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Unified description of thermal behaviors by macroscopic growth laws

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Unified description of thermal behaviors by macroscopic growth laws

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Abstract

Complex systems, in many different scientific sectors, show coarse-grain properties with simple growth laws with respect to fundamental microscopic algorithms. The known classification schemes of the growth laws refer to time evolution of biological and technical systems. We propose to apply the previous classifications to phenomenological analysis of thermal systems with a cross-fertilization among different sectors. As an example, the Fermi–Dirac distribution function and the electrical activation in implanted silicon carbide are discussed.

Introduction

Simulations of complex systems with a large number of interacting elementary parts are often difficult [1] and involve a large number of free parameters.

On the other hand, there is an impressive number of experimental verifications, in many different scientific sectors, that coarse-grain properties of systems, with simple laws with respect to fundamental microscopic algorithms, emerge at different levels of magnification.

In this respect, a useful tool is the general classification of growth laws in [2] which facilitates the cross fertilization among different fields of research. For example, the Gompertz law (GL) [3] applies to human mortality tables (i.e. aging) and tumor growth [4–6].

In general, a macroscopic growth problem is characterized by a function \( f(t) \), which describes the time evolution of some dynamical quantity, and by the specific rate, \( \alpha \), defined as \( (1/f)(df/dt) = \alpha(t) \). In the GL \( \alpha \) has an exponential dependence on time:

\[
(1/f)(df/dt) = \alpha(t) = a \ e^{bt},
\]

where \( a \) and \( b \) are constants. In aging \( f(t) \) indicates the survival probability, while with regards to tumor growth it corresponds to the number of cells \( N(t) \) (depending on the specific case \( a \) and \( b \) can be positive or negative).

For technical devices the specific rate of the survival probability has a power-law time behavior

\[
(1/f)(df/dt) = \alpha(t) = a \ t^n,
\]

with \( n > 1 \), called Weibull law (WL) [7, 8].

In the previous equations \( t \) is the time variable. However, formally, it can represent any parameter useful for describing the system.

We discuss the application of the growth laws to thermal behaviors, i.e. to the temperature, \( T \), dependence of dynamical quantities. The interpretation of the parameter \( t \) as \( 1/T \) (with the Boltzmann constant \( k_B = 1 \)) reproduces some typical laws of thermal systems and, as an example, the formalism will be applied to the Fermi–Dirac (FD) distribution function and to the electrical activation of the implanted silicon carbide (SiC) after annealing.

In section 2 we recall the classification of the growth laws; in section 3 one considers the generalization to thermal behaviors and the applications to FD distribution and to SiC; section 4 is devoted to comments and conclusions.

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1. Classification of growth laws

Many different biological systems evolve according to the simple equation
\[ (1/f)(df/dt) = \alpha(t), \]  
where \( \alpha \) is the specific growth rate.

A classification of the previous growth laws is obtained by considering the power expansion in \( \alpha \) of the function (see [2] for details)
\[ \Phi(\alpha) = \frac{d\alpha}{dt} = \Sigma_i b_i \alpha^i \quad i = 0, 1, 2 \ldots, \]
which for \( b_0 = 0 \) and \( b_1 = 0 \) for \( i > 1 \) gives a \( t \)-independent specific rate \( \alpha_0 \) and therefore an exponential growth; for \( b_0 \neq 0 \) and \( b_1 = 0 \) for \( i > 1 \) describes a linear \( t \)-dependent specific rate and again an exponential growth; at the first order in \( \alpha \), for \( b_0 = 0 \), \( b_1 = 0 \) and \( b_i = 0 \) for \( i > 1 \), reproduces an exponential behavior in \( t \) of the specific growth and therefore the GL; the second order term, \( O(\alpha^2) \), for \( b_0 = 0 \), \( b_1 \), \( b_2 = 0 \) and \( b_1 = 0 \) for \( i > 2 \) generates the logistic and generalized logistic growth for \( f(t) \).

The feedback effect, that is the dependence of the specific growth rate \( \alpha \) on the function \( f(t) \), can be easily derived by the dependence on \( t \) of the specific rate. For example, the GL for a growing number of cells, \( N(t) \), shows the well known logarithmic non linearity,
\[ \frac{1}{N(t)} \frac{dN(t)}{dt} = a - b \ln \frac{N(t)}{N_0} = b \ln \frac{N_\infty}{N(t)}, \]
and for the (generalized) logistic law one gets the typical power-law behavior
\[ \frac{1}{N(t)} \frac{dN(t)}{dt} = c \left[ 1 - \left( \frac{N(t)}{N_\infty} \right)^\gamma \right], \]
where \( a, b, c, \gamma \) are constants and the carrying capacity, \( N_\infty \), corresponds to fixed point where \( \alpha = 0 \).

