

Simulation of the writing and erasing processes in optical discs based on phase change material

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INTRODUCTION

During the last six months we built a fast dynamical simulation of the writing and erasing processes in optical phase change discs. Our simulation goes from optical simulation to thermodynamical simulation and can be used with growth and nucleation dominant material under static or dynamical conditions. The microstructure is easily obtained. We will give here an overview of the method and hypothesis we use to achieve our simulation.

PHYSICAL MODELS

OPTICAL MODEL

The optical part of the program is designed to optimize the stack of the optical disc in order to obtain wished properties like contrast, reflectivity and absorption. A multi-criteria approach is used to take into account all the properties during the optimization (Figure 1).

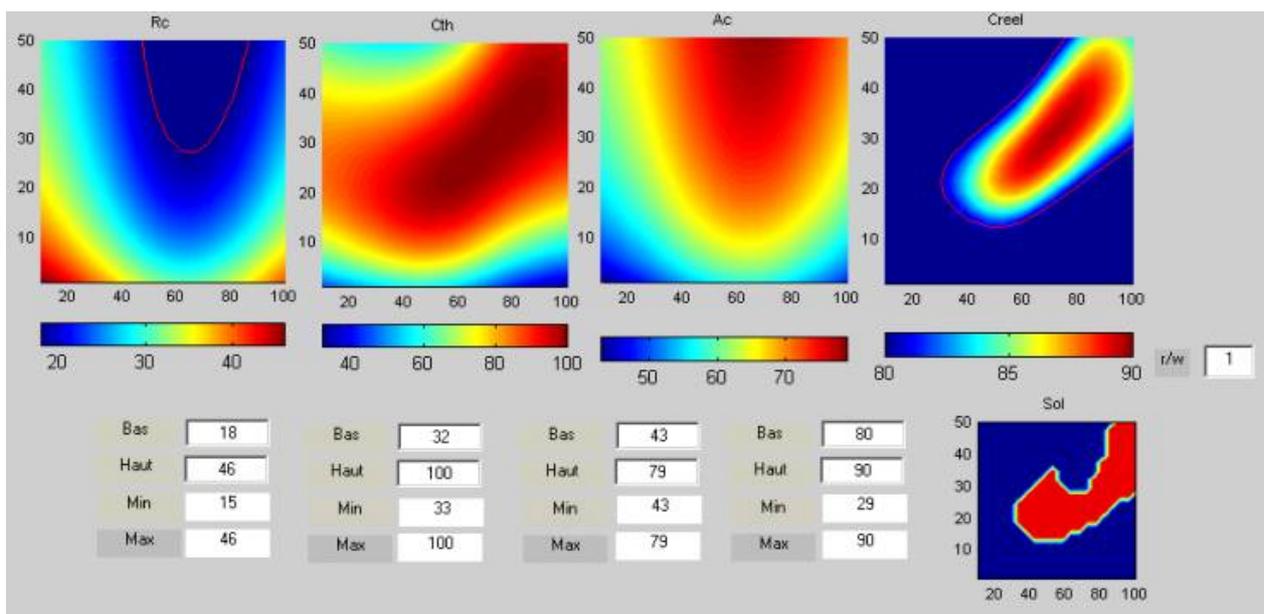


Figure 1 : An example of multi-criteria optimization of a stack. Solutions are represented by the red domain of the lower-right graph.

After this part of the work, we use optical simulation to obtain the electromagnetic field in the stack. The variation of this field versus time has the form of the laser pulse. The variation in the plane of the disc is represented by a function of the radius. This function can be the Airy function, a gaussian or whatever function we like. The variation with the coordinate along the optical axis are obtained by computing the electromagnetic field in the stack with a classical matrix formalism. We assume that the layers are homogeneous and the interfaces between them are plane.

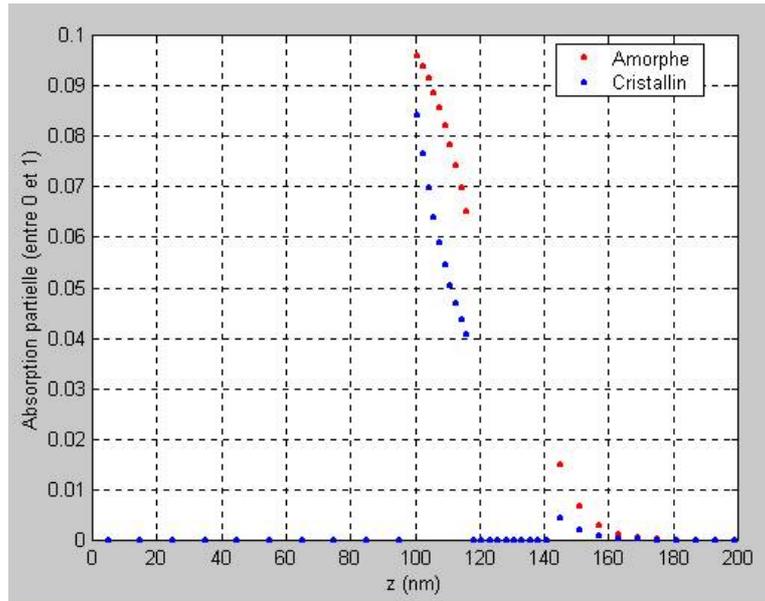


Figure 2 : Partial absorption (between 0 and 1) in a simple four-layer stack. Blue dots are for crystalline material and red dots are for amorphous material. Light comes from the left and z is the depth in the stack.

