STREEM AlGaN: STRain Engineering in Electronic Materials, AlGaN Edition

Visual Quick Start Guide

2016

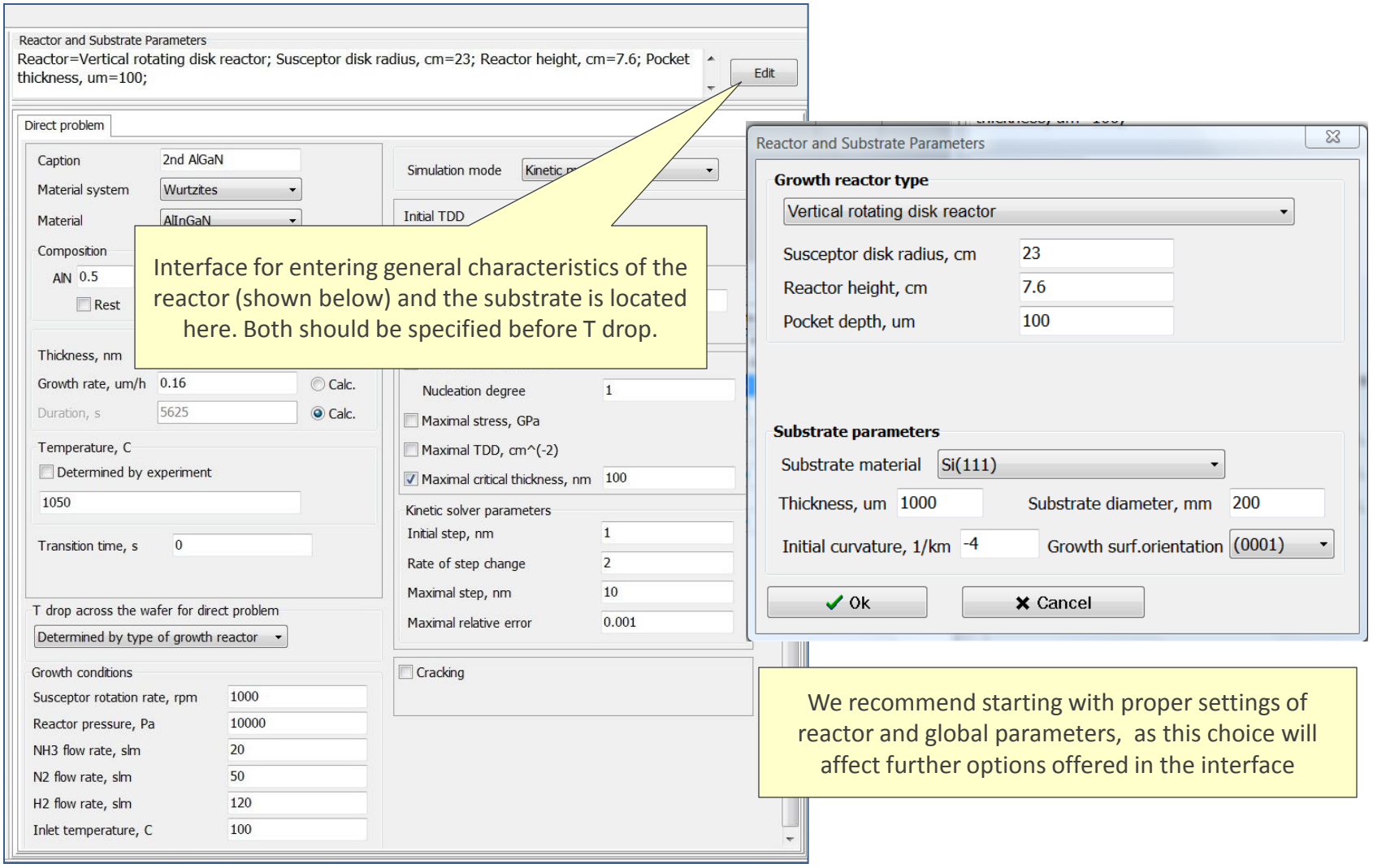
STR Group

Recommended Work Flow

Here is how we recommend to approach modeling a new heterostructure, assuming you are using experimental curvature data.

