

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 Substrate Parameters
 Reactor=Vertical rotating disk reactor; Susceptor disk radius, cm=23; Reactor height, cm=7.6; Pocket thickness, um=100; Edit

Direct problem

Caption: 2nd AlGaIn
 Material system: Wurtzites
 Material: AlInGaIn
 Composition: AlN 0.5
 Rest

Thickness, nm

Growth rate, um/h: 0.16 Calc.
 Duration, s: 5625 Calc.

Temperature, C
 Determined by experiment
 1050

Transition time, s: 0

T drop across the wafer for direct problem
 Determined by type of growth reactor

Growth conditions

Susceptor rotation rate, rpm	1000
Reactor pressure, Pa	10000
NH3 flow rate, slm	20
N2 flow rate, slm	50
H2 flow rate, slm	120
Inlet temperature, C	100

Simulation mode: Kinetic
 Initial TDD

Nucleation degree: 1
 Maximal stress, GPa
 Maximal TDD, cm⁻²
 Maximal critical thickness, nm: 100

Kinetic solver parameters
 Initial step, nm: 1
 Rate of step change: 2
 Maximal step, nm: 10
 Maximal relative error: 0.001

Cracking

Interface for entering general characteristics of the reactor (shown below) and the substrate is located here. Both should be specified before T drop.

Reactor and Substrate Parameters

Growth reactor type
 Vertical rotating disk reactor

Susceptor disk radius, cm: 23
 Reactor height, cm: 7.6
 Pocket depth, um: 100

Substrate parameters
 Substrate material: Si(111)
 Thickness, um: 1000 Substrate diameter, mm: 200
 Initial curvature, 1/km: -4 Growth surf. orientation: (0001)

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

Heating stages

#	Caption	Conflicts
1	heating	

Growth stages

#	Group	Caption	Material	Thickness	Growth Rate	Duration	Inv.Pr.	Conflicts
1		AlN nucleati	AlN	130	0.0616	7597.4		
2		1st AlGa	Al _{0.75} Ga _{0.25} N	100	0.257	2801.6		
3		2nd AlGa	Al _{0.5} Ga _{0.5} N	100	0.16	5625		
4		3rd AlGa	Al _{0.25} Ga _{0.75} N	100	0.2	5400		
5		1st GaN	GaN	218.33	1.5	500		
6		AlN interlaye	AlN	8	0.072	400		
7		2nd GaN	GaN	9.6	1.584	215		
8		AlN interlaye	AlN	8	0.096	300		
9		3rd GaN	GaN	1433.3	1.60	322		

Cooling stages

#	Caption	Conflicts
1	cooling	

Reactor and Substrate Parameters
 Reactor=Vertical rotating disk reactor; Susceptor disk radius, cm=23; Reactor height, cm=7.6; Pocket thickness, um=100;

Direct problem

Caption: 2nd AlGaN
 Material system: Wurtzites
 Material: AlInGaN
 Composition: AlN 0.5, InN 0, GaN (Rest)

Simulation mode: Kinetic model

Initial TDD: Inherited
 Initial stress: Inherited
 Large TD inclination
 Maximal stress, GPa: -1.5
 Maximal TDD, cm⁻²
 Maximal critical thickness, nm: 100

Kinetic solver parameters
 Initial step, nm: 1
 Rate of step change: 2

Growth conditions
 Susceptor rotation rate, rpm: 1000
 Reactor pressure, Pa: 10000
 NH3 flow rate, slm: 20
 N2 flow rate, slm: 50
 H2 flow rate, slm: 120
 Inlet temperature, C: 100

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

Edit the layer name and describe its composition

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

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

Reactor and Substrate Parameters
 Reactor=Vertical rotating disk reactor; Susceptor disk radius, cm=23; Reactor height, cm=7.6; Pocket thickness, um=100; Edit

Direct problem

Caption: 2nd AlGaIn
 Material system: Wurtzites
 Material: AlInGaIn
 Composition: AlN 0.5, InN 0, GaN (Rest) Rest

Thickness, nm: 250 Calc.
 Growth rate, um/h: 0.16 Calc.
 Duration, s: 5625 Calc.