For technical devices, the previous classification scheme has been generalized since the specific growth rate of Weibull law has a power dependence on \( t \) which is not reproduced by equation (4). The behavior \( \alpha(t) = t^n \), with \( n \) positive integer, corresponds to terms \( O(\alpha^{(n-1)/n}) \) in the expansion of \( \Phi(\alpha) \) and therefore for a general classification scheme of the specific growth/aging/failure rate of biological and technical systems one has to consider [9]:
\[ \Phi(\alpha) = \Sigma_{n=2}^\infty c_n \alpha^{(n-1)/n} + \Sigma_{n=1}^\infty b_n \alpha^n. \]
Note that: (a) \( 0 < (n - 1)/n < 1 \) and the \( n \)-th term in the power series in \( \alpha^{(n-1)/n} \) tends for large \( n \) to \( \alpha \), i.e. to the Gompertz law; (b) the term \( b_0 \neq 0 \), i.e. the exponential growth, can be neglected if one considers the GL, the generalized logistic or more complex growth laws for the biological systems (there is no problem to include this term in the expansion); (c) the first sum in the expansion has fractional powers. As a by-product of the proposed classification scheme one can easily evaluate the aging/failure of combined new bio-technical ‘manufactured products’ [9].

On the other hand, in many different systems it is often studied the dependence of the dynamical variables on the temperature \( T \) and one wonders about the role of ‘growth’ laws in such cases. In other terms the question concerns the information contained in equations (3), (4) if, for example, one interprets the variable \( t \) as \( 1/T \) (with the Boltzmann constant \( k_B = 1 \)), i.e. by considering the equations:
\[ \frac{1}{f(1/T)} \frac{df(1/T)}{d(1/T)} = \alpha(1/T), \]
with
\[ \Phi(\alpha) = \frac{d\alpha}{d(1/T)} = \Sigma_i c_i \alpha^i \quad i = 0, 1, 2 \ldots. \]
In the next section we shall analyze this aspect.

2. Thermal behavior

Let us now study some specific solutions of equations (8), (9) and the applications to the Fermi–Dirac distribution of a free gas and, in more details, to the electrical conductivity of Silicon Carbide (SiC).

For \( c_i = 0 \), \( i = 0, 1, 2, \ldots \), \( \alpha = \alpha_0 \) is a constant and \( f \) follows the the Boltzmann factor, i.e.
\[ f = f_0 \exp(\alpha_0/T); \]
if \( c_0 \neq 0 \) and \( c_1 = 0 \), \( i = 1, 2, \ldots \), there are corrections to the thermal Boltzmann spectrum, as observed in black-hole evaporation [10]; the case \( c_0 = 0 \), \( c_1 = 0, c_i = 0, i = 2, 3, \ldots \) reproduces...
the GL in the variable $1/T$ and for $c_0 = 0$, $c_1 = 0$, $c_2 = 0$ for $i \geq 3$ one gets the logistic (and generalized logistic) equation for $f$, that we discuss in more details in the following applications.

2.1. Fermi–Dirac distribution

The Fermi–Dirac distribution for a free fermion gas is given by

$$f(1/T)_{FD} = \frac{1}{1 + e^{\Delta/\alpha}},$$

where $\Delta$ is the difference in energy with respect to the Fermi energy. At fixed $\Delta$, as a function of $1/T$, $f$ satisfies a logistic equation. Indeed,

$$\alpha = \frac{1}{f_{FD}} \frac{df_{FD}(1/T)}{d(1/T)} = -\Delta(1 - f_{FD}),$$

According to the classification in [2], the logistic feedback in equation (11) corresponds to the class U2 [2], i.e. it is obtained by the expansion of $\Phi(\alpha)$ in equation (9) to second order in $\alpha$, as one easily verify by the chain of relations

$$\Phi(\alpha) = \frac{d\alpha}{d(1/T)} = -\Delta\left[ d\left( 1 - f_{FD} \right) \right]/d(1/T) = \Delta f_{FD} = \Delta\alpha(1 + \alpha/\Delta),$$

i.e. $c_1 = \Delta$ and $c_2 = 1$ in equation (9).

The fixed point $f_{FD} = 1$ is due to the Pauli principle and indeed the Bose–Einstein distribution,

$$f(1/T)_{BE} = \frac{1}{e^{E/T} - 1},$$

where $E$ is the energy, follows the $T$ evolution equation

$$\frac{1}{f_{BE}} \frac{df_{BE}(1/T)}{d(1/T)} = -E(1 + f_{BE}),$$

without saturation effect.