Optical properties are obtained by spectroscopic ellipsometry and can change with the thickness of the layer for a given material.

THERMAL MODEL

The thermal behavior of the stack is supposed to be given by the classical thermal diffusion equation :

$$\rho C \frac{\partial T}{\partial t} - k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) = q(x, y, z, t)$$

A simplification of our model is that the thermal properties are considered constant with time and spatial coordinates in each layer of the stack. Hence, if there is an amorphous mark, no difference can be made between the thermal properties of amorphous and crystalline states and dependence of the thermal properties against temperature cannot be taken into account. If we would like to take into account the evolution of the thermal properties in the plane of the layer and during time, we should solve the thermal diffusion equation in three dimensions and include at each time step the evolution of the material. Solving such a three dimensional non-linear problem is much more time-consuming than our approach and is not in the scope of our work. The use of the thermal diffusion equation implies also certain hypothesis concerning the number of collisions encountered by thermal phonons, this will be studied in the near future.

In the static case the heat source is obtained as indicated in the previous paragraph.

$$q(x, y, z, t) = \alpha \cdot P(t) \cdot I(\sqrt{x^2 + y^2}) A(z)$$

The equation is solved with a 2D finite element solver : pdetool used with Matlab. An example of such a thermal simulation for a crystalline phase change material in a four layer stack for a 100 ns laser pulse is shown in Figure 3. This result is obtained in around one minute on an old Pentium II 450MHz portable PC.

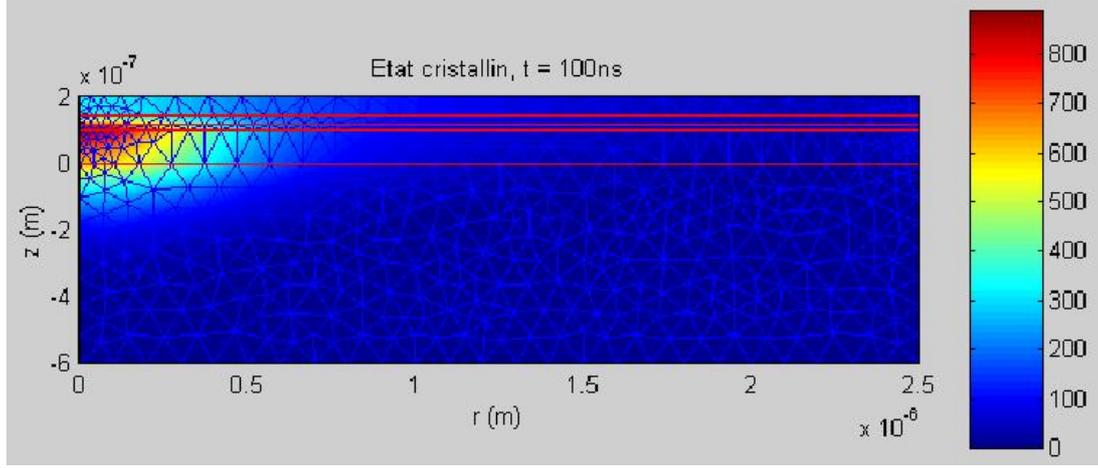


Figure 3 : Temperature profile in a four-layer stack. Phase change material is crystalline. Laser pulse is 100 ns long. Limits between the layers are shown by red lines. Light comes from the bottom along the left border. r is the radius from the optical axis. Temperature is given on the color scale at the right. Ambient temperature must be added to obtain the real temperature value.

In the dynamic case, the heat source is decomposed in small pulses arriving on the sample time after time.

$$q(x,y,z,t)=\sum_i \delta q_i(x,y,z,t)$$

δq_i is null outside the time interval defined by $[i.\Delta t ; i.\Delta t + \Delta t]$. The time step Δt is such that $P(t)$ and $A(z)$ are constant. We suppose also that $I(x,y)$ is the same for all the small pulses (the effects of writing or erasing on the shape of the focused beam are neglected). The heat source becomes :

$$q(x,y,z,t)=\alpha \cdot I(\sqrt{x^2+y^2}) \sum_i P_i \cdot A_i(z) \cdot \text{rect}\left(\frac{t-t_i}{\Delta t}\right)$$

To go further we introduce a crystalline fraction χ_i defined by :

$$A_i(z)=\chi_i \cdot A_c(z)+(1-\chi_i) \cdot A_a(z)$$

It follows a new expression of the heat source :

$$q(x,y,z,t)=\alpha \cdot I(\sqrt{x^2+y^2}) A_c(z) \sum_i P_i \cdot \chi_i \cdot \text{rect}\left(\frac{t-t_i}{\Delta t}\right) + \alpha \cdot I(\sqrt{x^2+y^2}) A_a(z) \sum_i P_i \cdot (1-\chi_i) \cdot \text{rect}\left(\frac{t-t_i}{\Delta t}\right)$$

