Do it yourself – automated thin film design using genetic algorithms

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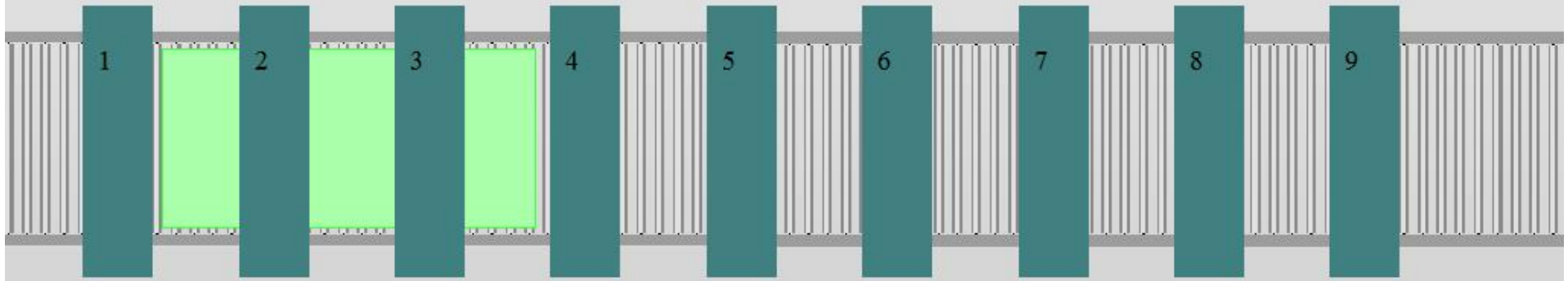
Motivation
A first simple design problem
Genetics: Solution by evolution
Simple 'real time' demonstrations
Advanced examples: Discussion of results

Motivation: Inline coater

Deposition chambers may be equipped with various types of cathodes.
What is the best choice for a given problem?



Available:

	SiO2	TiO2	ZnO	ITO	Ag	Cu	a-Si
Thickness range [nm]:	10 ... 30	5 ... 25	5 ... 25	20 ... 60	5 ... 15	5 ... 15	30 ... 80

0:00:17:525

First example: Car glass that can be heated for de-icing

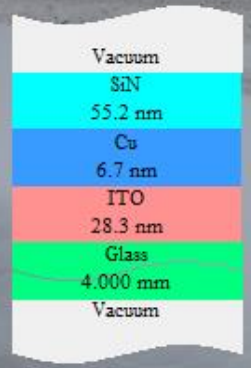
Design target

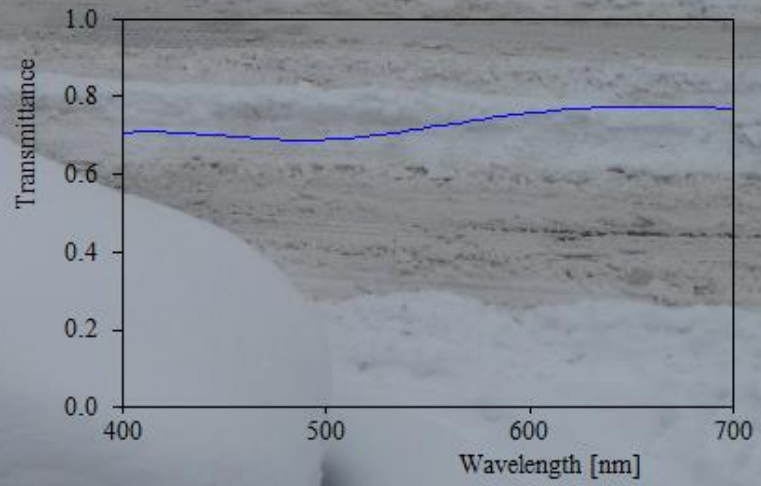
Integral quantity	**Current value**	**Target value**
Sheet resistance (SR)	2.9103	2.2000
Visible light transmittance (VLT)	0.726	1.000

$$Deviation = \frac{1}{10}(SR - 2.2)^2 + (VLT - 1)^2$$

$$Fitness = \frac{1}{0.0001 + Deviation} = 7.97$$

D	55.2	Stack 1 Layer 2 SiN: Layer thickness
D	6.7	Stack 1 Layer 3 Cu: Layer thickness
D	28.3	Stack 1 Layer 4 ITO: Layer thickness





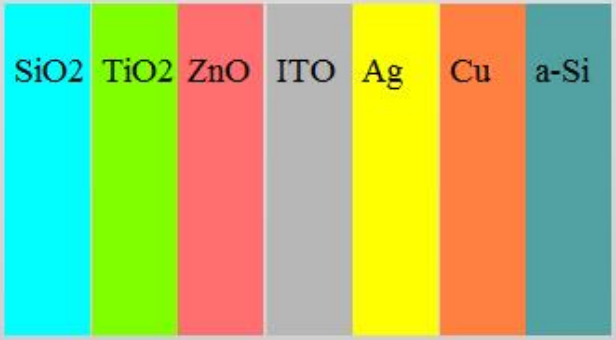
Genetics

128 bit represent a single layer (material selection and thickness)

100011011101101 ... 10110110110110001101011010101

64 bit represent a floating point number g
which is converted into a material index

$$N = truncate\left(1 + \frac{N_{Max} - 1}{1 + |g|}\right)$$



0010111101010101011011011 0 ... 011011011101110110

64 bit represent a floating point number f
which is converted into a thickness value

$$d = d_{min} + \frac{d_{max} - d_{min}}{1 + |f|}$$

N*128 bit represent a layer stack individual with N layers

1011011100111110001101101101101101101101101101011010110100110000001101101101010101010111111

Genetics

Start
Generate a large population (hundreds) of individuals with random genes

Ranking
Compute fitness for each individual, sort the population

Best individuals
move on to next generation without modifications

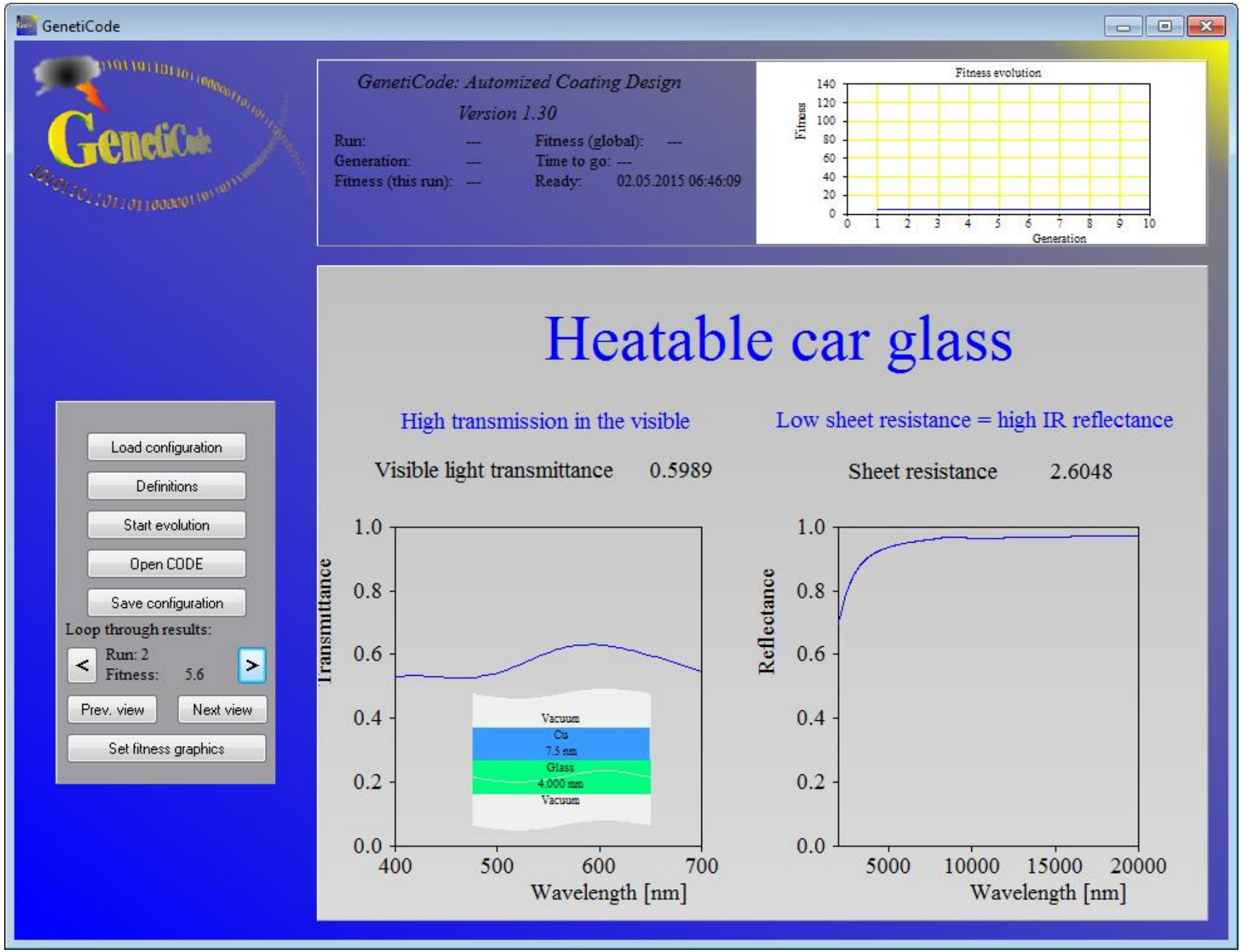
Mating
Combine genes of 2 individuals to produce children for next generation
Prefer individuals with high fitness

