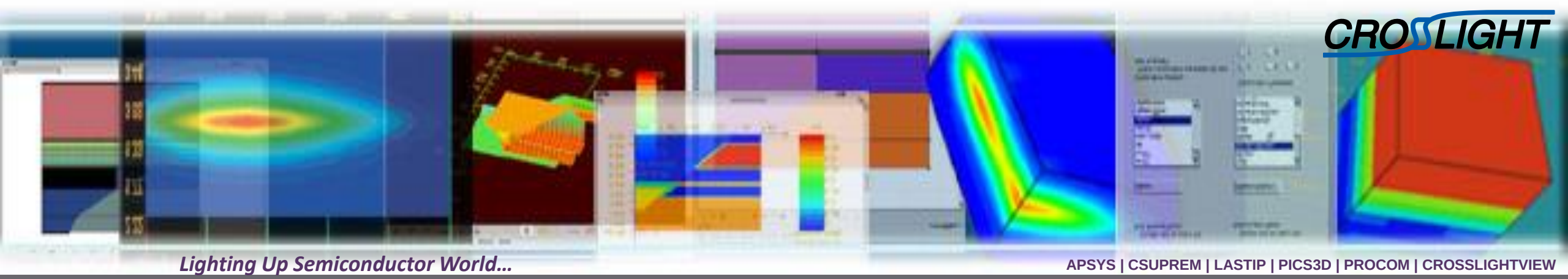
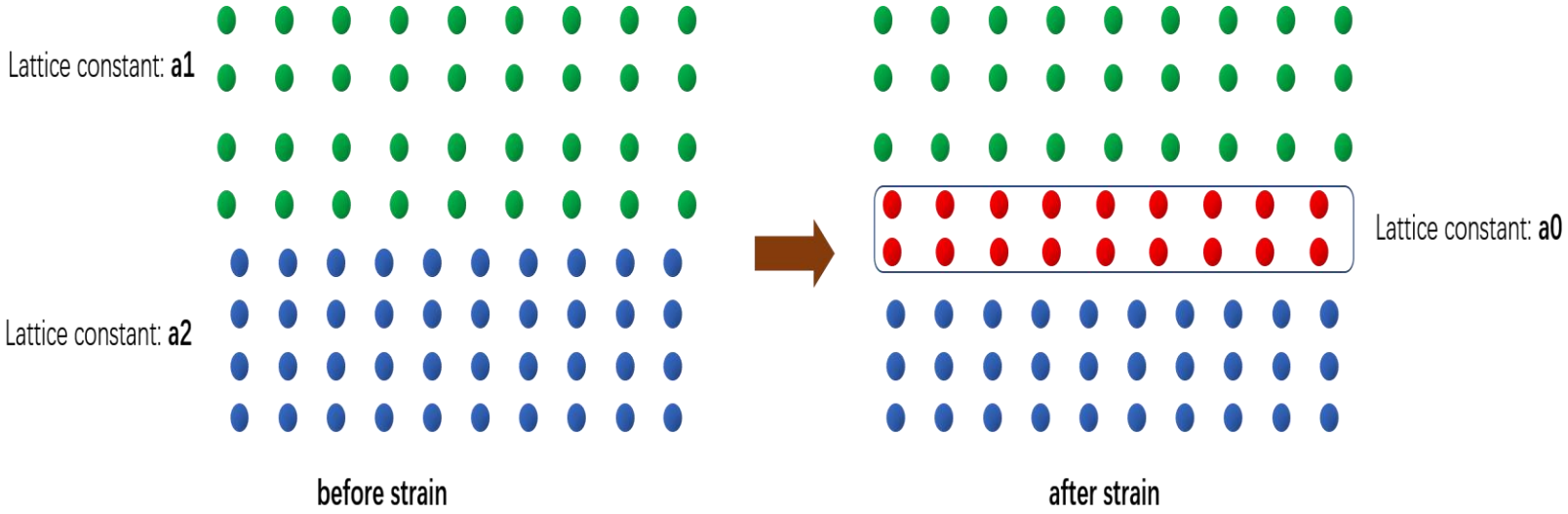