This expression is very interesting because it allows us to take into account the effects of the laser beam on the optical absorption of the phase change material and the effects of the displacement of the laser beam by simple linear combinations of two elementary thermal profiles. This elementary thermal profiles δT_c and δT_a are obtained with the following heat sources :

$$\begin{aligned} \delta q_c(x,y,z,t) &= \alpha \cdot I(\sqrt{x^2+y^2}) A_c(z) \cdot \text{rect}\left(\frac{t}{\Delta t}\right) \\ \delta q_a(x,y,z,t) &= \alpha \cdot I(\sqrt{x^2+y^2}) A_a(z) \cdot \text{rect}\left(\frac{t}{\Delta t}\right) \end{aligned}$$

The temperature is obtained using the following expression :

$$T(x,y,z,t) = \sum_i P_i \cdot \chi_i \cdot \delta T_c(t-t_i) + \sum_i P_i \cdot (1-\chi_i) \delta T_c(t-t_i)$$

This a very simple and fast method to obtain dynamic thermal profiles.

THERMODYNAMICAL MODEL

We will not give here the details of our thermodynamical model (it is the subject of the thesis of Bérangère Hyot which will be published very soon). We will only emphasize some interesting aspects of our model.

Nucleation can occur in a homogeneous or heterogeneous manner, but heterogeneous nucleation is usually the dominant mechanism. While homogenous nucleation occur in the volume of the phase change material (Figure 4), heterogeneous nucleation is supposed to occur on the interfaces of the phase change layer (Figure 5).

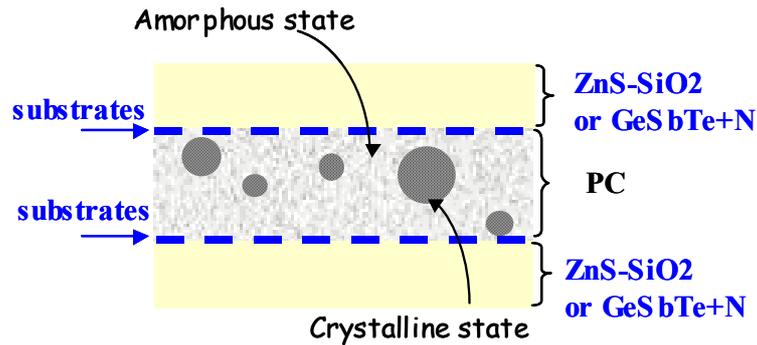


Figure 4 : Schematic representation of homogeneous nucleation.

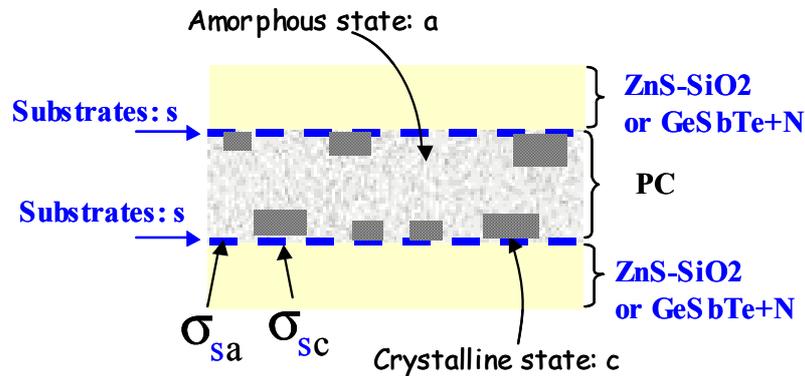


Figure 5 : Schematic representation of heterogeneous nucleation.

In the case of heterogeneous nucleation, the influence of the material adjacent to the phase change layer is represented by a simple factor which is the difference between two interface tensions : one between adjacent layer and crystalline phase change material and one between adjacent layer and amorphous phase change material.

Due to the very high heating and cooling rates encountered during the writing and erasing processes, we use, for both homogeneous and heterogeneous nucleation, a transient nucleation theory.

$$I(T,t) = I_{ss}(T) \exp\left(-\frac{\tau(T)}{t(T)}\right)$$

This theory gives the nucleation rate as a product of the steady-state nucleation rate $I_{ss}(T)$ given below and a correction factor depending on the isothermal holding time $t(T)$ and the transient time $\tau(T)$. The isothermal holding time, is equal to $\frac{1}{\frac{dT}{dt}}$ if we consider 1K isothermal increments. The steady-state nucleation rate has a classical expression :

$$I_{ss} = A_s \exp \left(- \frac{\Delta G^* (T)}{kT} \right)$$

Where ΔG^* is the excess free energy for the formation of a stable nucleus.