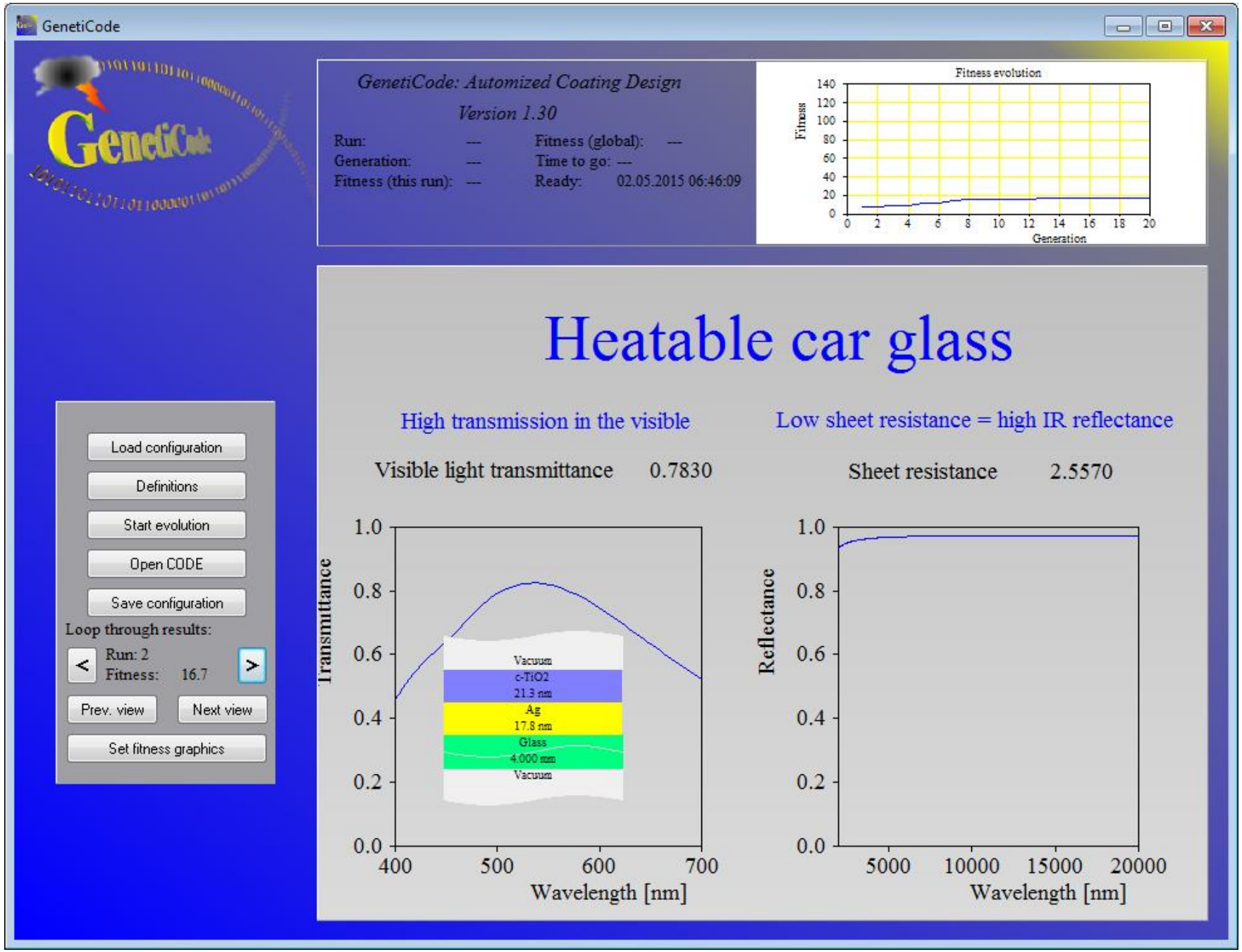
Mutation
With a certain probability: Exchange 2 genes at random positions

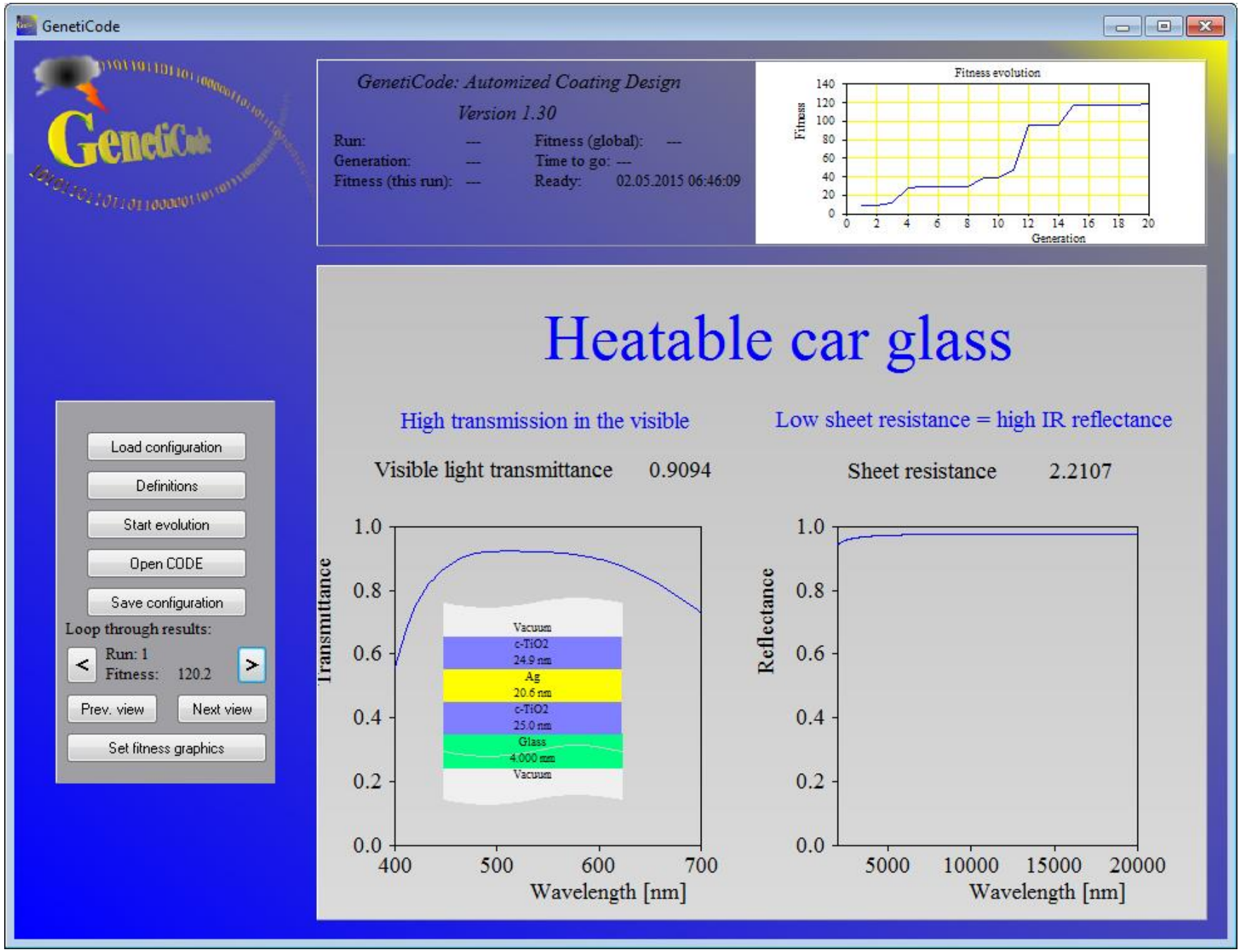
Next generation
with same number of individuals

End of evolution
Take the best individual as result
Eventually do refinement

First example: Car glass that can be heated for de-icing

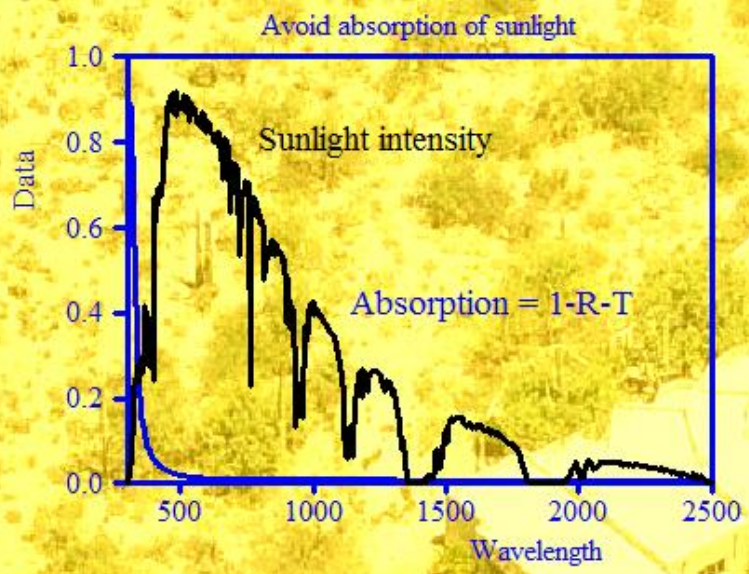

GenetiCode
GenetiCode: Automized Coating Design
Version 1.30
Run: ---
Generation: ---
Fitness (this run): ---
Fitness (global): ---
Time to go: ---
Ready: 02.05.2015 06:46:09
Fitness evolution
Fitness
Generation
Heatable car glass
High transmission in the visible
Low sheet resistance = high IR reflectance
Visible light transmittance 0.5989
Sheet resistance 2.6048
Transmittance
Wavelength [nm]
Vacuum
Cu
7.5 nm
Glass
4.000 mm
Vacuum
Reflectance
Wavelength [nm]
Load configuration
Definitions
Start evolution
Open CODE
Save configuration
Loop through results:
Run: 2
Fitness: 5.6
Prev. view
Next view
Set fitness graphics