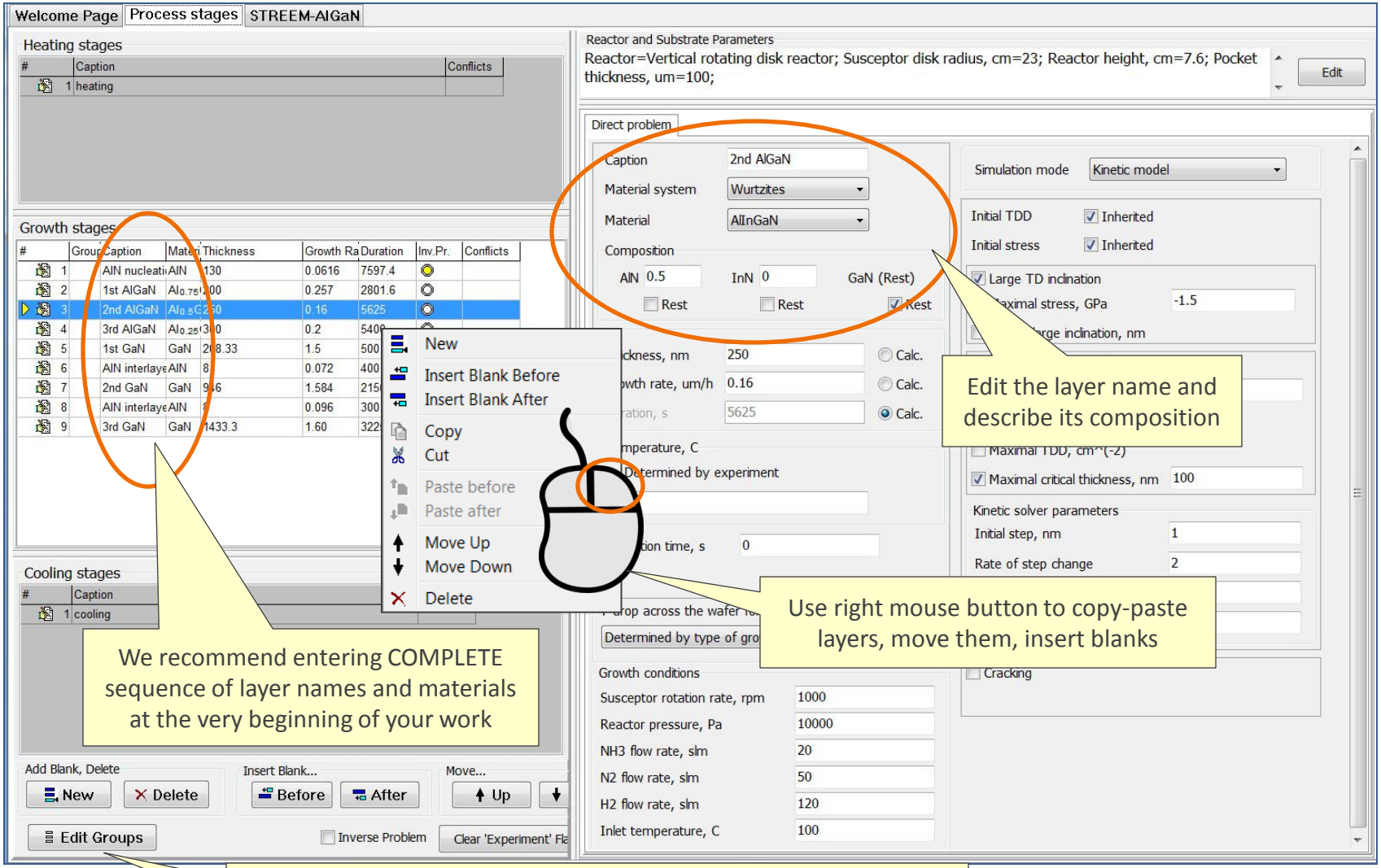
1) Look for a similar looking example or your own project file to use as a starting point. You will save a lot of time and avoid errors by editing a look-alike instead of creating a project from scratch.
2) Enter (or edit) reactor and substrate characteristics.
3) Set up a complete sequence of layers. Use copying layers or blocks of layer where possible. If you are planning to use experimental curve to set up time intervals of the layer growth, leave it for later – it will be much faster to specify intervals for all the layers once you have a complete list available.
4) Continue describing process stages by entering temperature and temperature drop sections.
5) Choose the appropriate simulation mode (strain/relaxation model). Nucleation layer should have Equilibrium mode (do not worry about the relaxation degree right now). Compressively strained layers should be simulated by Kinetic model with inheriting toggled on for both strain and TDD, except the first kinetic layer, where initial TDD should be assigned. For layers with tensile stress use Equilibrium model.
6) Set up the time intervals for the growth stages. If you are planning to use experimental data, go to Exp. Data Processing window and set up each layer's time (*Define Layer* button).
7) Run simulations. Compare the results with experimental curvature. Adjust relaxation degree of the nucleation layer to make respective segment of the curve fit.
8) Now, when the segment corresponding to nucleation layer fits, you can try adjusting initial TDD for the following layer. Initial stress should set to *Inherit* from the nucleation layer.

Reactor and Global Parameters



We recommend starting with proper settings of reactor and global parameters, as this choice will affect further options offered in the interface