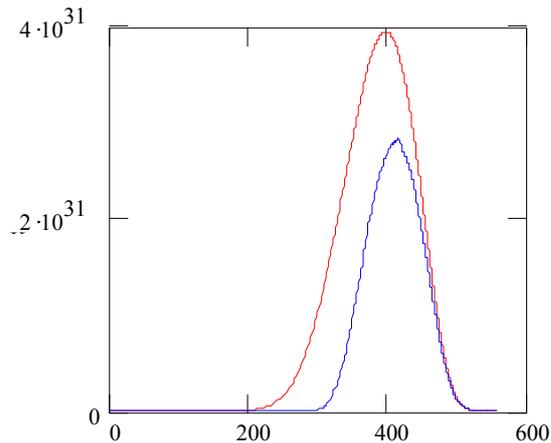


Figure 6 : Example of the influence of the heating rate on heterogeneous nucleation rate against temperature. The red curve represents the stationary nucleation rate, the blue curve represents the transient nucleation rate. We see that the difference is more important at low temperature when the heating rate is higher than at high temperature.

The growth rate is given by the classical following equation, where ΔG is the Gibbs energy for crystallization, γ , the atomic jump frequency and d , the interatomic distance.

$$V(T) = \gamma d \left(1 - \exp \left(- \frac{\Delta G(T)}{RT} \right) \right)$$

It is assumed here that the composition is the same between amorphous and crystalline state of the phase change material. A typical evolution of the growth rate with the temperature is shown on Figure 7.

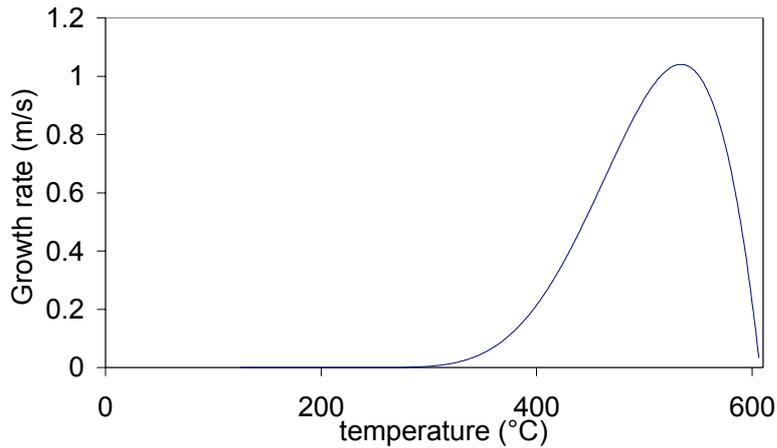


Figure 7 : Example of the evolution of the growth rate with temperature.

When there is a nucleation, the nucleus appear with a given size equal to the critical radius. On Figure 8 you can see, during a 100 ns static laser pulse, the evolution of temperature, nucleation rate, growth rate and critical radius. You clearly see here that nucleation will preferentially occur at a radius near 0.25 μm , because the heating rate is too high when the maximum nucleation temperature is reached at the center of the laser beam. This has to be balanced with the high growth rate at the center which could allow nuclei appeared there to grow over the nucleation annulus at 0.25 μm .

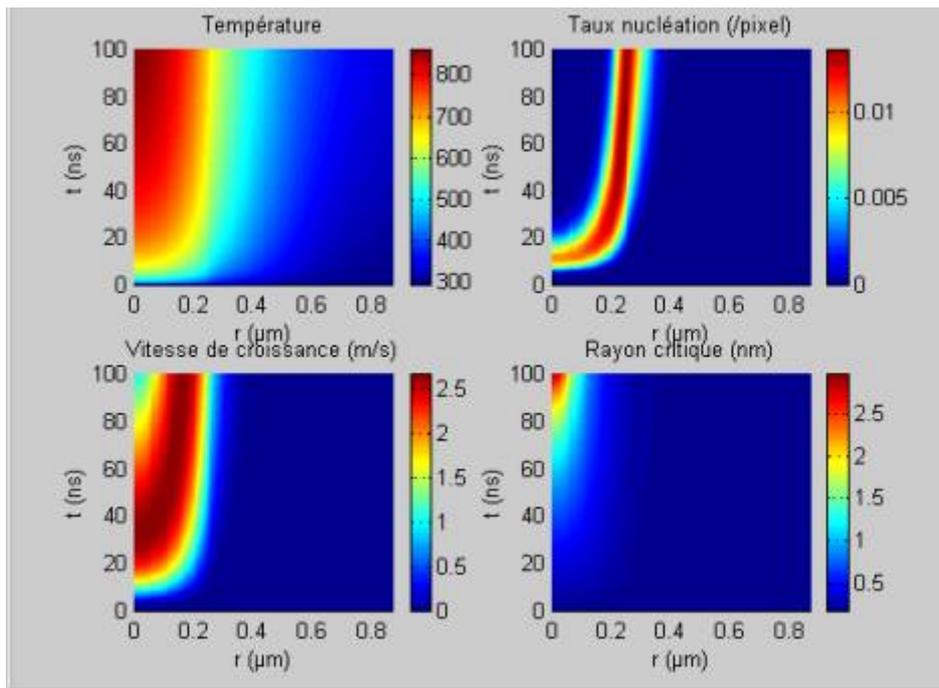


Figure 8 : Evolution, during a 100 ns static laser pulse, of temperature (upper-left), nucleation rate in a pixel during a time step (upper-right), growth rate (lower-left) and critical radius (lower-right). In each graph horizontal axis is the radius from the center of the beam and vertical axis is time.