Minimum Elastic Energy Stress Method in CSUPREM

© Crosslight Software, Inc., Vancouver, BC, Canada, (604)320-1704, www.crosslight.com

Stress Interface Layer

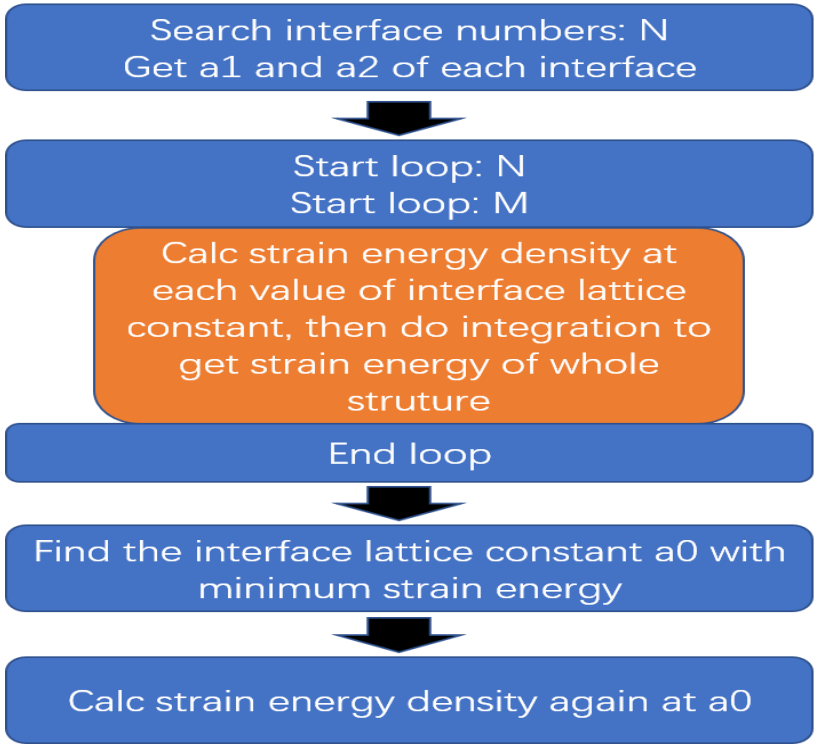


- Interface layer has lattice constant $a_1 < a_0 < a_2$ which creates strain
- Stress algorithm to find minimum elastic energy in entire structure

©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

Algorithm

- Assume interface layer is composed of N separate interfaces of thickness d, with a_0 varying for each interface
- Use a grid of M possible values for a_0 in the allowed $[a_1, a_2]$ range
- Compute strain energy for entire structure for all $M \times N$ possibilities



©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

Syntax Example (1)

```
option quiet
#
# nitride on silicon example

   line x loc=(-10) tag=l
   line x loc=-2.0 spac=0.2
   line x loc=0 spac=0.06 tag=m
   line x loc=2.0 spac=0.2
   line x loc=(10) tag=r

   line y loc=0 spac=0.06 tag=si
   line y loc=2 spac=0.2
   line y loc=5 tag=b

   region silicon xlo=l xhi=r ylo=si yhi=b
   bound expos xlo=l xhi=r ylo=si yhi=si
   initial ori=111
```


©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

Syntax Example (2)

```
deposit nitride thick=0.02 div=2
etch nitride left p1.x=0.0

#   material intrin.sig=1.4e10 nitride

#   stress temp1=1000 temp2=1000

material silicon latt.cons=5.4307
material nitride latt.cons= 7.6015
stress temp1=1000 temp2=1000 model="min.elastic.energy" times.try=30 interface.thick=0.15

#   plot.2d bound x.mi=-2.0 x.ma=2.0 y.ma=4.0 cl=f
#   select z=Sxy
#   contour val=-3.0e7
#end
struct out=exp8.str
```