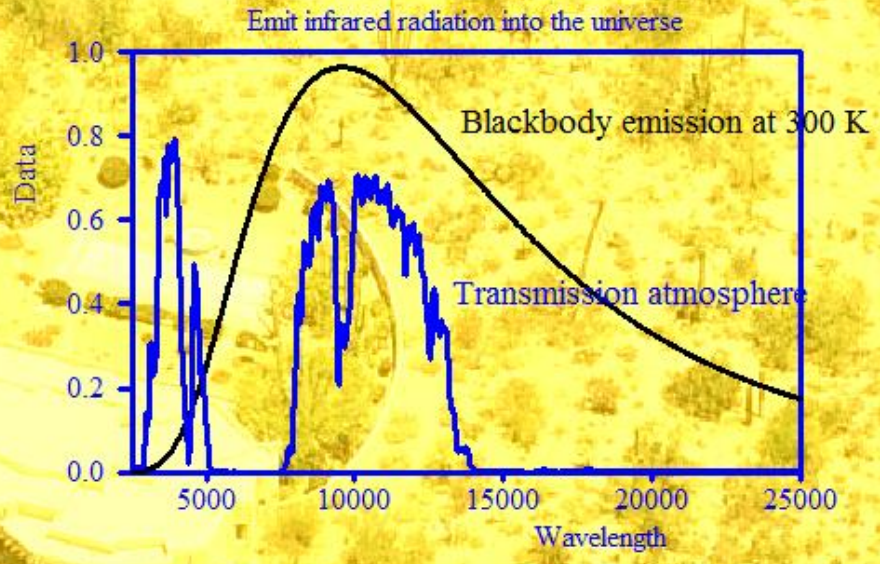

GenetiCode
GenetiCode: Automized Coating Design
Version 1.30
Run: ---
Generation: ---
Fitness (this run): ---
Fitness (global): ---
Time to go: ---
Ready: 02.05.2015 06:46:09
Fitness evolution
Fitness
Generation
Heatable car glass
High transmission in the visible
Low sheet resistance = high IR reflectance
Visible light transmittance 0.7830
Sheet resistance 2.5570
Transmittance
Wavelength [nm]
Vacuum
c-TiO2
21.3 nm
Ag
17.8 nm
Glass
4.000 mm
Vacuum
Reflectance
Wavelength [nm]
Load configuration
Definitions
Start evolution
Open CODE
Save configuration
Loop through results:
Run: 2
Fitness: 16.7
Prev. view
Next view
Set fitness graphics


GenetiCode
GenetiCode: Automized Coating Design
Version 1.30
Run: ---
Generation: ---
Fitness (this run): ---
Fitness (global): ---
Time to go: ---
Ready: 02.05.2015 06:46:09
Fitness evolution
Fitness
Generation
Heatable car glass
High transmission in the visible
Low sheet resistance = high IR reflectance
Visible light transmittance 0.9094
Sheet resistance 2.2107
Transmittance
Wavelength [nm]
Vacuum
c-TiO2
24.9 nm
Ag
20.6 nm
c-TiO2
25.0 nm
Glass
4.000 mm
Vacuum
Reflectance
Wavelength [nm]
Load configuration
Definitions
Start evolution
Open CODE
Save configuration
Loop through results:
Run: 1
Fitness: 120.2
Prev. view
Next view
Set fitness graphics

Hot day, full sunshine, high air condition bill - cooling coating?

Passive cooling requirements





Candidate: Coating on large glass pane

Cooling power =
Power emitted into space
- absorbed sunpower

Passive cooling invention

Candidate: Coating on large glass pane

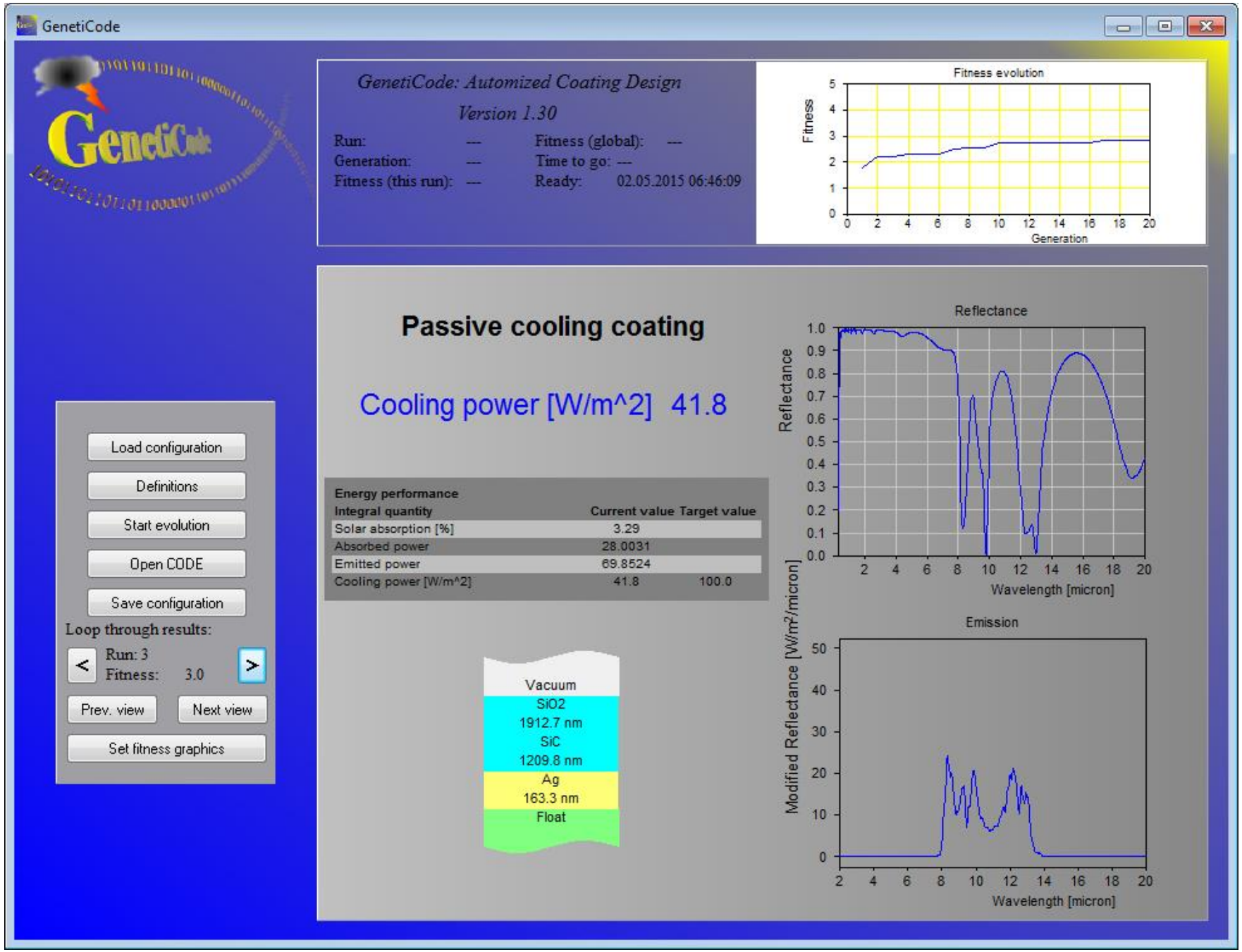
Cooling power =

Power emitted into space
- absorbed sunpower

Materials (vis and IR properties must be known) used for this problem:
- Ag (3 ... 200 nm)
- Au (3 ... 200 nm)
- Cu (3 ... 200 nm)
- SiO_2 (10 ... 2000 nm)
- TiO_2 (10 ... 2000 nm)
- SiC (10 ... 2000 nm)

Before we start genetics ...

Who is going to be the patent holder?
- this laptop?
- the person who pointed out the problem?
- the programmer of the software (yes!!!)
- those people who "invented" genetic algorithms?
- you as audience since you watch the invention happen?
- no-one?


GenetiCode
GenetiCode: Automized Coating Design
Version 1.30
Run: ---
Generation: ---
Fitness (this run): ---
Fitness (global): ---
Time to go: ---
Ready: 02.05.2015 06:46:09
Fitness evolution
Fitness
Generation
Passive cooling coating
Cooling power [W/m^2] 41.8
Energy performance
Integral quantity
Current value
Target value
Solar absorption [%] 3.29
Absorbed power 28.0031
Emitted power 69.8524
Cooling power [W/m^2] 41.8 100.0
Vacuum
SiO2
1912.7 nm
SiC
1209.8 nm
Ag
163.3 nm
Float
Reflectance
Wavelength [micron]
Emission
Modified Reflectance [W/m²/micron]
Load configuration
Definitions
Start evolution
Open CODE
Save configuration
Loop through results:
Run: 3
Fitness: 3.0
Prev. view
Next view
Set fitness graphics