Hence, even when we know the analytical models which represent the behavior of an optical phase change disc under a focused pulsed laser beam, it is not easy to forecast the size of the crystalline grains and the crystallization time without doing a numerical simulation of the writing and erasing processes.

CRYSTALLIZATION SIMULATION

PRINCIPLES

Given all the models, we can simulate the crystallization process. To do so, the phase change layer is discretized and represented by a fine plane grid with a 5 nm step for example. Temperature profile is computed on this grid and is supposed to be the same on both interfaces (it would be very easy to obtain specific temperature profiles on both interfaces). The crystalline microstructure is represented by a matrix of the same size as the temperature grid. In each pixel of the matrix several values are possible but zero is always for the amorphous state and non-zero values are always for crystalline state.

As shown before, the value of the temperature allows us to compute the nucleation rate in each pixel for each time step. To gain time the nucleation rate is computed only in the amorphous ununmolted pixels, because nucleation can not occur in pixels which are already crystallized. If this nucleation rate is less than one (which is the case in general) we cast a random number to decide if there will be a nucleation or not in the pixel during the time step. If the rate is greater than one we can force a certain number of nucleation to occur and cast a random number for the fractional part of the rate. At the moment, such a high rate only involves an alert message, because it is a very unusual situation often due to errors in the parameters. The position of the nucleus in the pixel is randomly obtained, with a uniform probability in the pixel (Figure 9). The identity card of the new nucleus is stored in an array comprising the name of the grain (a fractional number), its birth date, its size, the position of its center and its status. However the matrix representing the microstructure is not modified until the nucleus has reached a minimum size. Doing that we assume that a critical nucleus in a 5x5 nm pixel do not prevent new nucleations in the pixel.

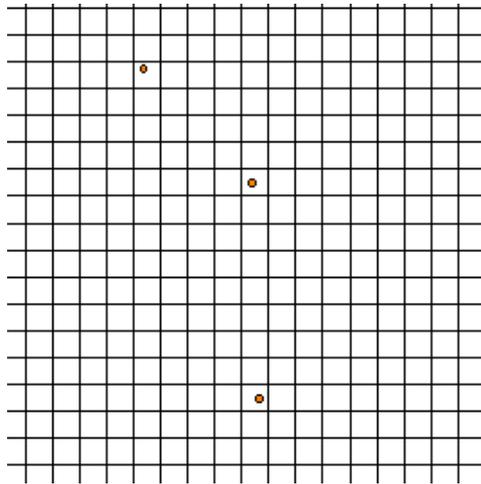


Figure 9 : Nuclei have appeared but they have no effect on the microstructure matrix.

At each time step, each nucleus in the array will grow. When the nucleus has reached a specified minimum size (for example 5 nm in diameter), the microstructure matrix is modified (Figure 10).

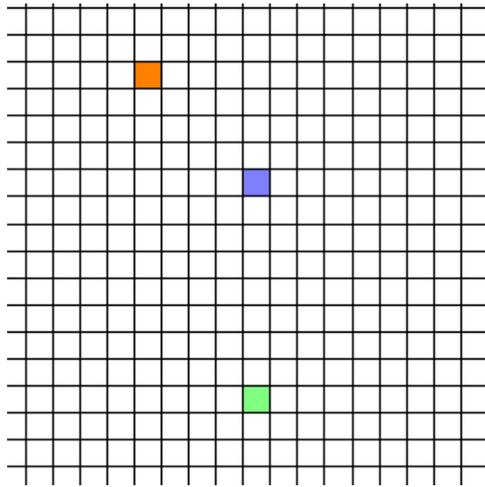


Figure 10 : Nuclei are sufficiently big to appear in the matrix.

The pixel corresponding to the location of the nucleus take a non zero value corresponding to the name of the nucleus. This two steps of the life and nucleus represent the birth and childhood of the grain. The analogy between the simulation and a life-and-death game can be used very far away as you will see below. When a nucleus appears in the matrix, its status is changed to tell to the program to change the matrix at each time step if necessary to take into account further growth of the grain. At each time step, the radius of the grain grows at a speed computed at the center of the grain. The matrix is changed at each pixels whose value is zero and whose centers are comprised in a circle whose size and position are equal to those of the grain. The modified pixels take the value of the name of the grain. It is easily seen that the grains will impinge on each other and automatically stop their growth in the direction where a grain is already present (Figure 11).

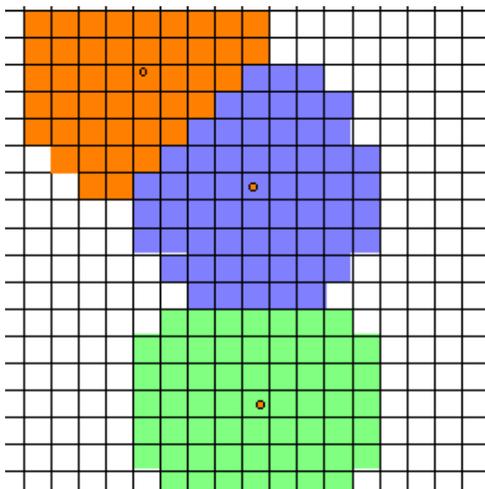


Figure 11 : Grains grow and impinge on each other, boundaries between grains are automatically drawn.