Lattice Constants

Stress Model

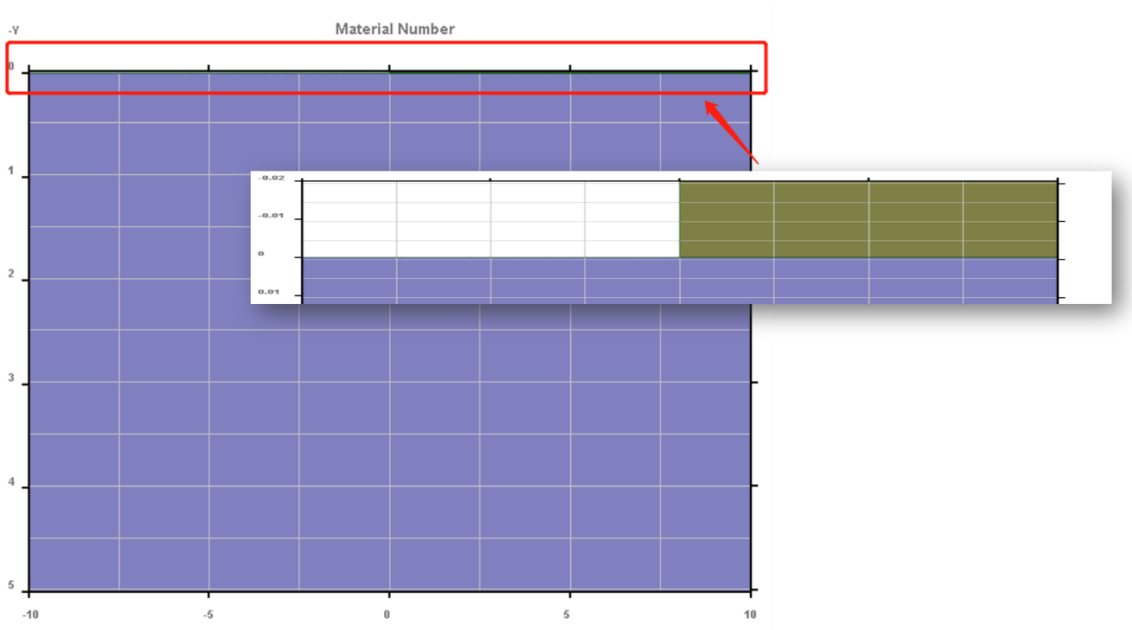
©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