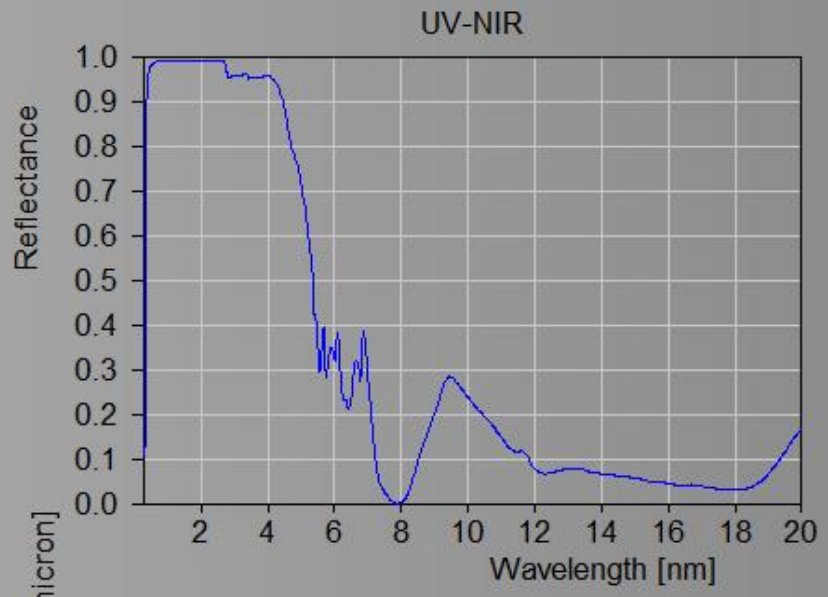
Passive cooling
Good and cheap solution:
Thin float glass/thick silver/ thick float glass

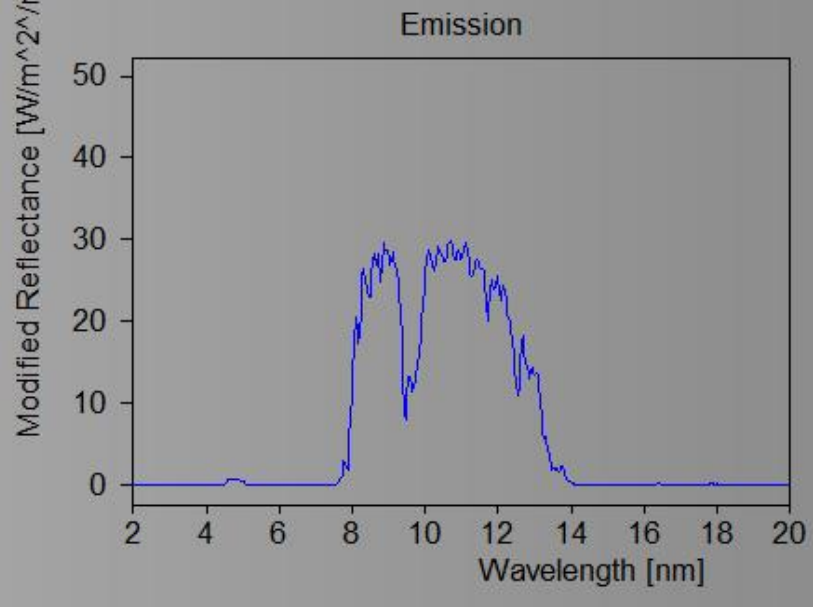
Cooling power [W/m^2] 85.0

Energy performance		
Integral quantity	**Current value**	**Target value**
Solar absorption [%]	4.18	
Absorbed power	35.5577	
Emitted power	120.5812	
Cooling power [W/m^2]	85.0	100.0

F		850.00	sunpower
F		300.000000	Blackbody:Temperature
D		42.5532	Stack 1 Layer 2 Float: Layer thickness
D		200.0	Stack 1 Layer 3 Ag: Layer thickness

Vacuum
Float
42.5532 micron
Ag
200.0 nm
Float



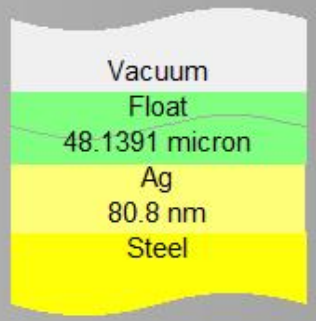


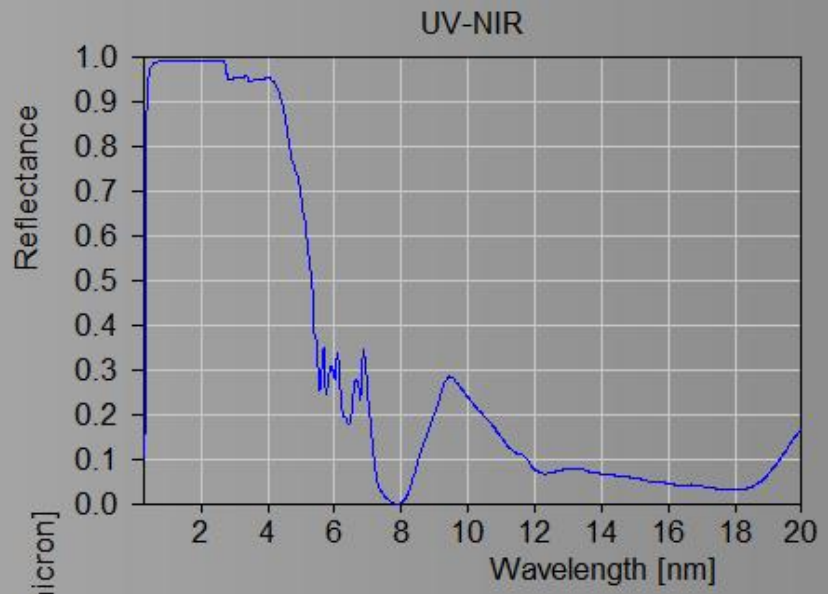
Passive cooling
Good and cheap solution:
Thin float glass / 80 nm silver/ steel

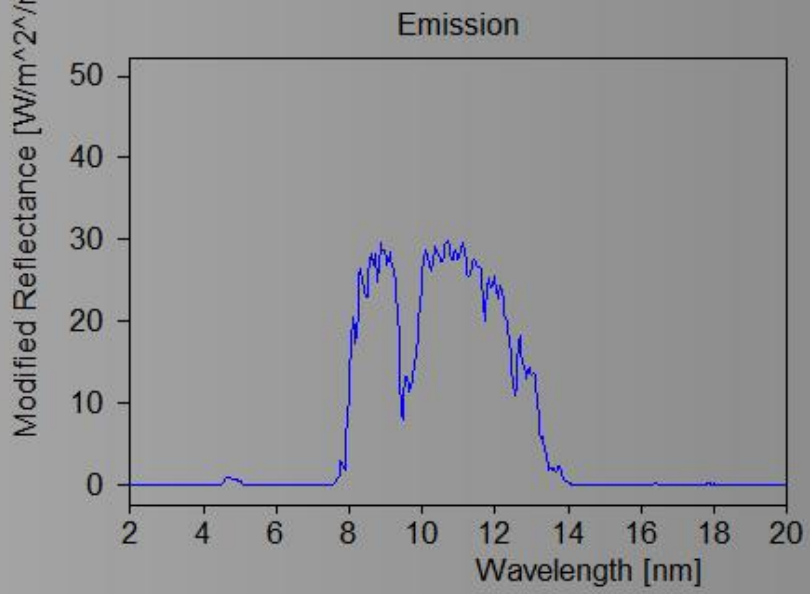
Cooling power [W/m^2] 80.3

Energy performance Integral quantity	Current value	Target value
Solar absorption [%]	4.76	
Absorbed power	40.4298	
Emitted power	120.7214	
Cooling power [W/m^2]	80.3	100.0

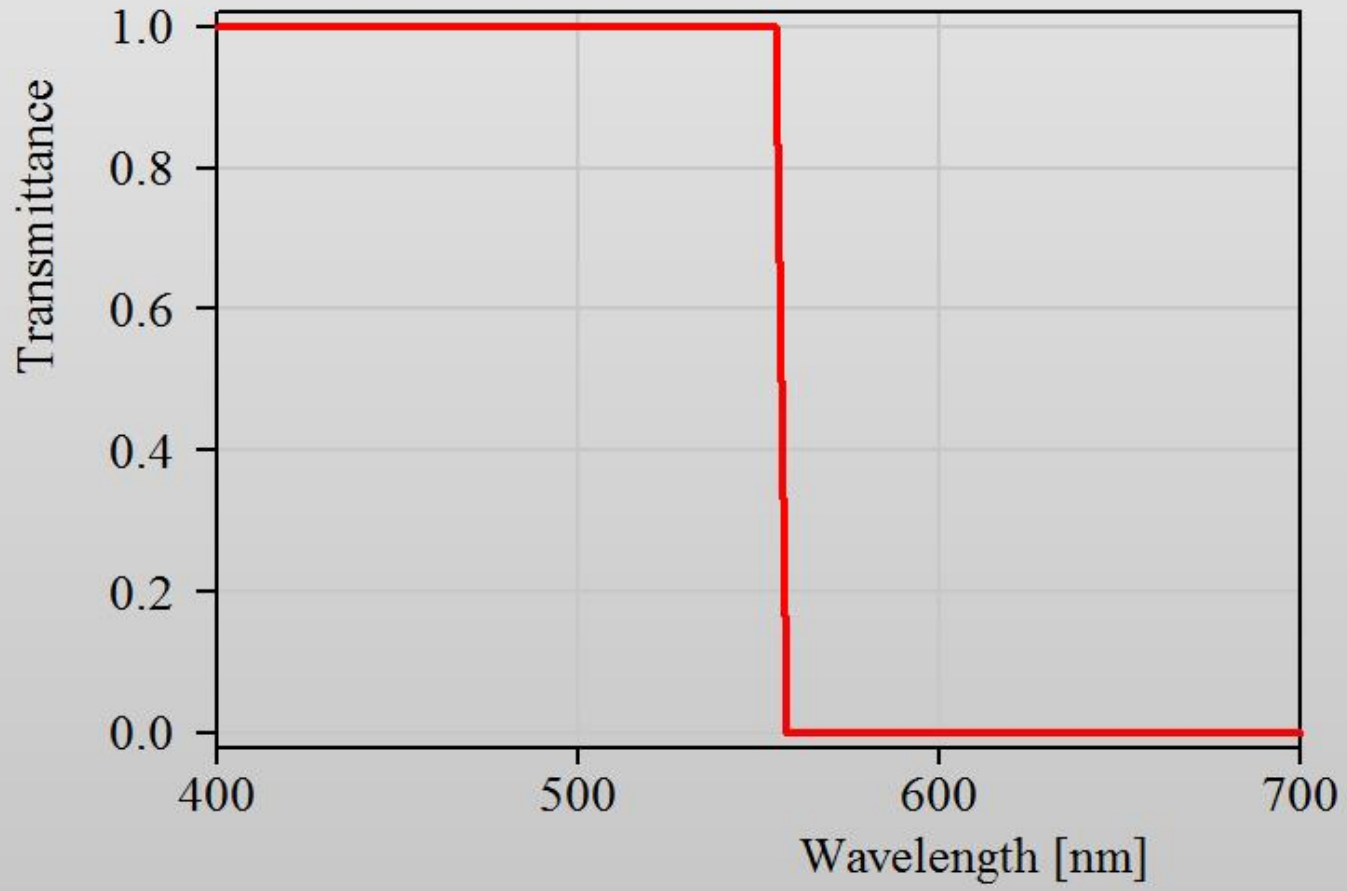
F	850.00	sunpower	
F	300.000000	Blackbody:Temperature	
D	48.1391	Stack 1 Layer 2 Float: Layer thickness	
D	80.8	Stack 1 Layer 3 Ag: Layer thickness	



