

# Advanced settings

## Parallelization

### Number of threads

The number of threads can be controlled using the command `<Maximum_Number_of_Threads>`

```
<Simulation_Parameter>
...
<Maximum_Number_of_Threads>12</Maximum_Number_of_Threads>
...
</Simulation_Parameter>
```

For an automatic setting, use 0 or do not specify this command. In this case, the number of threads will be set to half of the number of physical cores.

In any case, we recommended that `<Maximum_Number_of_Threads>` does not exceed the number of **physical** cores (note that when hyperthreading is activated, the number of physical cores is half the one on logical processors).

### Parallelization in case of combined Temperature-Voltage sweep

In the case where a combined Temperature-Voltage sweep is used, there are two levels of parallelization. The first is at the level of the command `<Threads>` in the `<SweepParameters>` section.

```
<SweepParameters>
  <SweepType>Temperature-Voltage</SweepType>
  ...
  <Threads>6</Threads> <!-- Parallelization for Temperature-Voltage sweep -->
</SweepParameters>
```

The second level of parallelization occurs in the `<Simulation_Parameter>` section:

```
<Simulation_Parameter>
...
<Maximum_Number_of_Threads>2</Maximum_Number_of_Threads>
...
</Simulation_Parameter>
```

In this example, the total number of threads will be `<Threads>* <Maximum_Number_of_Threads> = 6*2 = 12`.

## Definition of graded alloy and graded interfaces

There are two possibilities to define graded alloy profile.

### Linearly graded alloys

To define a linear graded alloy profile, two materials first need to be defined in the `<Material>` section For example,

```
<Material>
  <Name>GaAs</Name>                                <!-- Binary material -->
  <Alias>mat1</Alias>
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
</Material>

<Material>
  <Name>Al(x)Ga(1-x)As</Name>                        <!-- Ternary material -->
  <Alloy_Composition>0.15</Alloy_Composition> <!-- alloy composition x -
->
  <Alias>mat2</Alias>
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
</Material>
```

Then, in the layer definition (named `<Superlattice>`), the following can be used to define a layer with a linear alloy profile, with composition starting from the material 1 and ending with the material 2 composition.

```
<Layer> <!-- all the material parameters will be linearly interpolated
between the <Material1> and the <Material2> -->
  <Material1>mat1</Material1>
  <Material2>mat2</Material2>
  <Thickness unit="nm">5.0</Thickness>
</Layer>
```

## Scattering processes

### Contributions of individual scattering processes

The following command allow to display self-energies and spectral functions for some specific mechanisms, like e.g. scattering due to optical phonons:

```
<Scattering>
...
<Separate_Scattering>yes</Separate_Scattering>
...
```

## </Scattering>

This command is only for analysis purpose, and has no influence on the other calculated quantities. It only involves an additional calculation of self-energies and Green's functions. In each basis folder, a folder with the name of the scattering process will appear, containing the retarded self-energy and the spectral function arising only from the specific scattering mechanism. Hence this spectral function gives the contribution to broadening of an individual scattering process.

### Homogeneous Coulomb scattering

To speed up the calculation, it is possible to consider the assumption of homogeneously distributed Coulomb scatterers (ionized impurities and other charge carriers) using the following command:

```
<Scattering>
...
<Homogeneous_Coulomb>yes</Homogeneous_Coulomb>
...
</Scattering>
```

### Output format for 2D plots

By default, 2D plots are output in a [VTK format](#) (.vtr extension). [Gnuplot](#) files (.plt extension) are also generated (in a file explorer, double click on the file to generate the gnuplot figure).

In addition, to output 2D plots in a [AVS/Express format](#) (.fld extension), the following command “<FLD\_format>” can be added in the <Output> section of the input file.

The following commands can be used to control the output formats:

```
<Output>
...
<VTK_format>yes</VTK_format>
<FLD_format>yes</FLD_format>
<Gnuplot_format>yes</Gnuplot_format>
...
</Output>
```

### Scaling 1D wavefunctions

In order to scale the output of the square of the wavefunctions (1D plots), the following command can be used:

```
<Output>
...
<ScaleWaveFunction>0.1</ScaleWaveFunction>
...
```

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</Output>

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