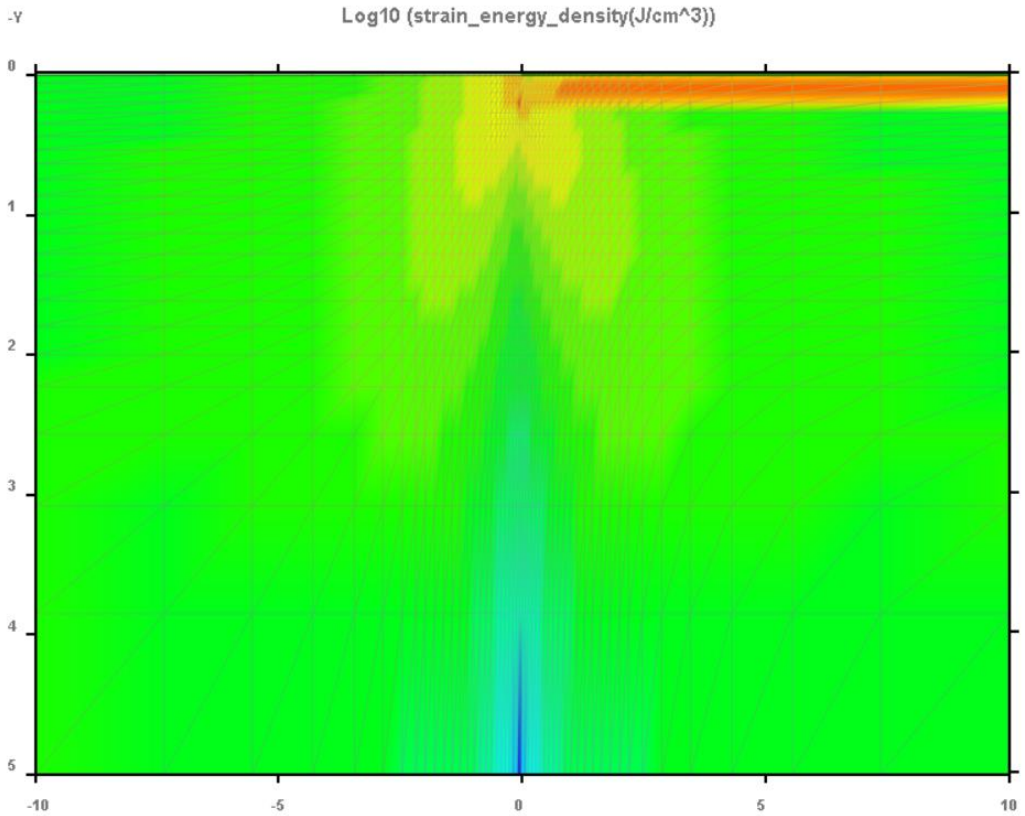
Model Output

```
--->" material silicon latt.cons=5.4307"

--->" material nitride latt.cons= 7.6015"

--->" stress temp1=1000 temp2=1000 model="min.elastic.energy"  times.try=30 interface.thick=0.15"
stress model: min.elastic.energy
--- Start batch calculations for device elastic energy ---
    number of interface type: 1
    try 30 data points of lattice constant for each interface
[Interface] [Try NO.] [a1]     [a2]     [a.share] [Elastic energy]
    1          1       5.43070 7.60150 5.43070 1.158197e+003
    1          2       5.43070 7.60150 5.50556 1.062656e+003
    1          3       5.43070 7.60150 5.58041 9.823818e+002
    1          4       5.43070 7.60150 5.65527 9.173740e+002
    1          5       5.43070 7.60150 5.73012 8.676326e+002
    1          6       5.43070 7.60150 5.80498 8.331577e+002
    1          7       5.43070 7.60150 5.87983 8.139493e+002
    1          8       5.43070 7.60150 5.95469 8.100072e+002
    1          9       5.43070 7.60150 6.02954 8.213317e+002
    1         10       5.43070 7.60150 6.10440 8.479225e+002
    1         11       5.43070 7.60150 6.17925 8.897799e+002
    1         12       5.43070 7.60150 6.25411 9.469036e+002
    1         13       5.43070 7.60150 6.32896 1.019294e+003
    1         14       5.43070 7.60150 6.40382 1.106950e+003
    1         15       5.43070 7.60150 6.47867 1.209874e+003
    1         16       5.43070 7.60150 6.55353 1.328063e+003
    1         17       5.43070 7.60150 6.62838 1.461519e+003
    1         18       5.43070 7.60150 6.70324 1.610241e+003
    1         19       5.43070 7.60150 6.77809 1.774230e+003
    1         20       5.43070 7.60150 6.85295 1.953486e+003
    1         21       5.43070 7.60150 6.92780 2.148007e+003
    1         22       5.43070 7.60150 7.00266 2.357796e+003
    1         23       5.43070 7.60150 7.07751 2.582850e+003
    1         24       5.43070 7.60150 7.15237 2.823171e+003
    1         25       5.43070 7.60150 7.22722 3.078759e+003
    1         26       5.43070 7.60150 7.30208 3.349613e+003
    1         27       5.43070 7.60150 7.37693 3.635733e+003
    1         28       5.43070 7.60150 7.45179 3.937120e+003
    1         29       5.43070 7.60150 7.52664 4.253773e+003
    1         30       5.43070 7.60150 7.60150 4.585693e+003
lowest elastic energy : 8.100072e+002
--- Done! ---
```