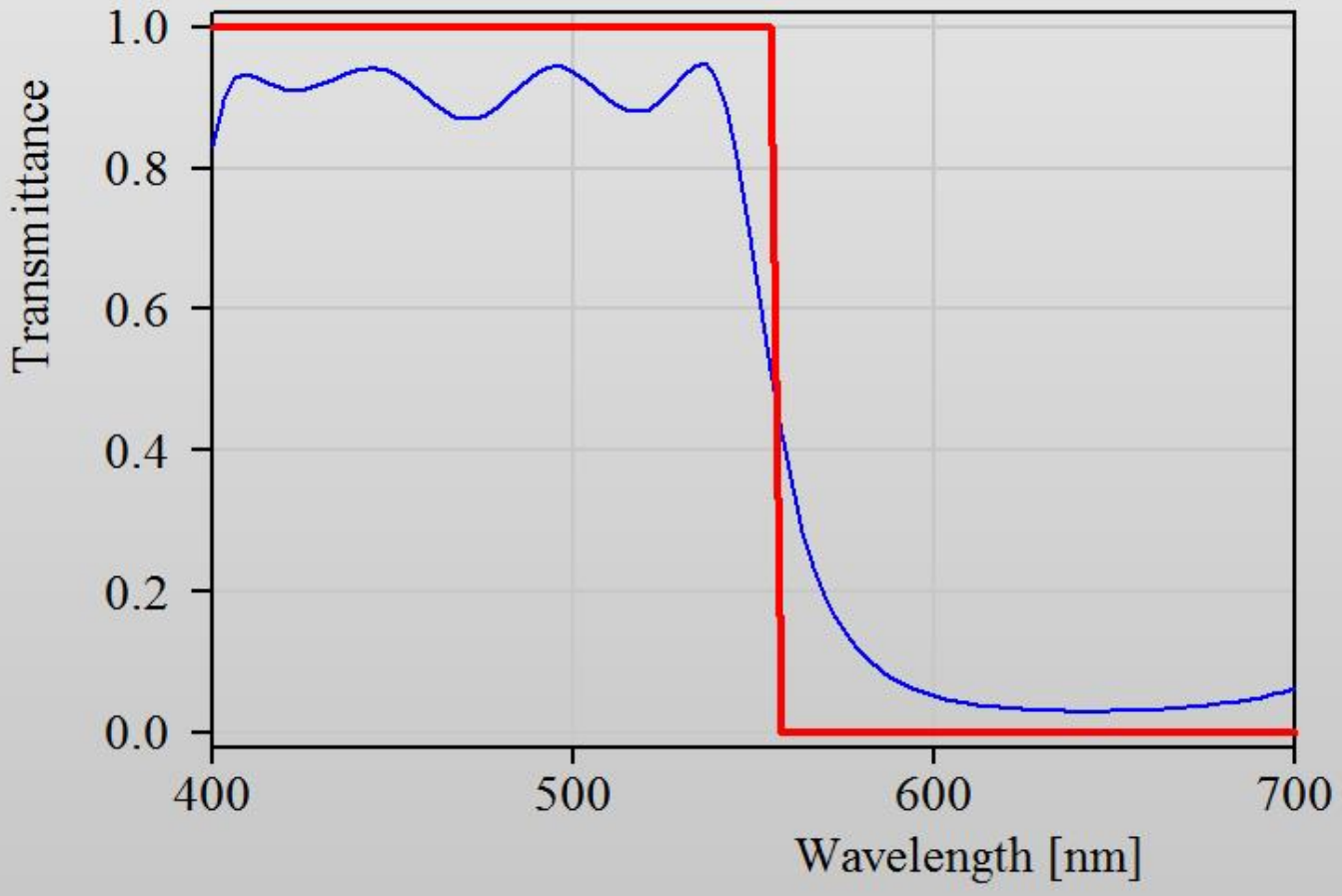


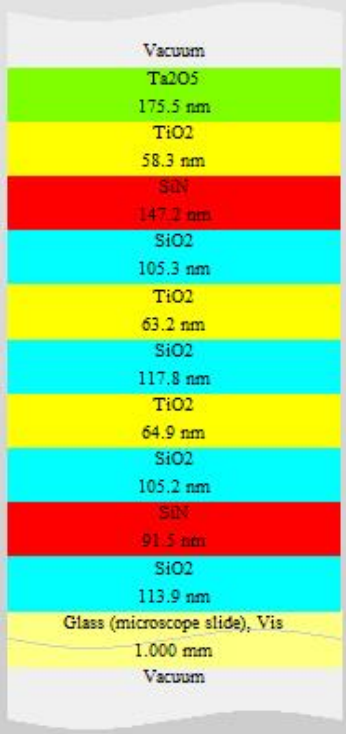


Handling problems with many layers
Edge filter on glass, visible transmission
Red curve: Target spectrum