Entering the Layer Sequence



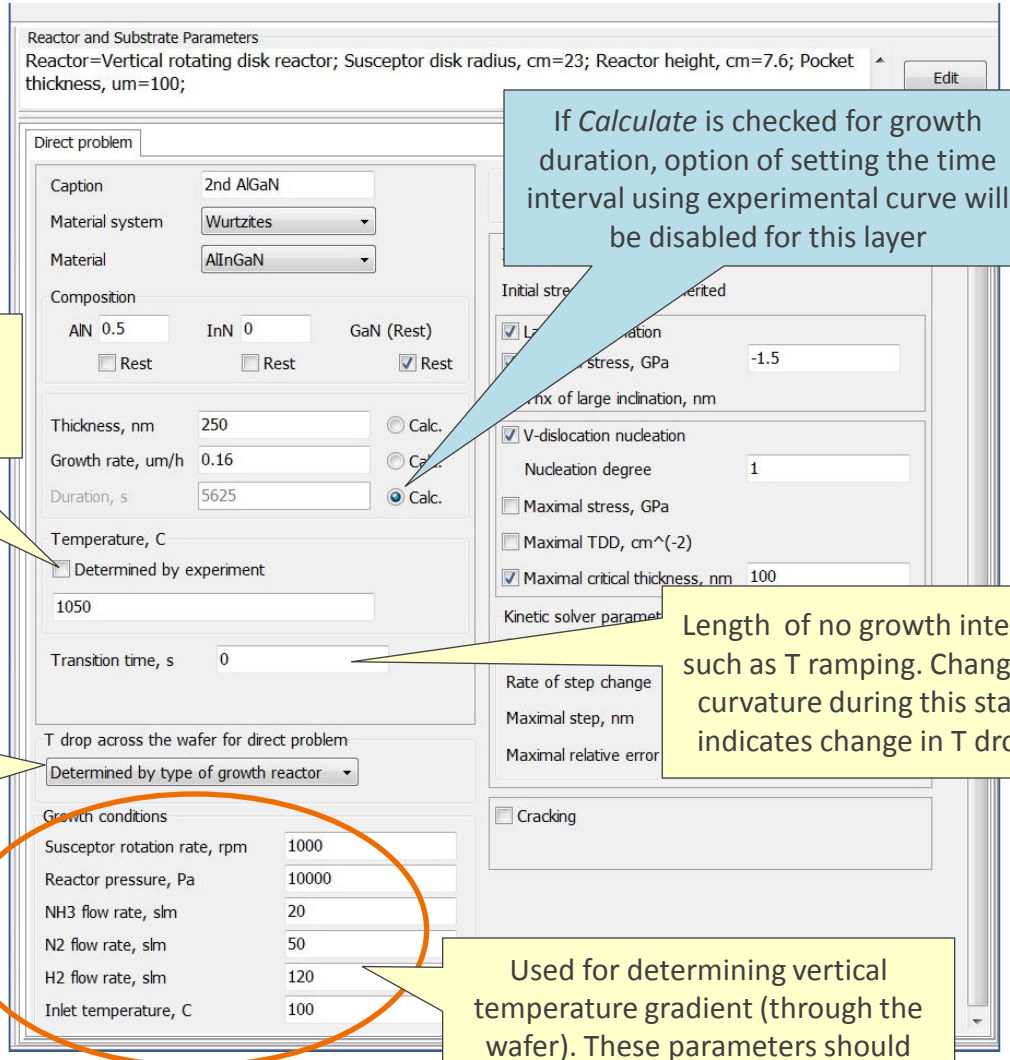
Edit the layer name and describe its composition

Use right mouse button to copy-paste layers, move them, insert blanks

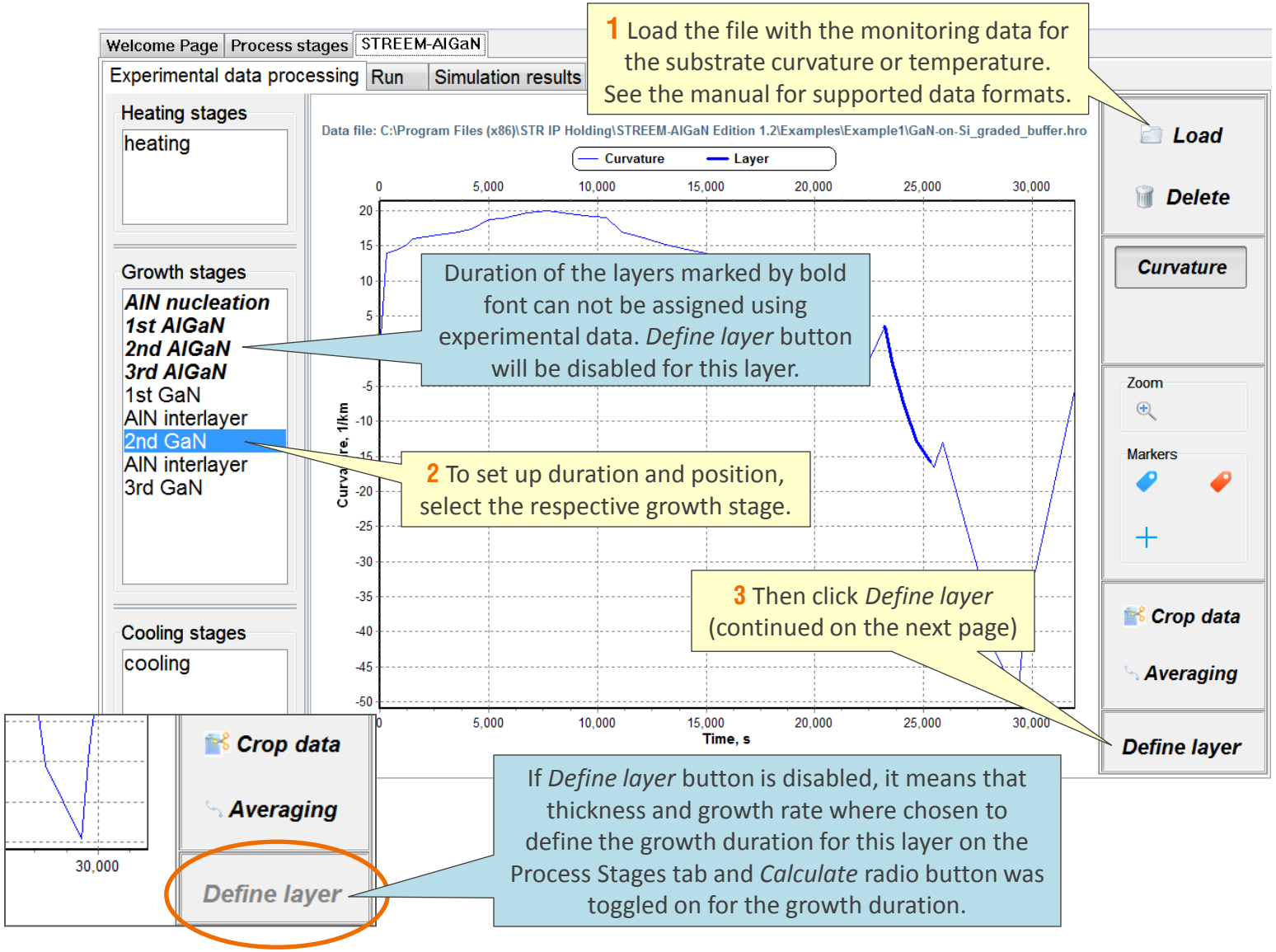
We recommend entering COMPLETE sequence of layer names and materials at the very beginning of your work