©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

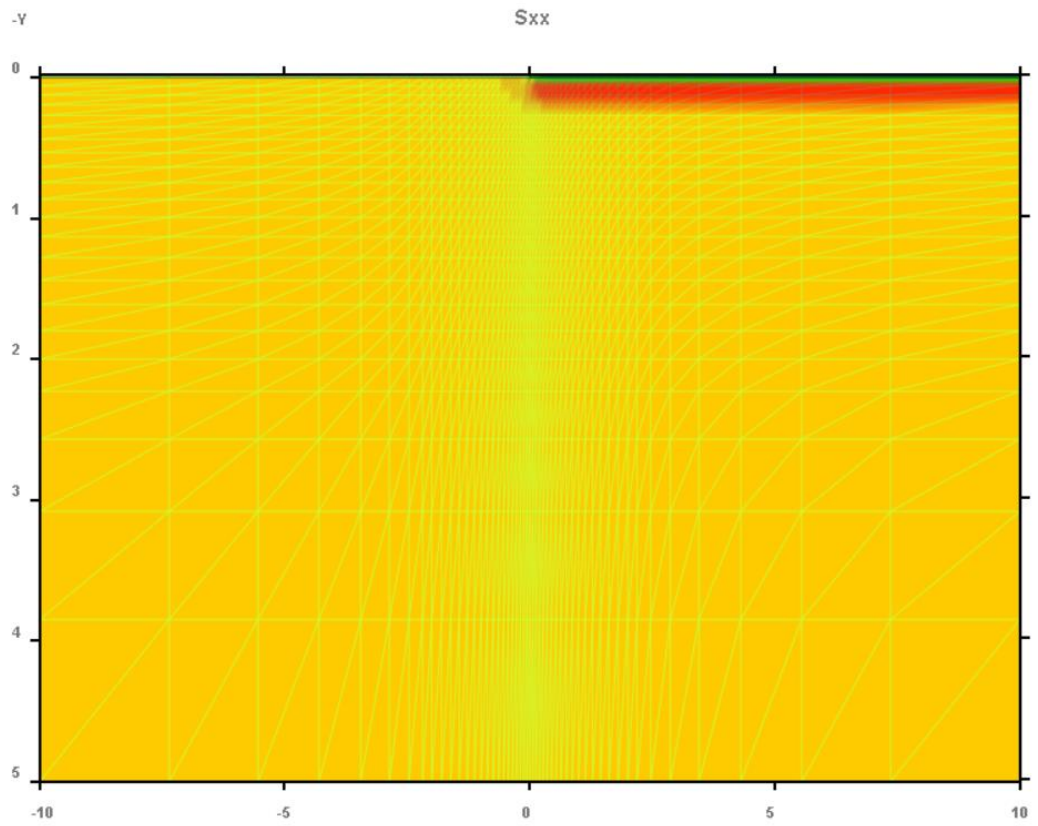
Results

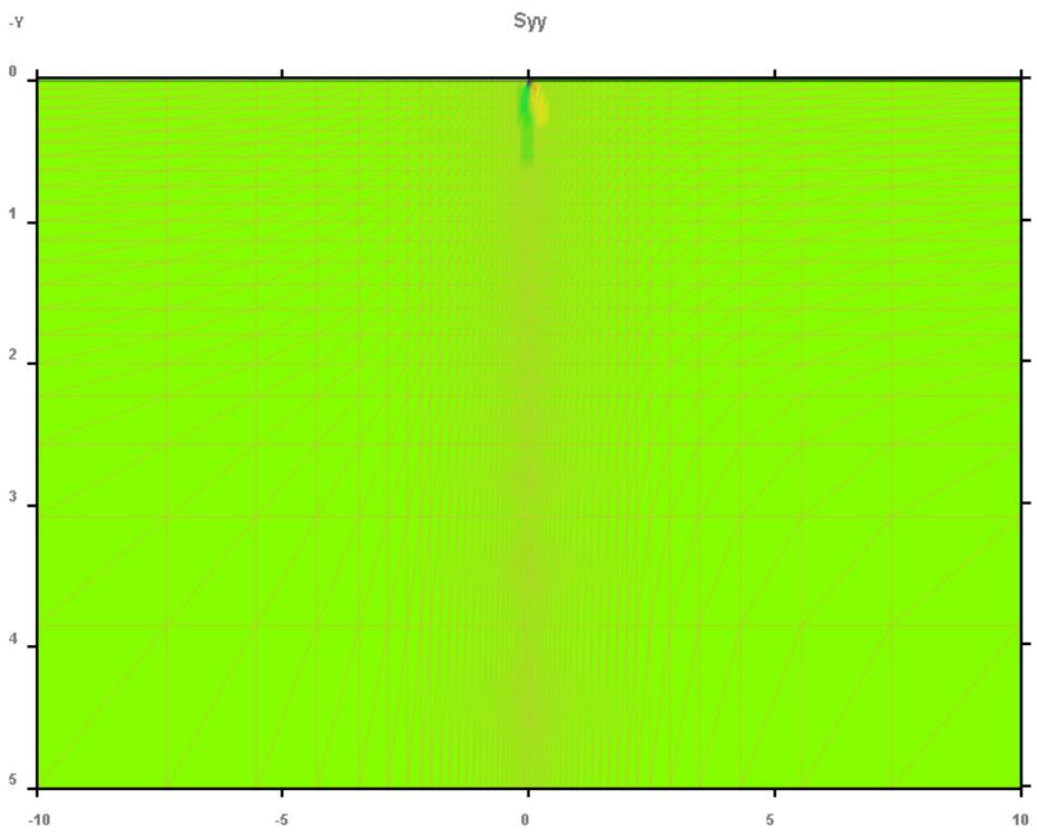