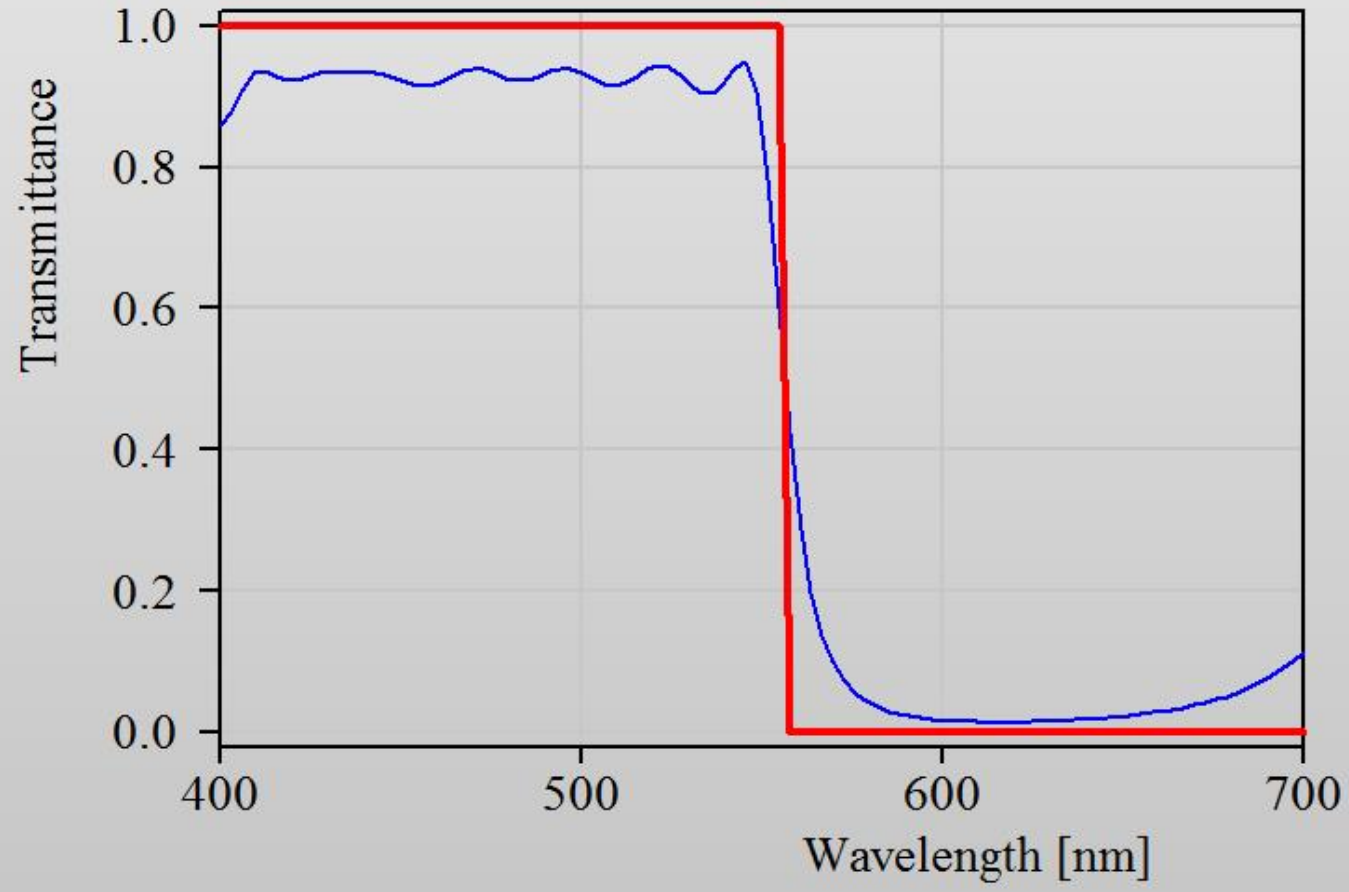


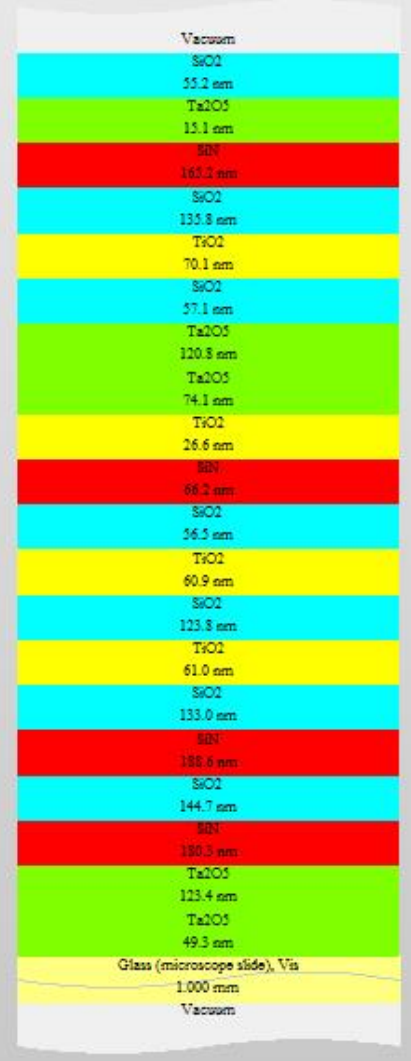
Genetics solution using 10 layers





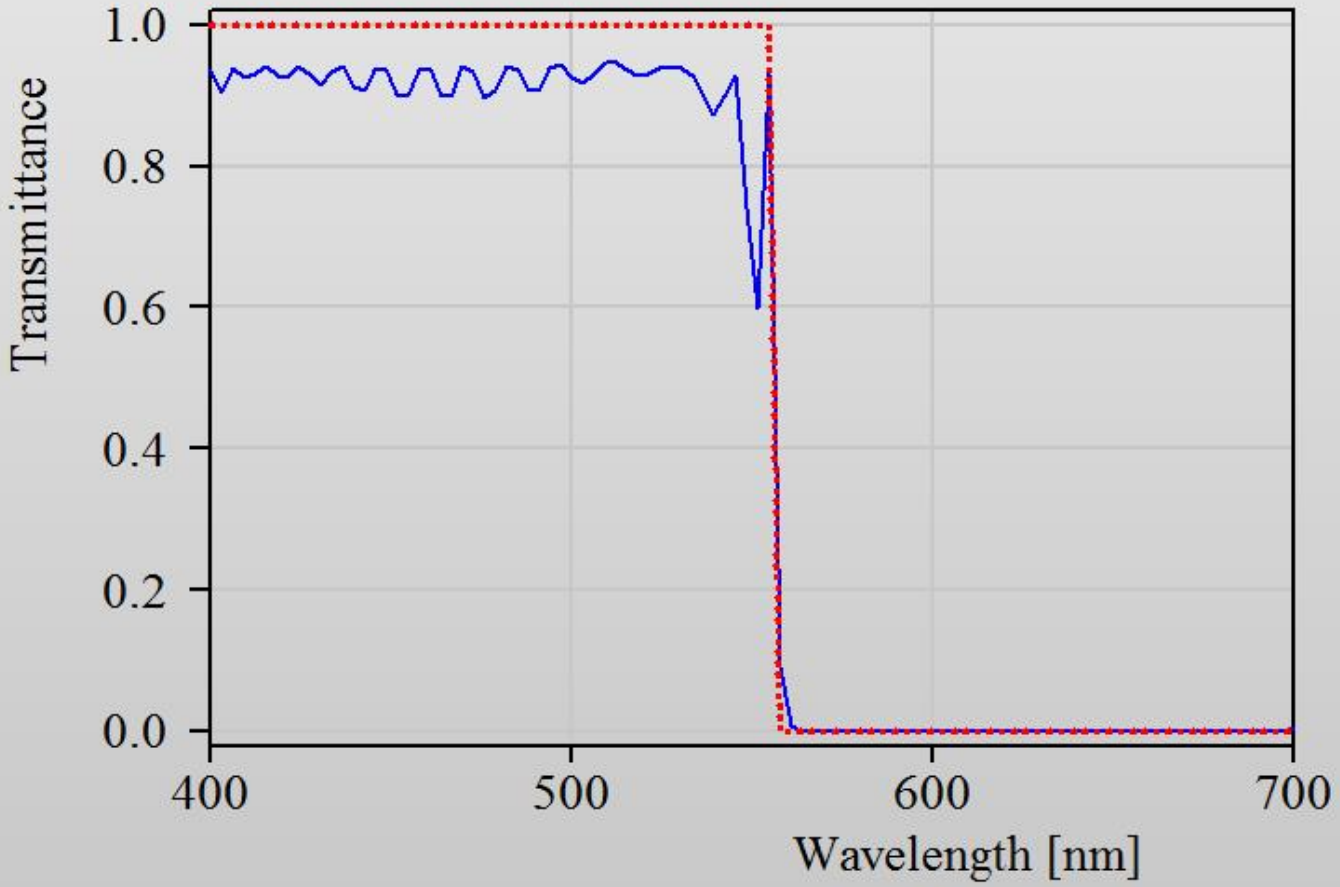
Genetics solution using 20 layers

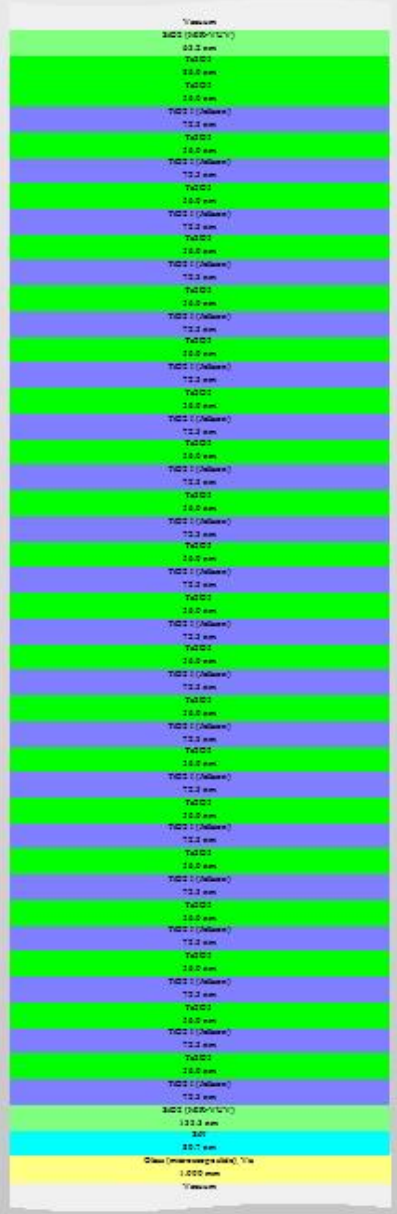




Speed up genetics giving a hint: Use Bragg reflectors for high reflectance

Genetics solution for 6 layers: A / B / [C / D /]^20 E / F / glass / air

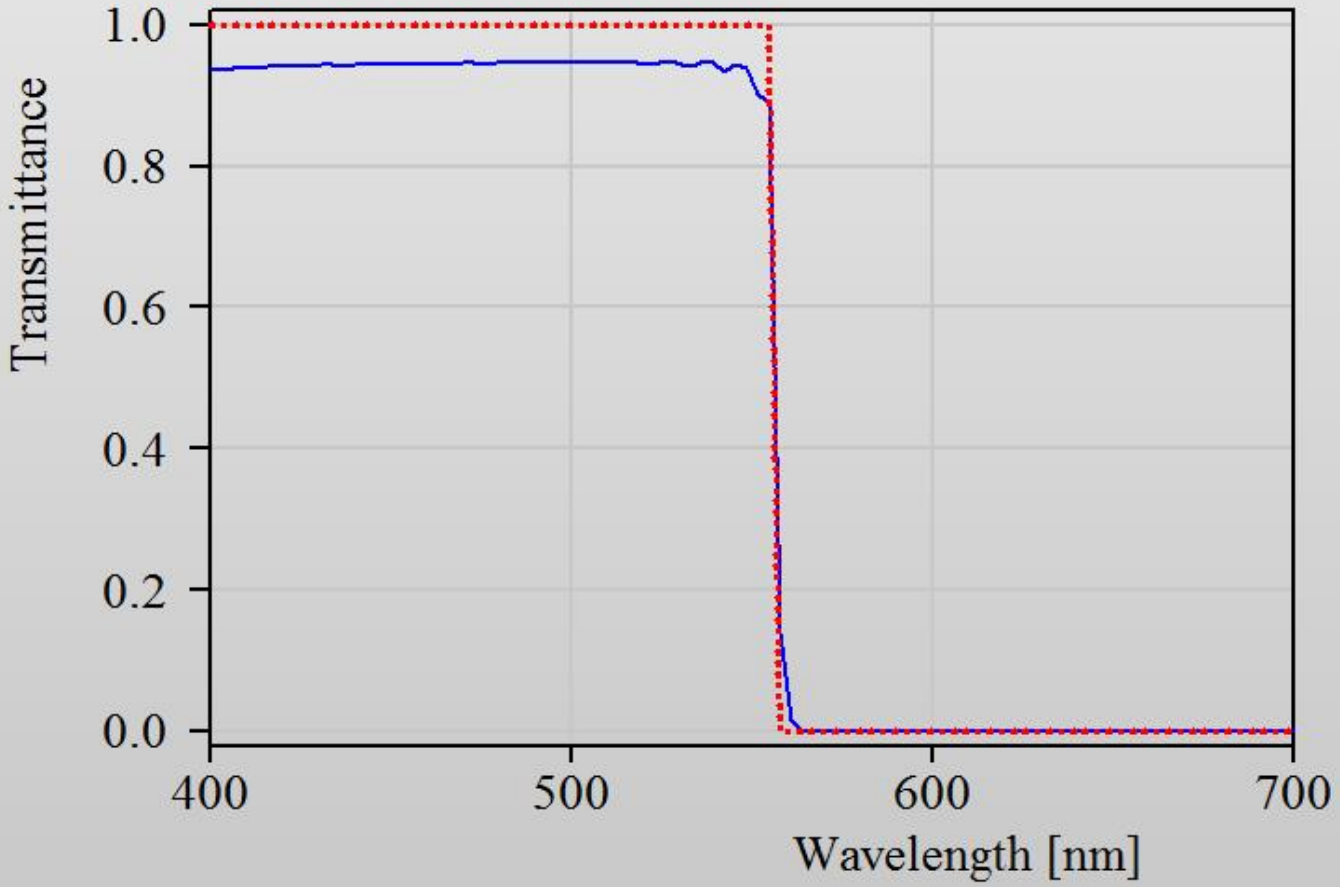


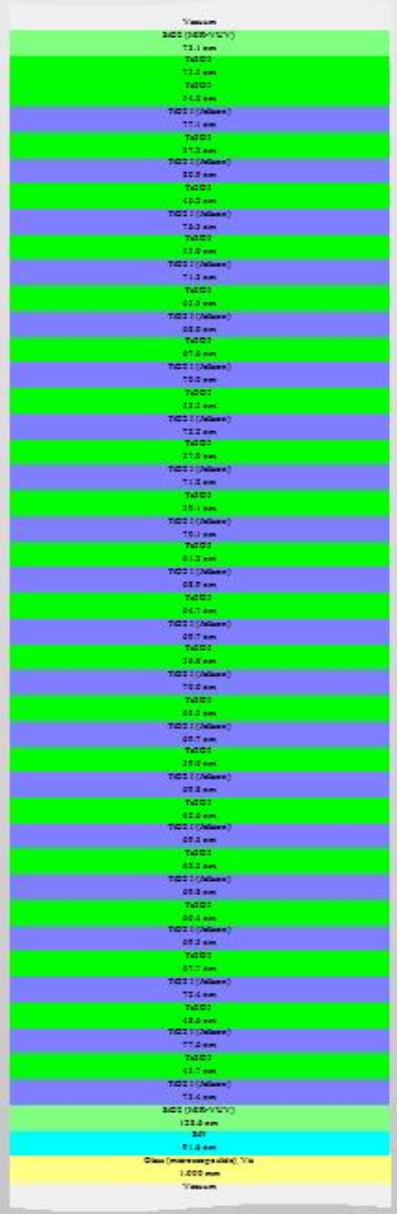