Use grouping to specify periodic structures, for instance, superlattices. It would allow you to treat them as a single object

Editing the Layer Parameters



Defining Growth Stage Duration and Position Using Experimental Data

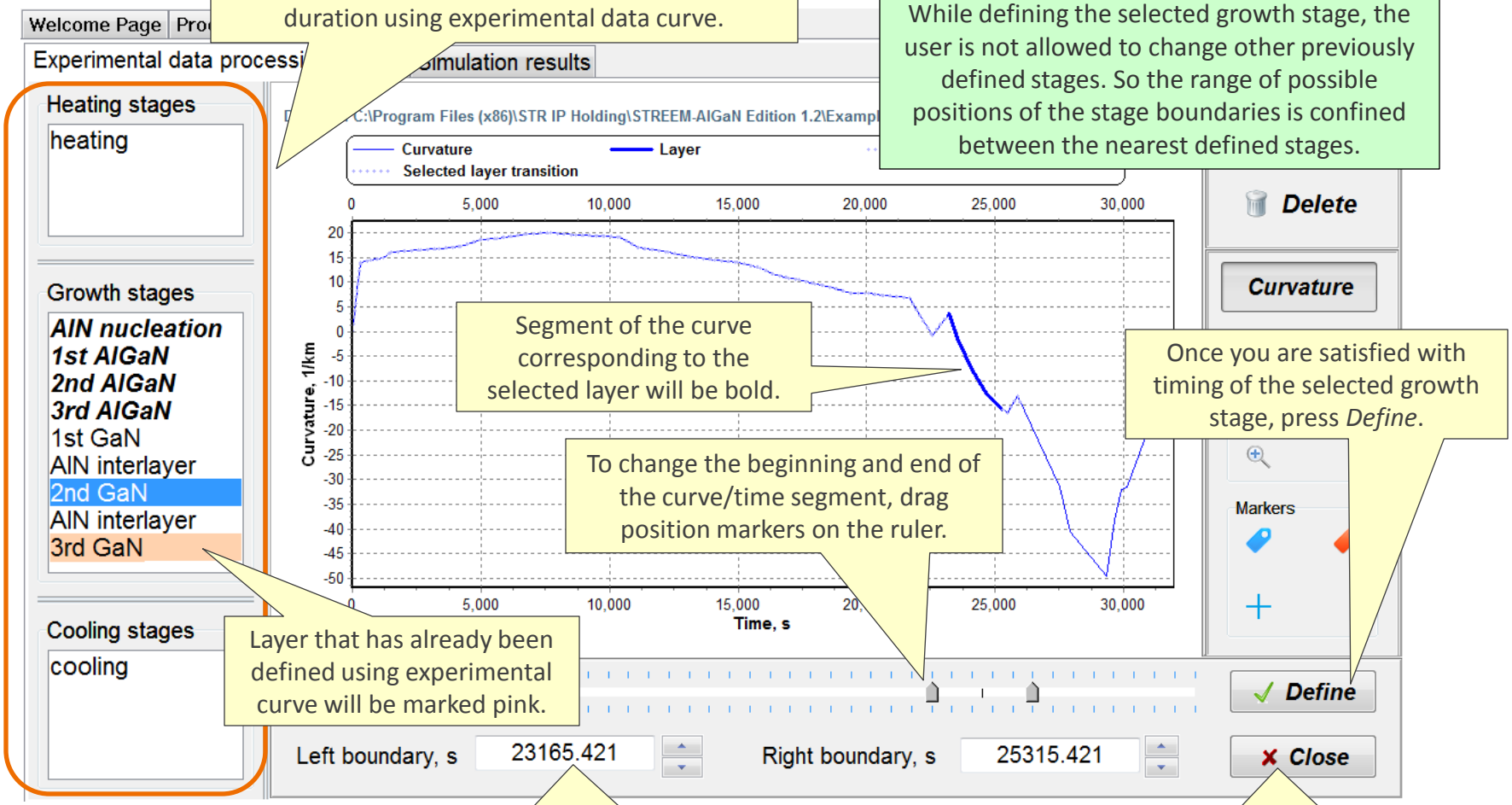


Defining Duration and Position of the Growth Stages (Continued)

To significantly reduce effort for the case set up , we recommend that you have complete list of growth stages before you start defining their duration using experimental data curve.