Temperature, C
 Determined by experiment
 1050

Transition time, s: 0

T drop across the wafer for direct problem
 Determined by type of growth reactor

Growth conditions

Susceptor rotation rate, rpm	1000
Reactor pressure, Pa	10000
NH3 flow rate, slm	20
N2 flow rate, slm	50
H2 flow rate, slm	120
Inlet temperature, C	100

Initial stress, GPa: -1.5
 V-dislocation nucleation
 Nucleation degree: 1
 Maximal stress, GPa
 Maximal TDD, cm⁻²
 Maximal critical thickness, nm: 100

Kinetic solver parameters
 Rate of step change
 Maximal step, nm
 Maximal relative error

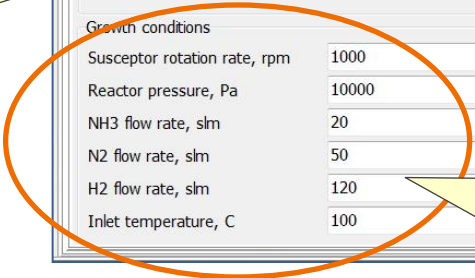
Cracking

If checked, will link to respective time interval of experimental data for temperature

Automatic (by type of reactor) calculation of T drop is recommended. Alternative is manual set up. It can be used when the information about the experiment is insufficient (can't use auto mode), or when we know the temperature drop with guaranteed high accuracy

If *Calculate* is checked for growth duration, option of setting the time interval using experimental curve will be disabled for this layer

Length of no growth interval such as T ramping. Change in curvature during this stage indicates change in T drop.



Used for determining vertical temperature gradient (through the wafer). These parameters should not be used for fitting

1 Load the file with the monitoring data for the substrate curvature or temperature. See the manual for supported data formats.

2 To set up duration and position, select the respective growth stage.

3 Then click *Define layer* (continued on the next page)

Duration of the layers marked by bold font can not be assigned using experimental data. *Define layer* button will be disabled for this layer.

If *Define layer* button is disabled, it means that thickness and growth rate where chosen to define the growth duration for this layer on the Process Stages tab and *Calculate* radio button was toggled on for the growth duration.

The screenshot shows the 'Process stages' tab for 'STREEM-AIGaN'. The 'Growth stages' list includes: AIN nucleation, 1st AIGaN, 2nd AIGaN, 3rd AIGaN, 1st GaN, AIN interlayer, 2nd GaN (highlighted in blue), AIN interlayer, and 3rd GaN. The central graph plots Curvature (1/km) on the y-axis (ranging from -50 to 20) against Time (s) on the x-axis (ranging from 0 to 30,000). Two data series are shown: 'Curvature' (blue line) and 'Layer' (red line). The 'Layer' line shows a step-like increase in curvature over time, with some fluctuations. The 'Define layer' button in the bottom toolbar is circled in orange. A callout box points to the '2nd GaN' stage in the list, and another callout points to the 'Define layer' button. A third callout points to the 'Layer' data series in the graph.



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.

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

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

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.

