or input lifetimes directly with zero dislocation density. Use of both dislocation density and lifetimes is possible, but in this case the lifetimes must describe the contribution of the defects except to the dislocations.

Some people claim that Indium fluctuations may improve IQE by capturing carriers and preventing them to reach dislocations. We have developed a model to describe this effect. The model needs characteristic fluctuations in the energy of the conduction and valence bands. It is assumed that DOS decays exponentially inside the energy gap. Details are given in Sec. 6.2.1 of SiLENSe Physics Summary.

The sum U_n+U_p is suggested to be nearly equal to the characteristic decay energy of the low-energy (long wavelegths) wing of the emission spectrum. It was experimentally found to about ~50 meV for different structures. Then, we suggest that U_n/U_p ratio equal to the ratio between band offsets dEc/dEv = 7/3 . So, the default values are 35 and 15 meV for conduction and valence bands, respectively.

Degree of relaxation in layer properties

By default, SiLENSe assume that all layers are grown pseudomorphically. There is an idea that at high In content real QWs are partially relaxed. In SiLENSe, the user can specify a degree of strain relaxation for each layer. Please keep in mind that if you set some strain relaxation in QWs, you have to simultaneously set complete strain relaxation in the next barrier or electron blocking layer. Otherwise, next layer will inherit lattice constant from the underlying QW. Example of an SQW structure with 50% strain relaxation is supplied with the program. Section 2 of SiLENSe Physics Summary contains all details of computation of the strain and the piezoelectric field.

Can I specify more than one periodic structure?

The current version of SiLENSe supports only one periodic structure. It will be improved in the next version. Right now, you can use copy/paste option for two or more layers at once.