©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

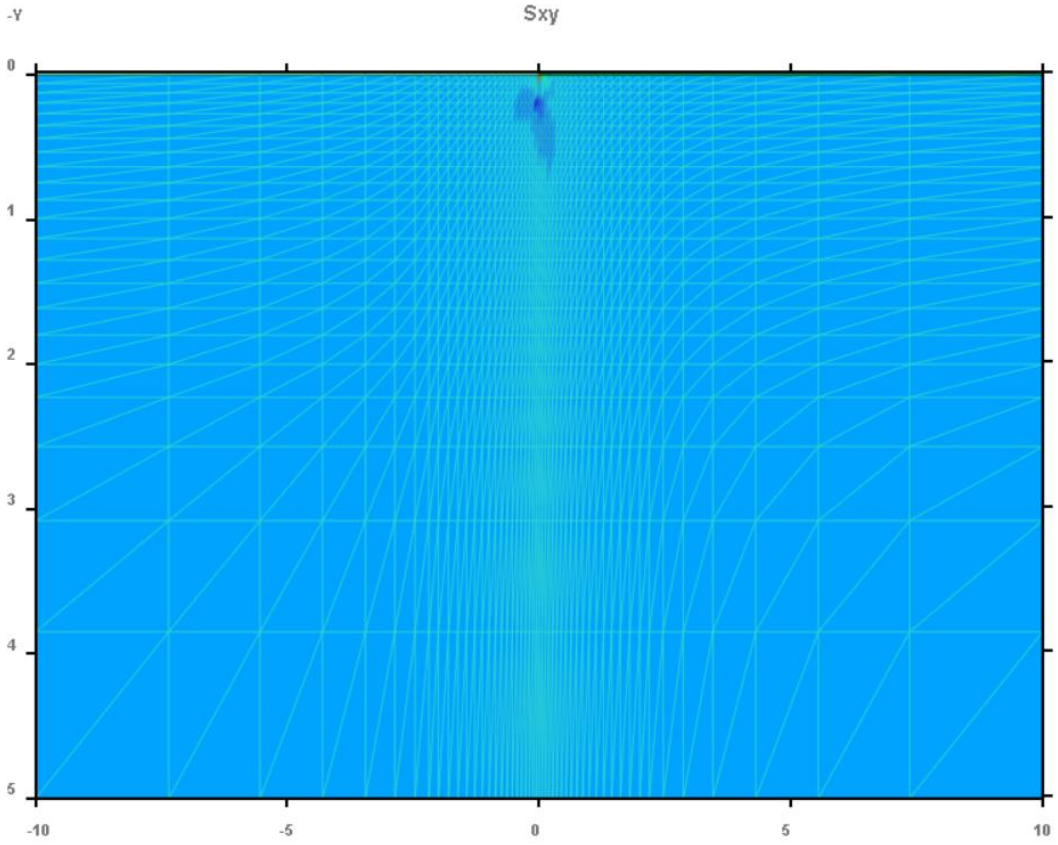
Results (2)