As you can imagine, if the grain becomes big, the growth speed on its border is not the same as in the center and not constant on the border. We need a simple way to take into account the variation of the growth speed of a grain on its border. To do so we introduced a kind of reproduction rule : when a grain becomes too big, its growth is stopped and several nuclei are put on its border (Figure 12). Each nucleus has its own location and name and null size. Growth rate will be different for each new nucleus, in order to cope with anisotropic growth of the grains. Those nuclei are considered to be the sons of the bigger one. They have an inheritance : the integer part of the name of the father. Each nucleus is recognized by its fractional part. This way of thinking allows us to retrieve the microstructure by displaying the integer part of the names put in the microstructure matrix. The father is considered as hibernating : it doesn't grow anymore but can be awoken by specific events. We think it is simpler than a vectorial approach of the displacement of the crystalline front of each grain.

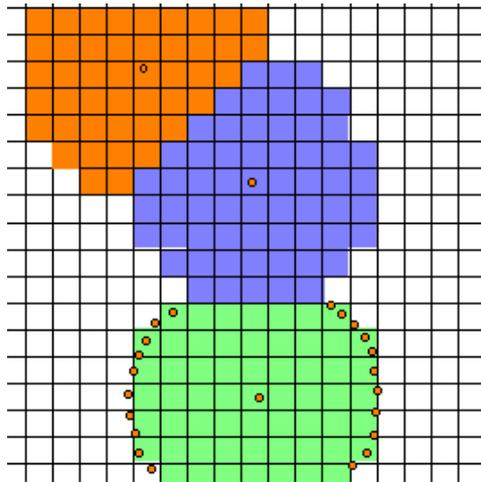


Figure 12 : When a grain becomes too big its growth is stopped and numerous nuclei are put on its border. It is illustrated here only on the green grain. After that each nucleus is free to grow with its own speed computed on the border of the father grain.

So our grain can be born, grow and hibernate. Sadly they can also die. Death occur during the childhood if the nucleus pixel is crystallized by another grain before the nucleus has reached the minimum size to appear in the microstructure matrix or if the temperature of the pixel raises above the melting temperature. When a grain has already appeared in the microstructure matrix, it can die by melting only. Two kind of melting are taken into account : complete melting and partial melting (Figure 13). Whether partial melting is realistic on a physical basis can be the subject of discussion, perhaps is there a minimum grain size under which partial melting can not occur.

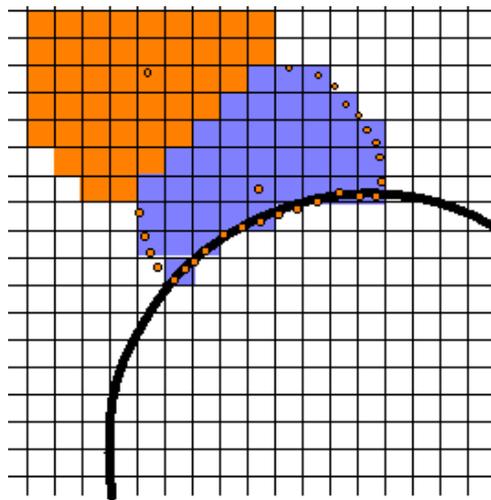


Figure 13 : The molten area is under the black curve. The green grain is totally molten. The blue one is partially molten, new nuclei are put on its border. The red grain is not changed.

In complete melting all the pixels of a grain are above the melting temperature, the grain is removed from the microstructure matrix (pixels are put to zero) and erased from the array. If some part of the grain is under the melting temperature (grain on the border of the molten area) the treatment is more complex. Molten pixels of the grain are put to zero value and sons of the grain are put on the border between the grain and the molten area in unmolten pixels. The partially molten grain is considered as hibernating, and new nuclei are put on its boundary with amorphous area. Nuclei have null beginning size. Those nuclei will grow if the temperature stays under the melting point. Nevertheless, further increase of the size of the molten area will kill the newly formed nuclei.

At the end of the simulation for a sequence of small pulses, we can store the microstructure matrix and the array of nuclei and grains to use it with a new sequence of small pulses. Hence it is possible to write an amorphous mark and to erase it after. Finally, we have to say that the initial state of the microstructure matrix can be amorphous or crystalline. In this case the microstructure matrix is initialized. Presently the same process of simulation is used with two steps of homogeneous temperature : one temperature for nucleation and one for growth. The kind of microstructure we obtain is shown in Figure 14. It is a very crude manner to initialize the matrix but it should be possible to make a more realistic simulation of the initialization process.

EXAMPLES

Here are some illustrative examples of the kind of results we obtain with our simulation. On Figure 14 you can see the initial crystalline microstructure.