The classification U2 implies that two physical constants completely specify the macroscopic evolution rate in $T$, independently on the microscopic details. A more complex system, in a complete different sector, will be discussed in the next subsection.

2.2. Silicon Carbide electrical activation

Silicon Carbide is a wide bandgap semiconductor with high thermal conductivity and other outstanding properties [11, 12] used in a large series of electronic devices. An accurate, microscopic, modeling of its electrical properties is currently not available and phenomenological approaches are often proposed [13]. The previous 'thermal growth' classification immediately suggests various empirical models of the electrical activation as a function of the annealing temperature at fixed implantation dose. The first model is obtained by considering equation (8) for the electrical activation, $I$, and by considering the first order expansion $\Phi(\alpha) = c_1 \alpha$, which corresponds to the GL, i.e.

$$I_k = I_0 e^{k_1 \alpha/(1 + \alpha)} e^{\alpha/(1 - \alpha)},$$

where $k_0$ is a constant and $I_0 = 1$, i.e. 100 % of possible activation of the implanted ion, for low implantation dose ($< 10^{14}$ cm$^{-2}$).

The second and third empirical models are obtained by considering the expansion of $\Phi(\alpha) = c_1 \alpha + c_2 \alpha^2$ which generates the logistic behavior,

$$I_l = \frac{1}{1 + k_1 e^{a_1/T}},$$

where $k_l$ and $a_1$ are constants depending on $c_1$ and $c_2$ (and on the boundary conditions of the differential equations), and the generalized logistic curve

$$I_g = \left[ \frac{1 + k_2 e^{a_2/T}}{1 + k_2} \right]^{-\rho},$$

where, again, $k_2$, $a_2$, $\rho$ are constants related to $c_1$, $c_2$.

In figures 1, 2 the previous different 'thermal growth' models are compared with various data on electrical activation, for low dose Al, N, P- SiC implanted, as a function of the annealing temperature.

The previous analysis can be easily generalized to take into account that, at large implantation dose ($> 10^{14}$ cm$^{-2}$), high temperature thermal processes reduce the maximum electrical activation.
Figure 1. Electrical activation for SiC implanted with Al for different annealing temperature form [11, 14–17]. The values of the parameters are: \( a_i = 72.1619 \, ^\circ\mathrm{C}, k_i = 7.59 \times 10^{-11}, a_g = 92.4396 \, ^\circ\mathrm{C}, k_g = 4.07 \times 10^{-16}, \rho = 0.59, k_e = -8.15 \times 10^{-19} \) and \( c_i = 63.9806 \, ^\circ\mathrm{C} (1 \, \text{eV} = 11.6045 \, ^\circ\mathrm{K}) \).

Figure 2. Annealing-temperature dependence of electrical activation ratio in nitrogen- or phosphorus-implanted SiC[11]. The implantations were performed at room temperature (total implant dose: \( 10^{14} \, \text{cm}^{-2} \)). Parameters: \( a_i = 72.7409 \, ^\circ\mathrm{C}, k_i = 1.12 \times 10^{-21}, a_g = 66.6759 \, ^\circ\mathrm{C}, k_g = 6.44 \times 10^{-20}, \rho = 0.96, k_e = -1.57 \times 10^{-18} \) and \( c_i = 53.544.9 \, ^\circ\mathrm{C} \).
More precisely, implantation doses in the range \(10^{10} - 10^{17} \text{ cm}^{-2}\) correspond to dopant atom densities of \(2 \times 10^{18} - 10^{20} \text{ cm}^{-3}\), for a deep box profile of 400 nm, and in [18, 19] it has been shown that in phosphorus implanted SiC, at the fixed annealing temperature of 1600 °C, the maximum electrical activation decreases to 20%–40% of the implanted ion density.

This result implies that at large implantation dose the ‘carrying capacity’ decreases: if, for example, the electrical activation follows the logistic equation

\[
\frac{1}{I_0} \frac{dI}{d(1/T)} = a_t (1 - I_t),
\]

the saturation value (i.e. the carrying capacity) can be easily (re-)introduced by rescaling \(I_t \rightarrow I_t / I_0^0\), with \(I_0^0\) depending on the dopant atom density. By assuming the other parameters of the logistic curve in figure 2 are independent on the implanted ion density, the behavior of the electrical activation as a function of the annealing temperature for different implantation doses is predicted in figure 3 (see figure caption).