Refinement: Improvements after genetics

Convert A / B / [C / D /]^20 E / F to 44 single layers with individual thickness

Fit 44 thickness values using a downhill method

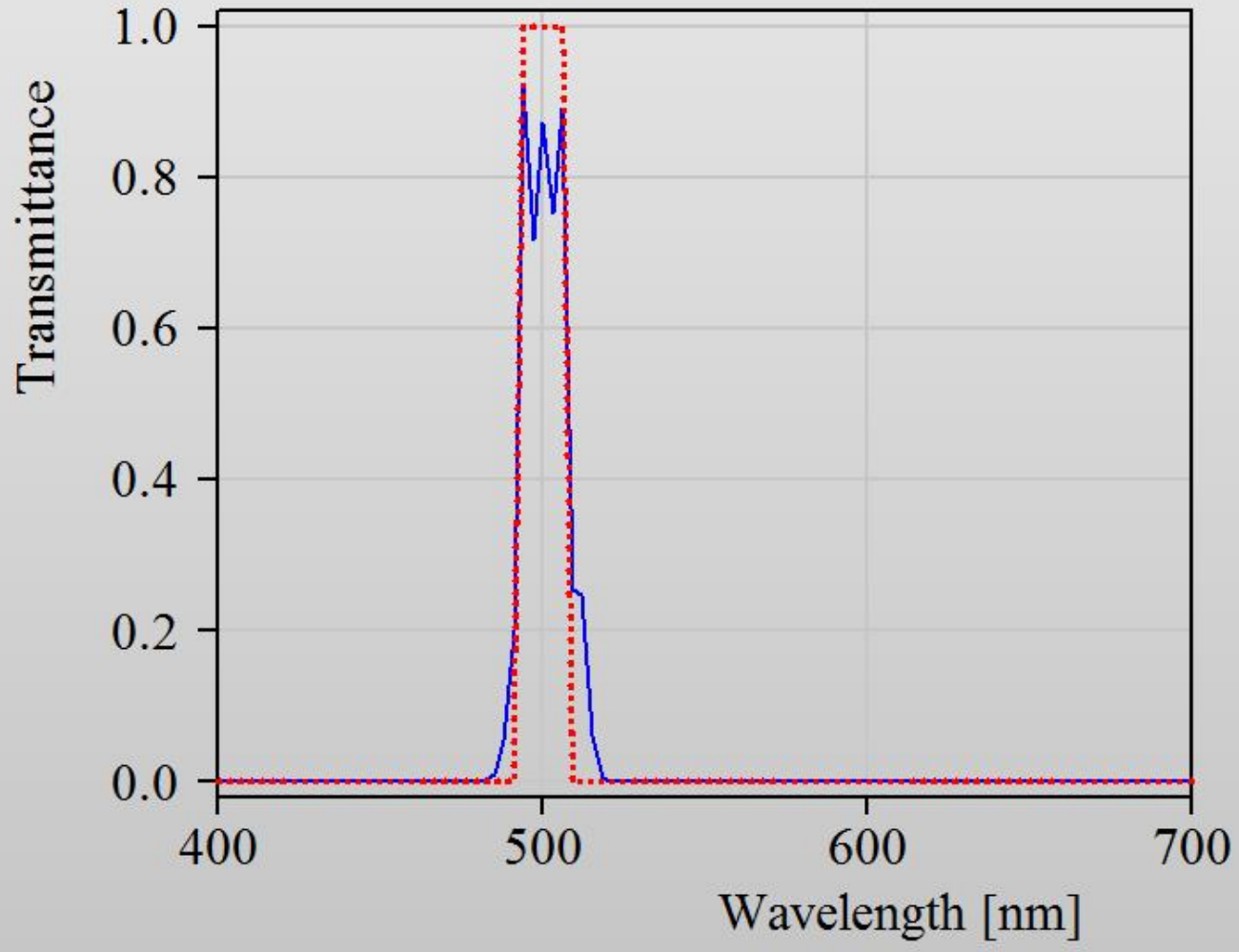


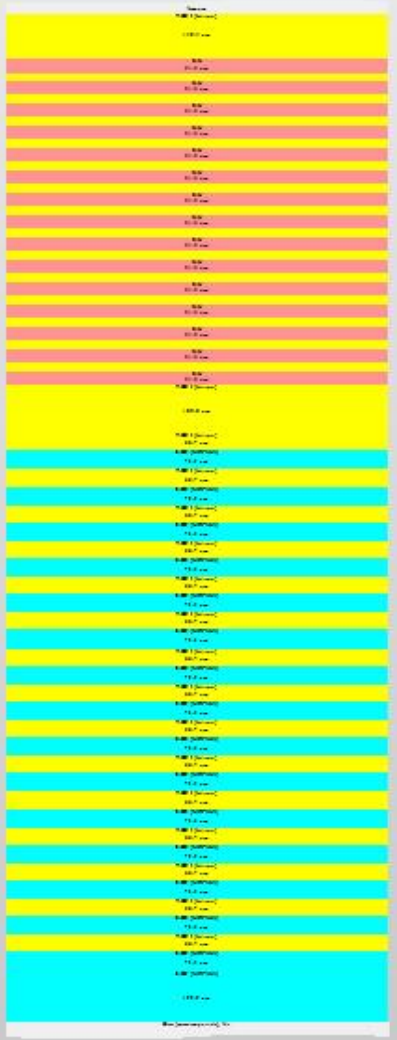


Bandpass filter

Help genetics: Use 2 Bragg reflectors and a cavity layer

Layer structure: A / [B / C /]^15 D / [E / F /]^15 G / glass / air

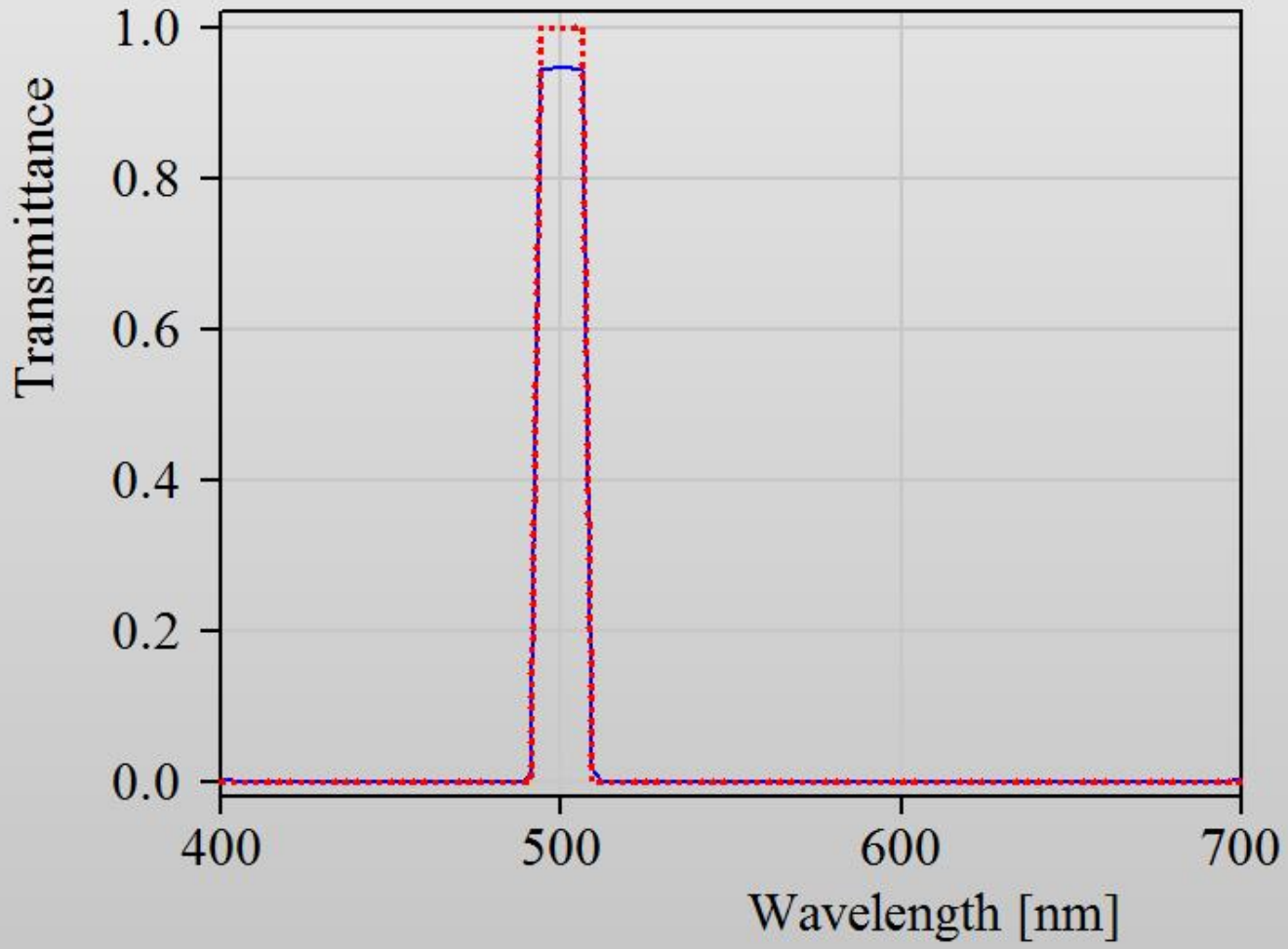


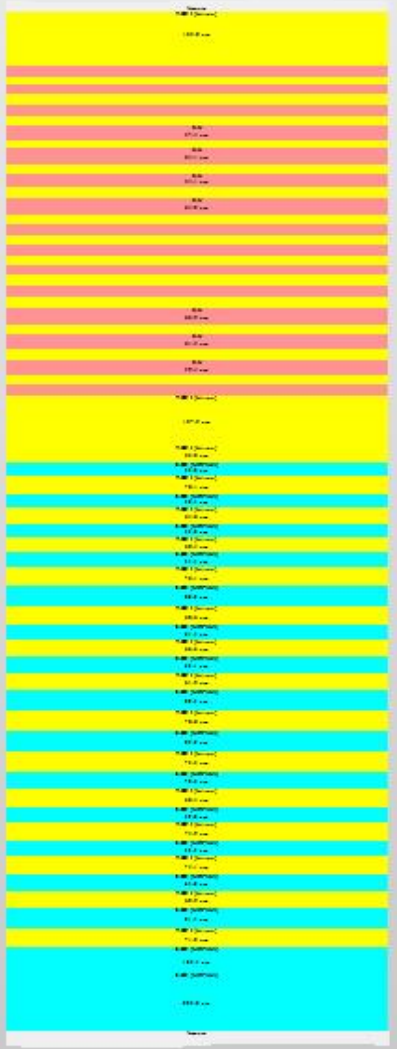