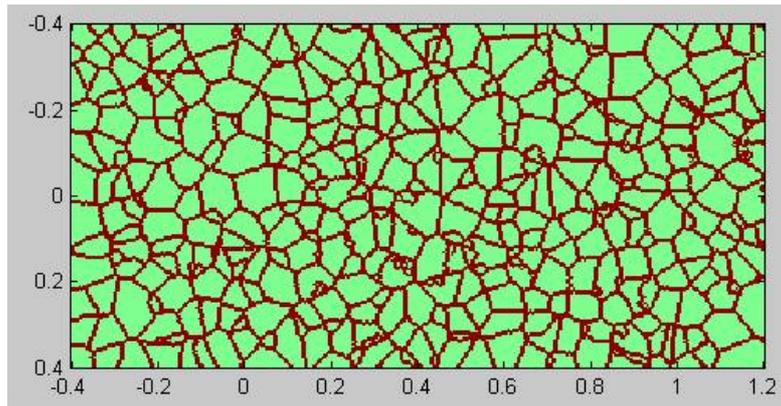


Figure 14 : Example of a crystalline microstructure obtained after our crude initialization. Limits between grains are in brown.

Figure 15, Figure 16 and Figure 17 show the evolution of the shape of an amorphous mark when the sample is lighted with two successive laser pulses followed by a cooling pulse and continuous erase power.

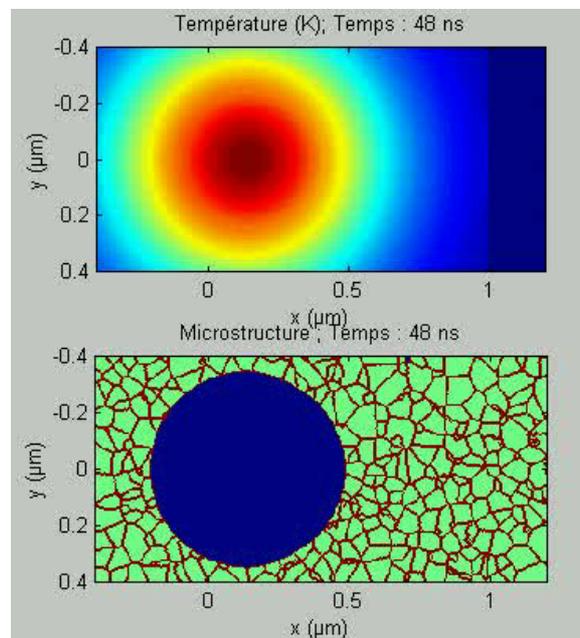


Figure 15 : Shape of the amorphous mark just after the end of the first laser pulse. The upper graph shows the temperature.

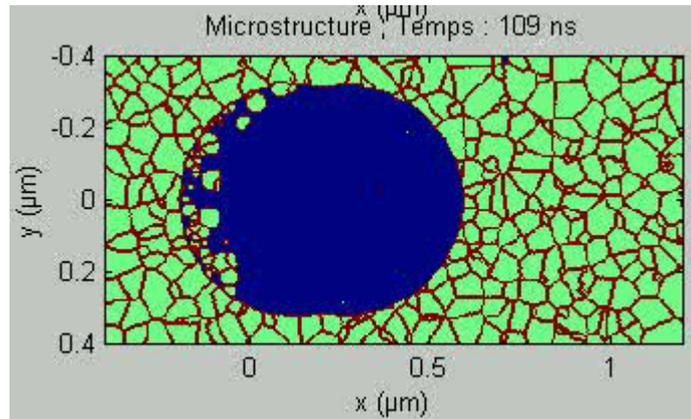


Figure 16 : Shape of the amorphous mark after the second laser pulse.

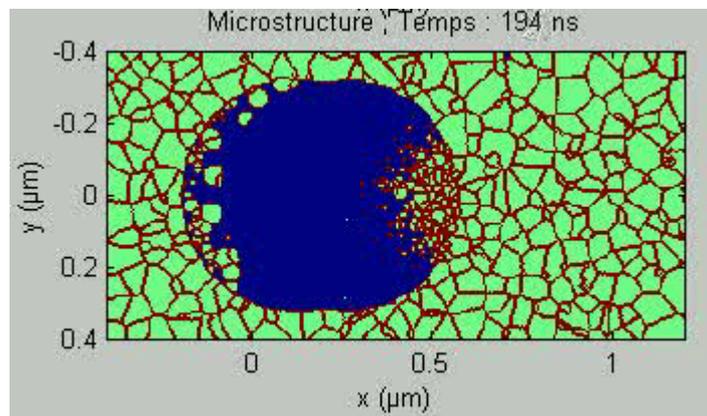


Figure 17 : Shape of the amorphous mark when laser power is set at the erase power after the cooling pulse.

At the end of this simulation, the shape of the amorphous mark and the data on the nuclei and crystalline grains are stored. Those data can be retrieved to be used as a new initial state.

Figure 18 shows a short amorphous mark. Figure 19 and Figure 20 show erasure of this amorphous mark with nucleation dominant mechanism and growth dominant mechanism.