©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

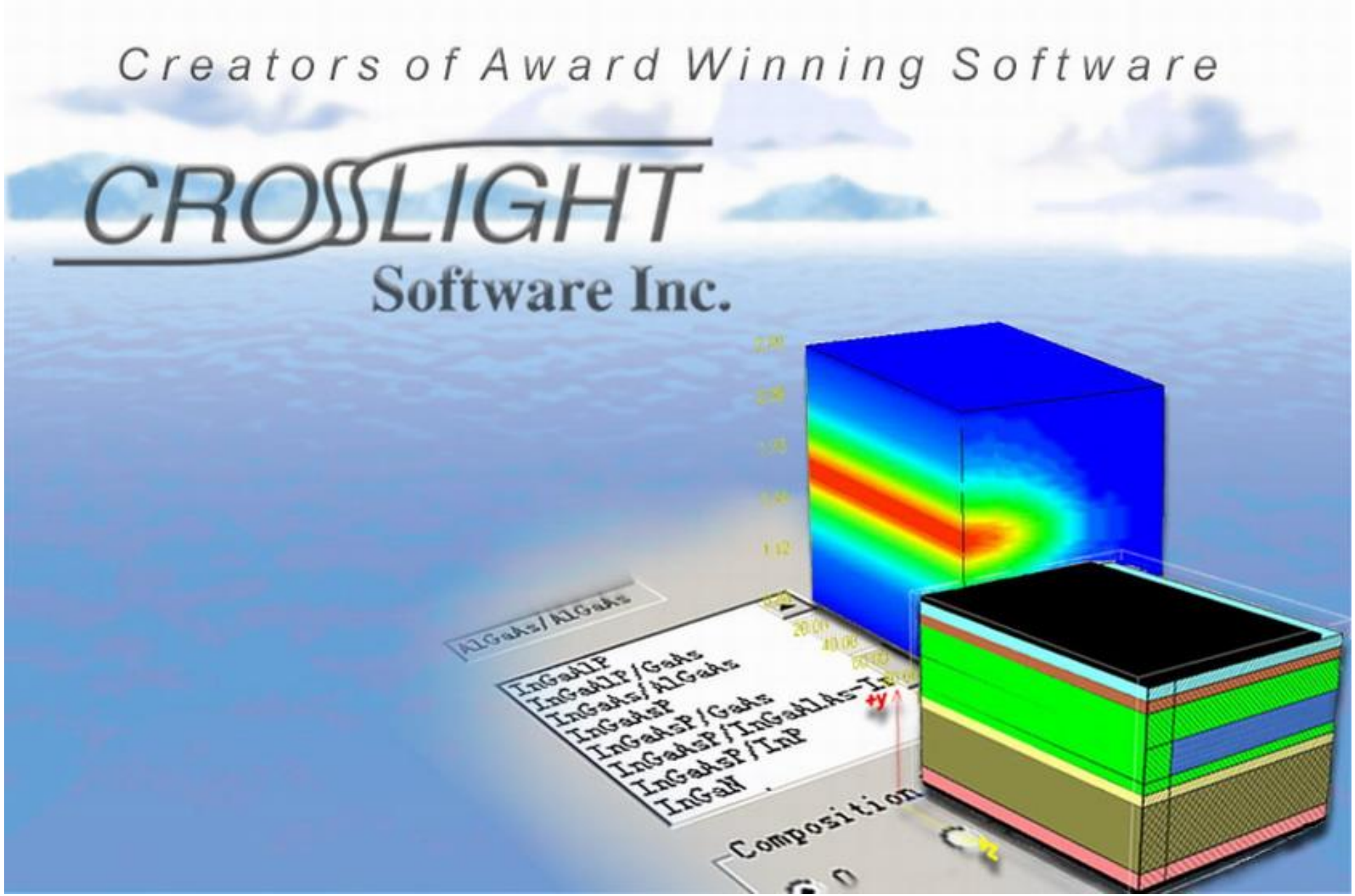
Results (3)



©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com

Thanks for your attention!

©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com



©2020 Crosslight Software, Inc., Vancouver, BC, Canada www.crosslight.com