Time intervals between defined growth stages will be filled with transition stages.

While defining the selected growth stage, the user is not allowed to change other previously defined stages. So the range of possible positions of the stage boundaries is confined between the nearest defined stages.



Segment of the curve corresponding to the selected layer will be bold.

Once you are satisfied with timing of the selected growth stage, press *Define*.

To change the beginning and end of the curve/time segment, drag position markers on the ruler.

Layer that has already been defined using experimental curve will be marked pink.

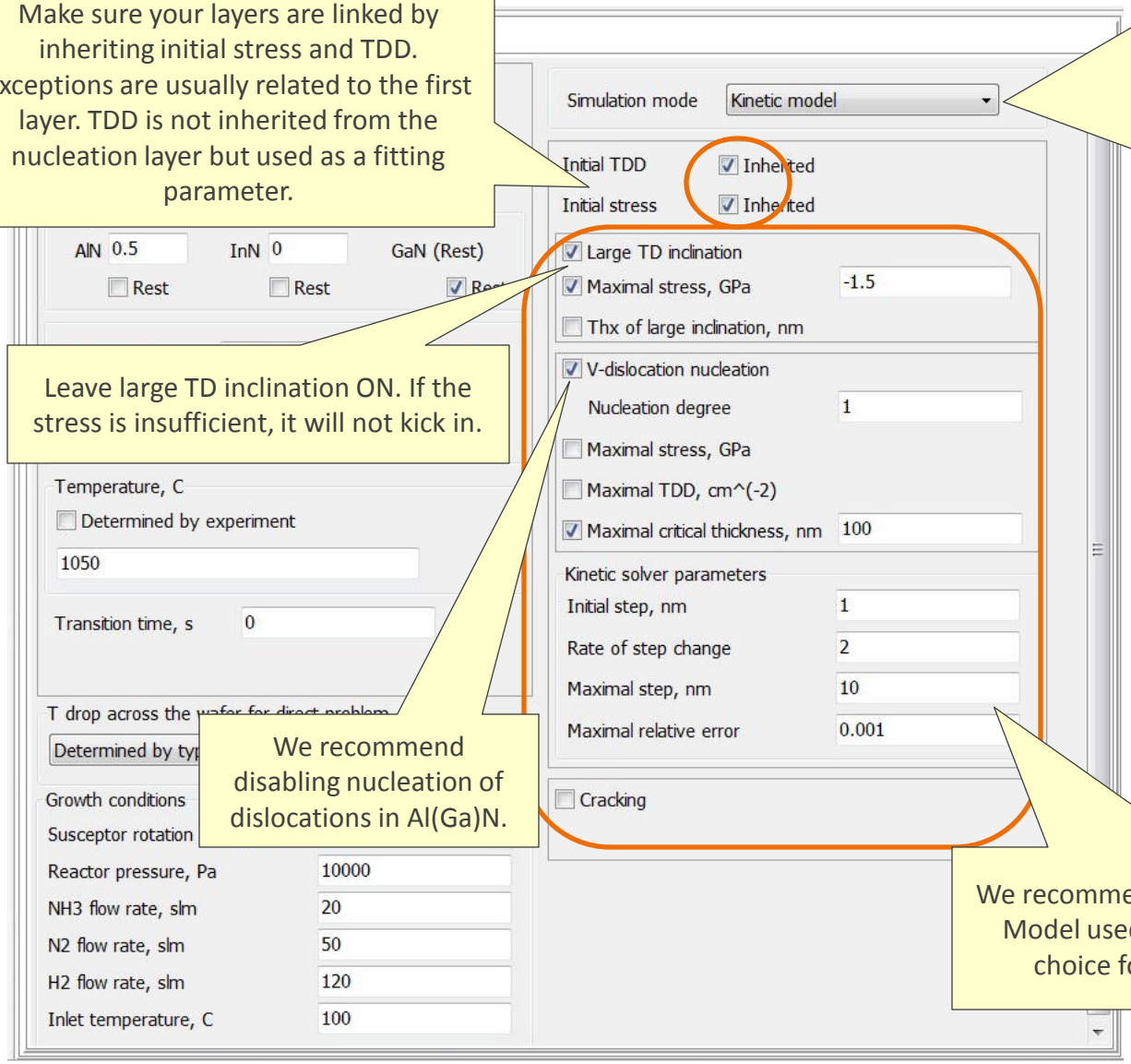
Alternatively, you can assign beginning and end times for the selected growth stage in numerical format.

If you do not need to choose a different growth stage to work on, you can close the panel.