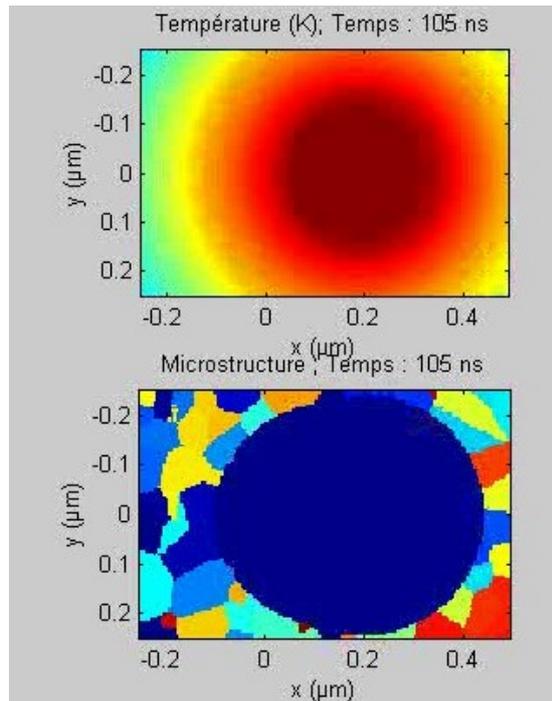


Figure 18 : Written amorphous mark (dark blue). Red grains are young grains. Blue grains are older ones.

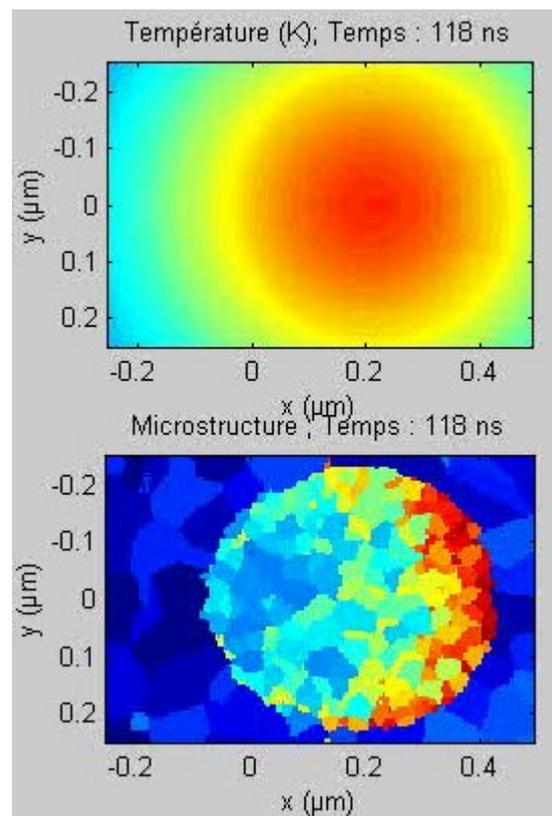


Figure 19 : DC erasing of the amorphous mark showing crystallization with nucleation and growth mechanisms.

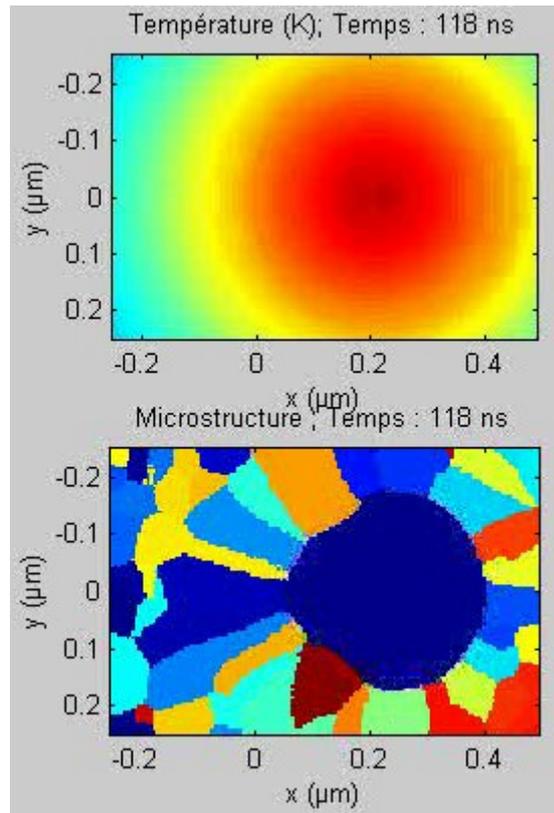


Figure 20 : Partial erasing of an amorphous mark showing growth-dominant mechanism (nucleation was inhibited).

CONCLUSION

Our program is now working well and allows us to simulate writing and erasing processes in growth-dominant and nucleation-dominant phase change materials. A complete dynamic simulation roughly lasts from ten to sixty minutes depending on the pulse duration between 100 and 1000 ns, on a Pentium III 650MHz with 128 Mo RAM. This complete tool can give valuable results only if several parameters are provided. We are now working on the measurement and determination of those parameters. Difficulties occur for example to determine the viscosity of the molten material. We are opened to collaboration with other researchers on those aspects of the problem.