3. Comments and conclusions

The previous analysis shows that a thermal behavior can be considered as a macroscopic ‘growth’ with specific feedback effects. Therefore, independently on the microscopic complexity of the considered system, the thermal evolution can be predicted on the basis of few parameters which define the specific growth rate. In this respect, the macroscopic behavior of very different systems follows similar trend and, in particular, we have shown that the electrical activation of implanted silicon carbide as a function of the annealing temperature can be described by growth laws typical of the evolution of biological systems.

The proposed general classification raise the fundamental question why very different physical systems satisfy similar growth laws. This important aspect can be more easily discussed by considering a macroscopic quantity, \(f(t)\), following the time evolution

\[
\frac{df}{dt} = \alpha f - \beta f^2,
\]

which, according to the different values of \(\alpha = 0\) and \(\beta = 0\), describes Gompertz, logistic or generalized logistic growth. By defining \(\tau = \alpha t\) and \(k = \beta / \alpha\) one gets

![Figure 3. Maximum electrical activation as a function of annealing temperature for different implanted ion density, \(d < 10^{17} \text{ cm}^{-2}\) (\(I_0 = 1\); \(10^{14} \text{ cm}^{-1}\) (\(I_0 = 0.9\)); \(3 \times 10^{15} \text{ cm}^{-1}\) (\(I_0 = 0.55\)); \(3 \times 10^{16} \text{ cm}^{-1}\) (\(I_0 = 0.3\)).]
\[
\frac{df}{d\tau} = 1 - kf
\]  

which implies that there is a typical time scale of the process, related to \(\alpha\), and that the system has a carrying capacity, i.e. a value \(f^* = 1/k\) where there is no growth, i.e the specific rate has a fixed point. These two dynamical ingredients are common to many different systems, of course with different meanings.

In cellular growth there is a characteristic time due to cell doubling and a carrying capacity related to the available metabolic resources [20].

The carrying capacity (i.e. the saturation point) for SiC electrical activation is essentially due to the presence of defects and to solid solubility: there is a maximum number of defects that can contribute to the electrical activation.

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References

[1] Wolfram S 1984 Nature 311 419
[2] Castorina P, Delsanto P P and Guiot C 2006 Classification scheme for phenomenological universalities in growth problems in physics and other sciences Phys. Rev. Lett. 96 188701  
Castorina P, Delsanto P P and Guiot C 2006 Classification scheme for phenomenological universalities in growth problems in physics and other sciences Phys. Rev. Lett. 96 188701 Erratum
[3] Gompertz B 1825 On the nature of the function expressive of the law of human mortality and a new mode of determining life contingencies Phil. Trans. R. Soc. 115 513
[4] Steel G G 1977 Growth Kinetics of Tumours (Oxford: Clarendon)
[5] Wheldon T E 1988 Mathematical Models in Cancer Research (Bristol, UK: Adam Hilger Publisher)
[6] Norton L A 1988 A Gompertzian model of human breast cancer growth Cancer Res 48 7067–71
[7] Barlow R E and Proshan F 1975 Statistical theory of reliability and life testing Probability models (Canada: Holt, Rinehart and Winston)
[8] Rigdon S E and Basu A P 2000 Statistical Methods for the Reliability of Repairable Systems (New York: Wiley)
[9] Castorina P and Blanchard P 2012 Unified approach to growth and aging in biological, technical and biotechnical systems SpringerPlus 1 7
[10] Parikh M K and Wilczek F 2000 Hawking radiation as tunneling Phys. Rev. Lett. 85 5042
[11] Kimoto T and Cooper J A 2014 Fundamentals of silicon carbide technology: growth, characterization Devices and Applications (Hoboken, NJ, USA: Wiley)
[12] Choyle W J, Matsunami H and Pend G 2013 Silicon Carbide: Recent Major Advances (Berlin, Germany: Springer) (https://doi.org/10.1007/978-3-642-18870-1)
[13] Simonka V, Hessinger A, Wienbub J and Selberherr S 2018 Empirical model for electrical activation of aluminum- and boron-implanted Silicon Carbide IEEE Transaction of Electron Devices 65 674
[14] Saks N S et al 2004 App. Phys. Lett. 5195
[15] Parasini A et al 2015 J. Appl. Phys. 118 035101
[16] Negro J et al 2004 J. Appl. Phys. 96 4916
[17] Trefler T et al 1997 Phys. Status Solidi 162 277
[18] Handy E M, Rao M V, Holland O W, Jones K A, Derenge M A and Papanicolaou N 2000 Variable-dose 1017–1020cm-3 phosphorus ion implantation into 4H-SiC 88 1–6
[19] Calcagno L private communication
[20] Castorina P and Zappala D 2006 Physica A 365 473–80