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

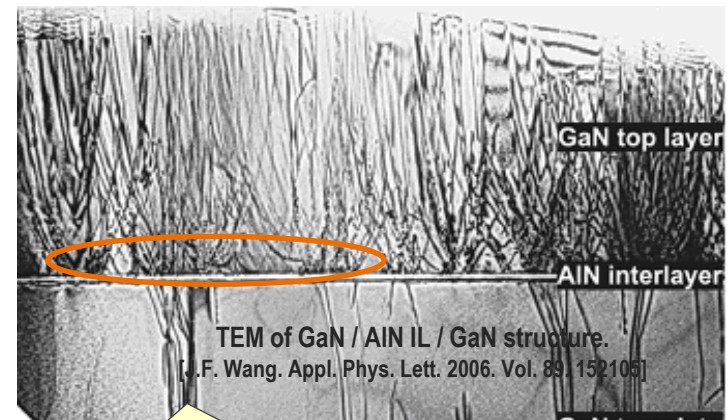
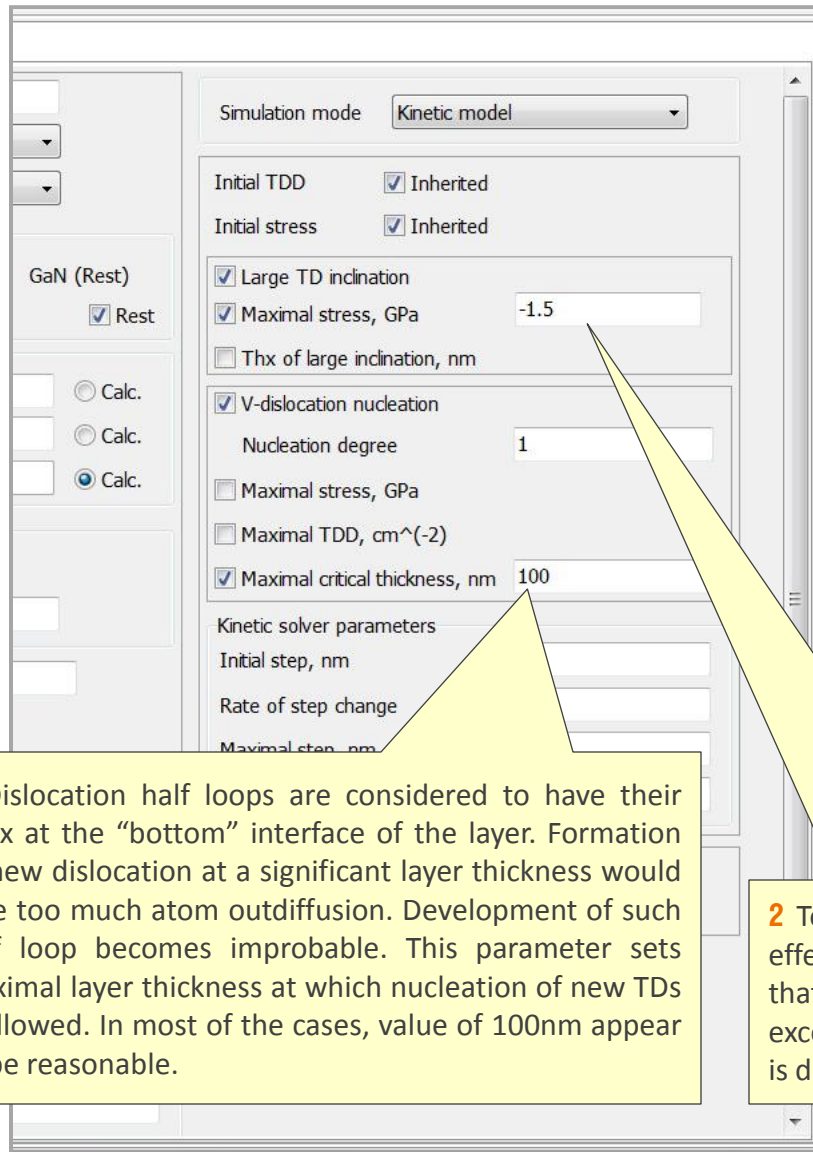
We recommend disabling nucleation of dislocations in Al(Ga)N.

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

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

The screenshot shows a software interface for simulation settings. The 'Simulation mode' is set to 'Kinetic model'. Under 'Initial TDD' and 'Initial stress', the 'Inherited' checkbox is checked. In the 'Kinetic model' section, 'Large TD inclination' and 'Maximal stress, GPa' (-1.5) are checked. 'V-dislocation nucleation' is checked with a 'Nucleation degree' of 1. 'Maximal critical thickness, nm' is set to 100. Under 'Kinetic solver parameters', 'Initial step, nm' is 1, 'Rate of step change' is 2, 'Maximal step, nm' is 10, and 'Maximal relative error' is 0.001. The 'Cracking' checkbox is unchecked. On the left, material layers are listed: AlN 0.5, InN 0, and GaN (Rest). Growth conditions include reactor pressure (10000 Pa), NH3 flow rate (20 slm), N2 flow rate (50 slm), H2 flow rate (120 slm), and inlet temperature (100 C).



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.

Simulation mode: Equilibrium model

Number of steps: 50

Relaxation degree: Al(Ga)N IL 0.36966

Cracking

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

Number of steps: 50

Relaxation degree: Al(Ga)N IL 0.36966

Cracking

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.

Direct problem

Caption: 2nd AlGaIn

Material system: Wurtzites

Material: AlInGaIn

Composition

AlN: 0.5 InN: 0 GaN: 0

Rest Rest Rest

Doping

Si Concentration, cm⁻³

Thickness, nm: 250 Calc.

Growth rate, um/h: 0.16 Calc.

Duration, s: 5625 Calc.