Simulation Mode / Relaxation Model

Make sure your layers are linked by inheriting initial stress and TDD. Exceptions are usually related to the first layer. TDD is not inherited from the nucleation layer but used as a fitting parameter.

Simulation Modes:
Pseudomorphic – same as equilibrium with zero relaxation
Equilibrium – allows to specify expected relaxation degree. Use for **nucleation layer** (relaxation degree for NL is usually >0.9), tensile strain, cracking. Use number of steps 20+
Kinetic – uses software capabilities to predict compressive stress relaxation via dislocation inclination and nucleation. Should be chosen for compressively strained layers
Experimental – uses your data or results of solving inverse problem

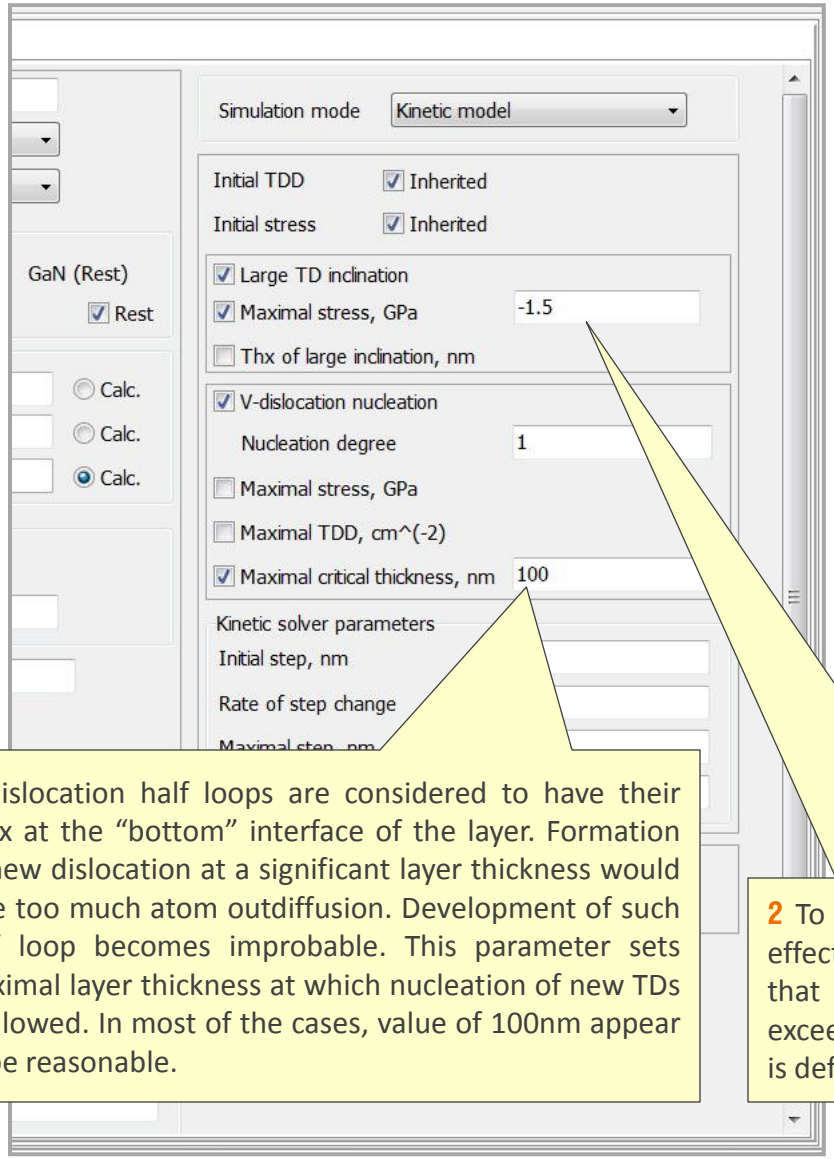


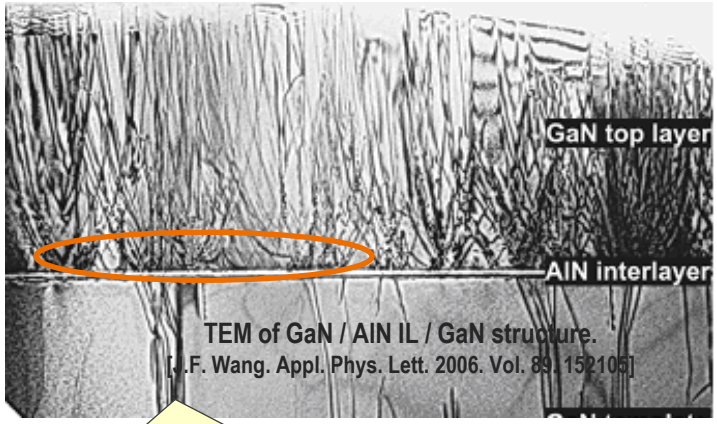
Leave large TD inclination ON. If the stress is insufficient, it will not kick in.

We recommend disabling nucleation of dislocations in Al(Ga)N.