Bandpass filter: Refinement after genetics

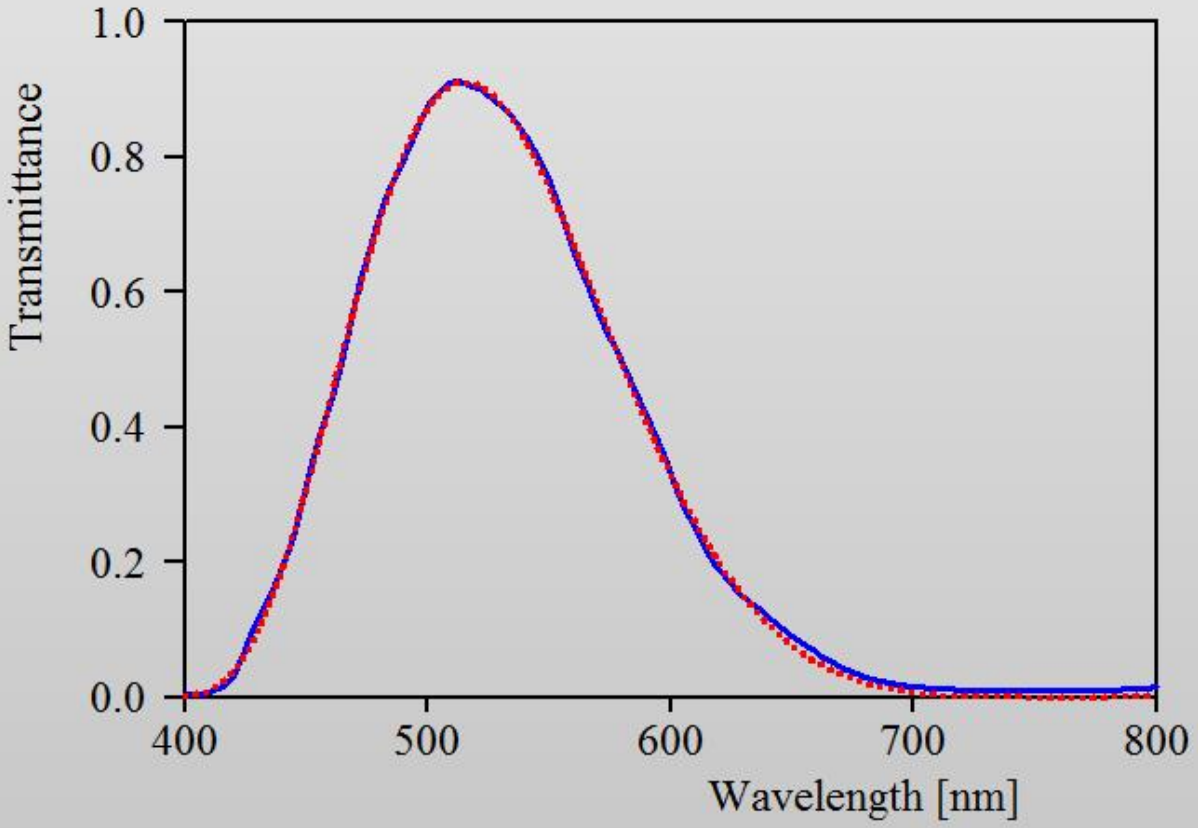
Convert A / [B / C /]^15 D / [E / F /]^15 G to 63 individual layers

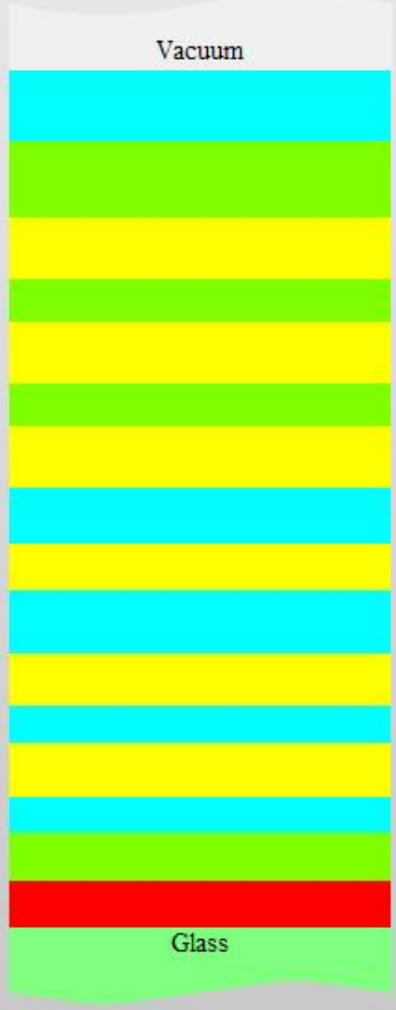
Fit layer thicknesses





Optical filter reproducing human eye sensitivity
Genetics result using 16 layers after refinement
Selected materials: SiN, SiO2, TiO2,Ta2O5





Genetic algorithms

- suitable for automatic coating design
- need a little push, eventually

- main problem: definition of the problem