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 InGaIn growth leading to strong dependence of In incorporation on stress at growth surface. AlGaIn 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 InGaIn for the account of chemical processes during AlInGaIn growth and self-consistent modeling of strain relaxation and In content.

Direct problem

Caption: 2nd AlGaIn

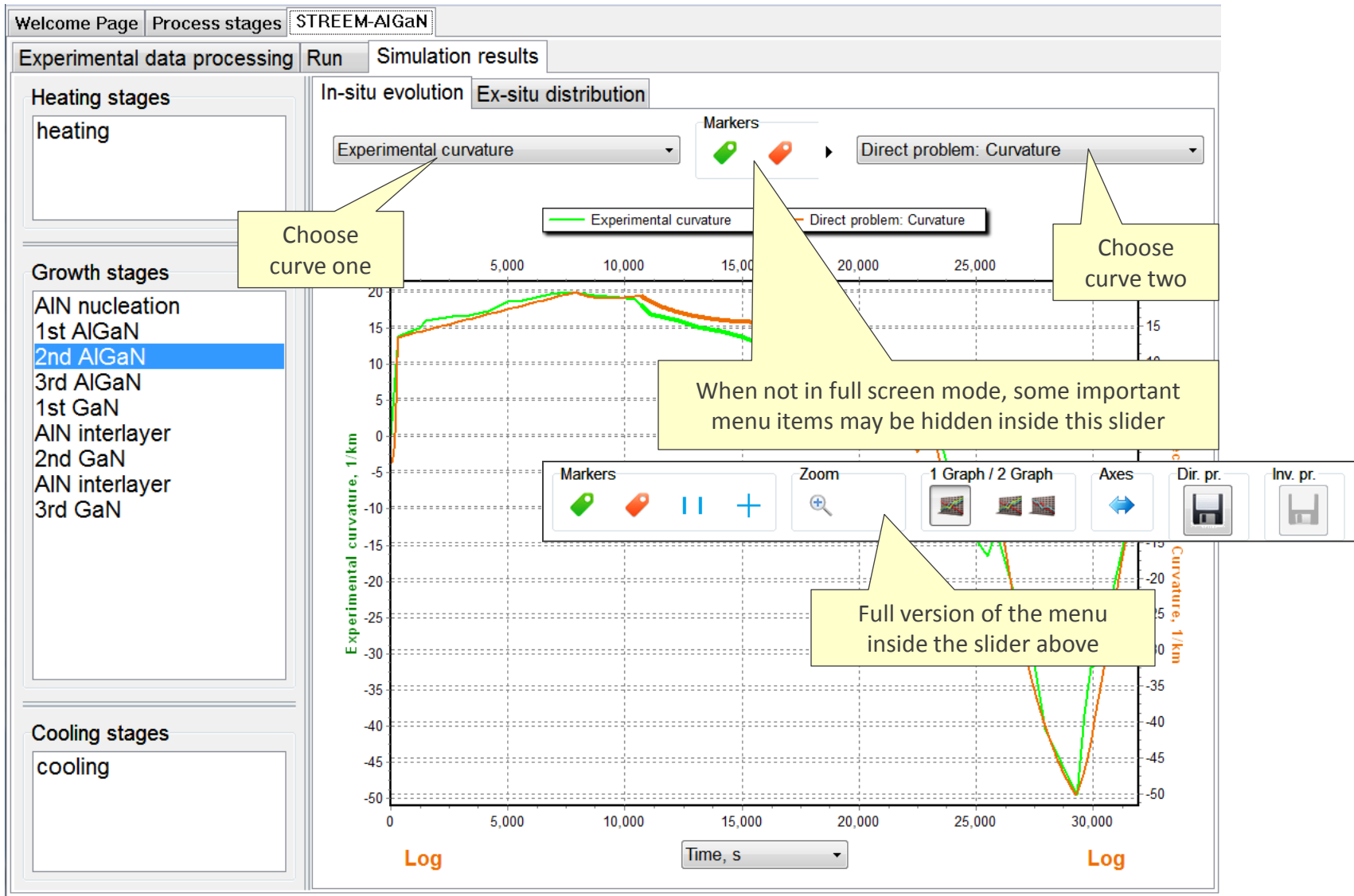
Material system: Wurtzites

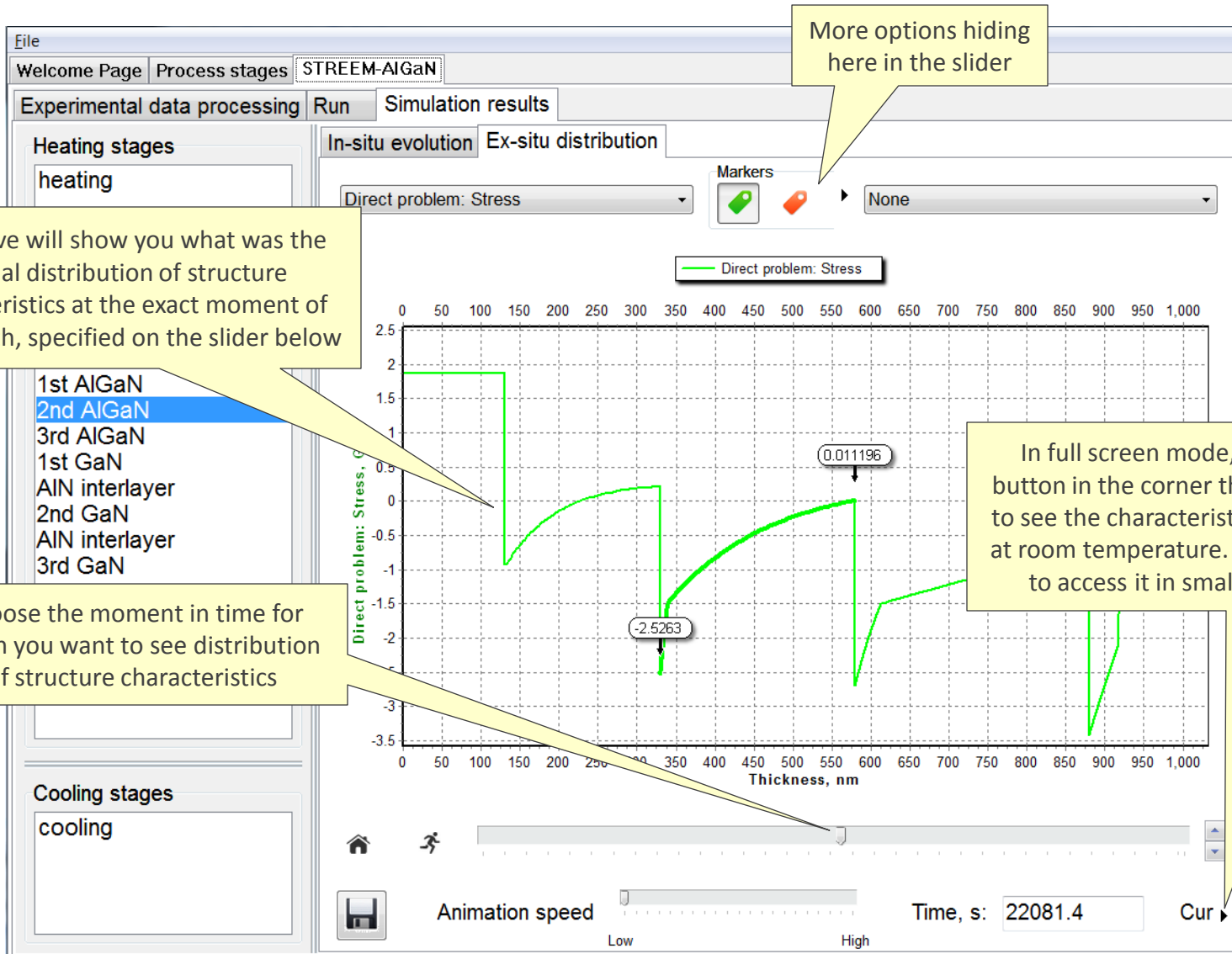
Material: AlInGaIn

Composition

AlN: 0.5 InN: 0 GaN (Rest)

Rest Rest





This curve will show you what was the spatial distribution of structure characteristics at the exact moment of the growth, specified on the slider below

- 1st AlGaIn
- 2nd AlGaIn
- 3rd AlGaIn
- 1st GaN
- AlN interlayer
- 2nd GaN
- AlN interlayer
- 3rd GaN

More options hiding here in the slider

Choose the moment in time for which you want to see distribution of structure characteristics

In full screen mode, there is RT button in the corner that allows one to see the characteristic distribution at room temperature. Use this slider to access it in small windows.