We recommend using the settings of Kinetic Model used in this example as a default choice for most of the calculations

Physical meaning of some parameters



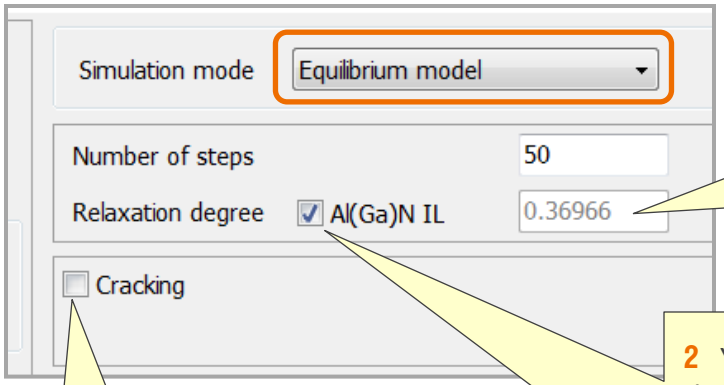


1 Compressive stress is relaxed by the inclination of TDs and the implemented kinetic model predicts variation of the inclination angle. However, as of today, it does not extend smoothly to the case of very large stress values. In that case, TDs incline quite radically (shown above), which allows them to reduce stress from initial value of, for instance, about - 10 Gpa to - 1,5 Gpa in some 20-40 nm.

2 To account for this very important effect, we have a separate model that kicks in once the stress value exceeds certain threshold value, that is defined here as a parameter.

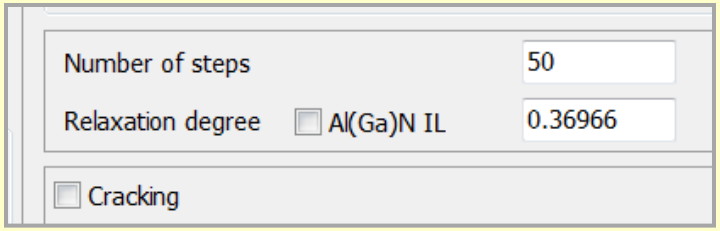
3 Dislocation half loops are considered to have their apex at the “bottom” interface of the layer. Formation of new dislocation at a significant layer thickness would take too much atom outdiffusion. Development of such half loop becomes improbable. This parameter sets maximal layer thickness at which nucleation of new TDs is allowed. In most of the cases, value of 100nm appear to be reasonable.

Physical meaning of some parameters (continued)



1 STREEM offers an option of automatic setting of relaxation degree in equilibrium model when used for thin Al(Ga)N layers under tensile strain. Calculation of this parameter is based on the experimental data we have and it takes into account all relaxation mechanisms including microcrack-induced strain relief.

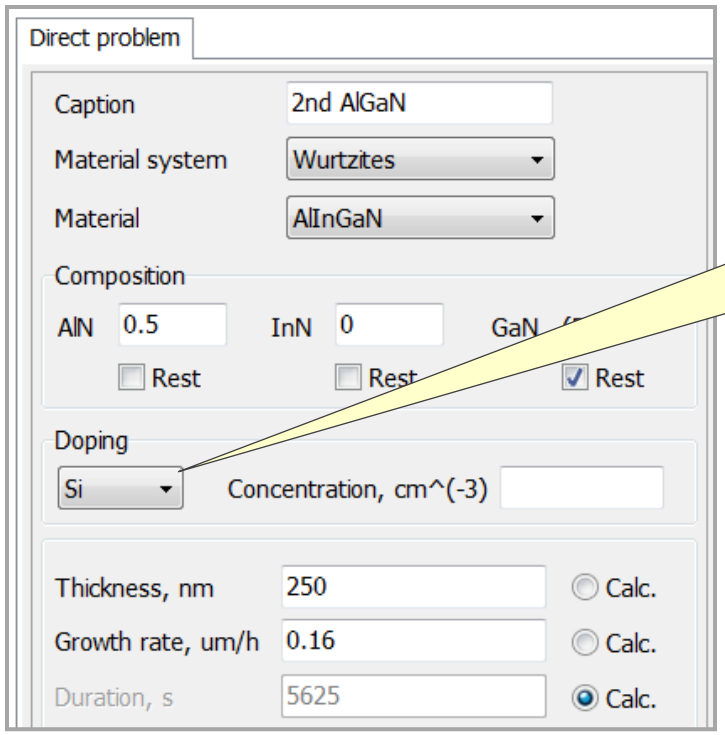
2 You can override this automatic value by un-checking the *Relaxation degree* box and, since the value will become editable, inputting the new parameter



3 This cracking refers to a cracking only and does not account for an initial slight relaxation via misfit dislocations formation. So it is recommended to use Cracking option for analysis of possible cracking in thick layers, particularly during structure cooling.

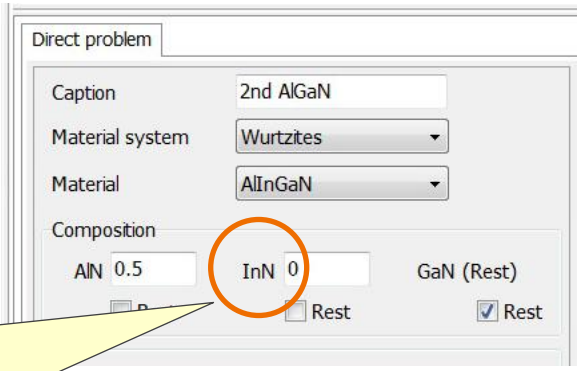
If automatically predicted relaxation degree for thin Al(Ga)N interlayer seems very low, it might still be a perfectly reasonable number reflecting the fact that micro-cracking only starts once the layer reaches certain thickness.

Physical meaning of some parameters (continued)



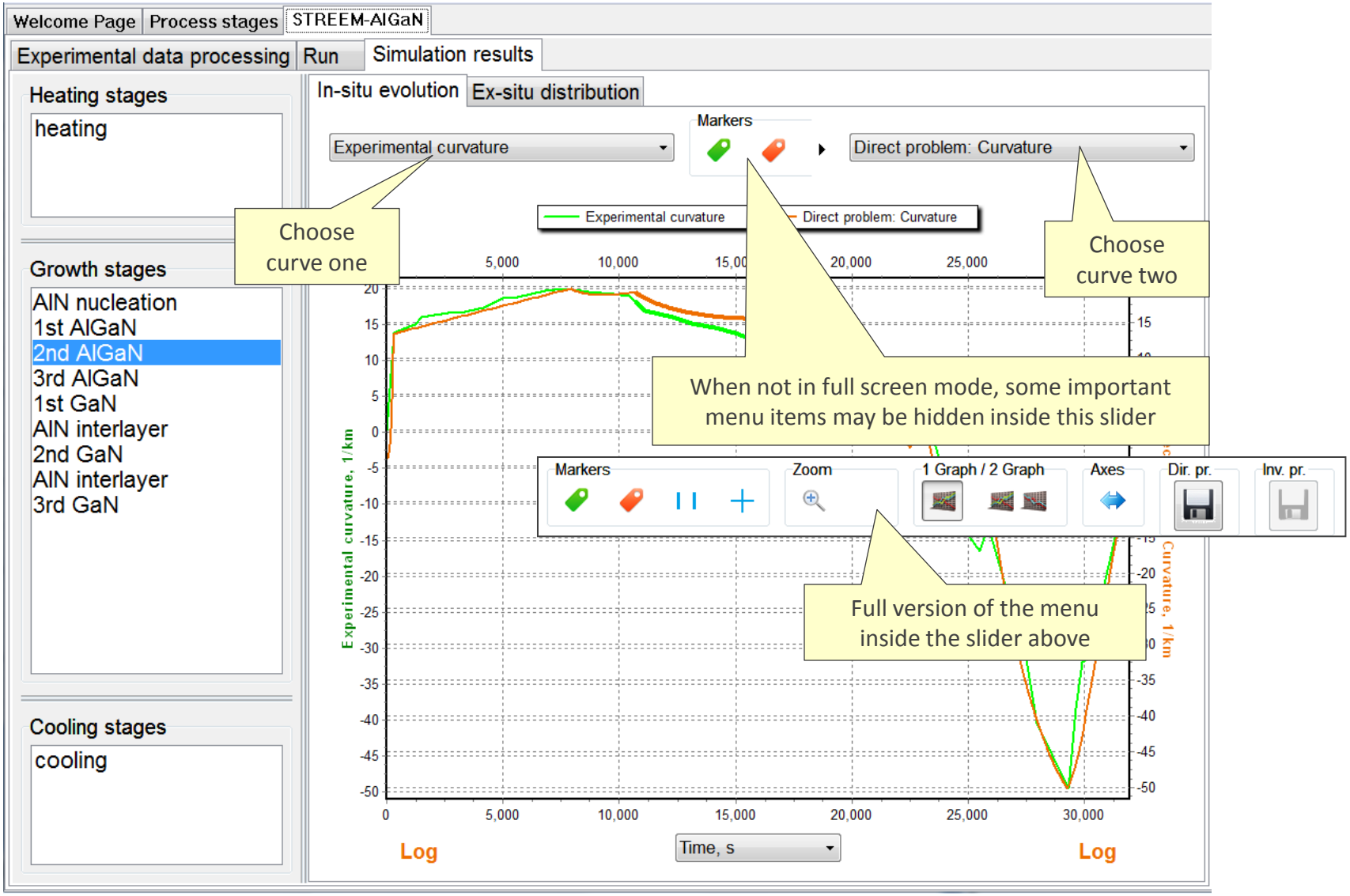
1 STREEM allows one to take into account the effect of **Si doping** on relaxation of compressively stressed layers. Presence of Si atoms increases inclination of threading dislocations thus accelerating the stress relief.

2 Please, note that inclination of dislocation in initially compressively strained layers is known to cease only once the stress becomes slightly tensile. The stress value at which dislocation stop inclining also depends on Si concentration.



3 A note on layers containing In. While STREEM supports simulation of stress relaxation in layers containing In, one should use this capability with caution, remembering that In segregation plays an important role in InGaN growth leading to strong dependence of In incorporation on stress at growth surface. AlGaN version of STREEM does not account for the effect of stress on In composition and careful treatment of this parameter becomes the responsibility of the user. You can use STREEM InGaN for the account of chemical processes during AlInGaN growth and self-consistent modeling of strain relaxation and In content.

Evolution of “Visible” Characteristics in Time



Detailed View for a Moment in Time