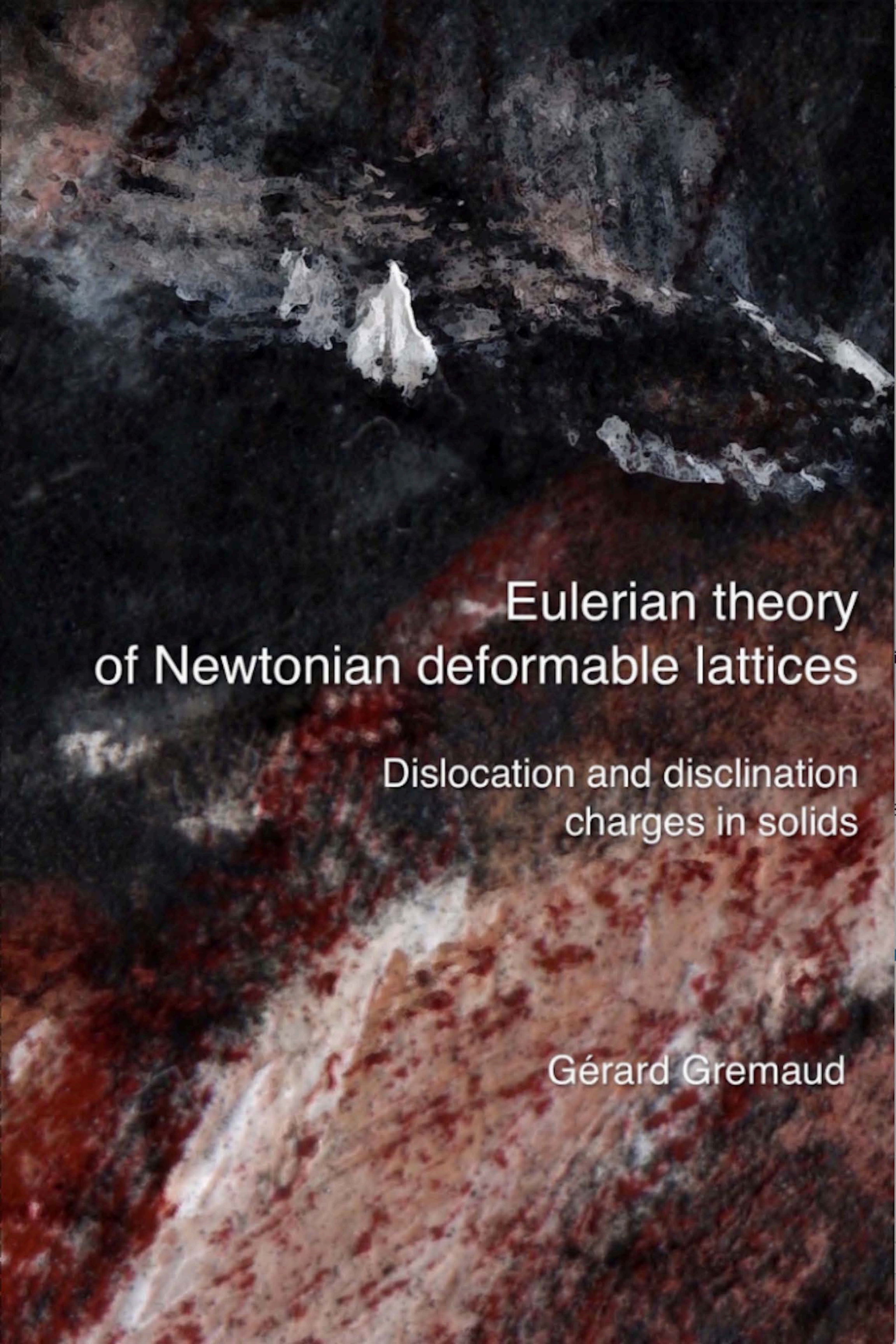

Eulerian theory of Newtonian deformable lattices

Dislocation and disclination charges in solids

Gérard Gremaud

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Introduction

In this book, one summarizes autonomously a first book[1] published during year 2013, which lays methodically the foundations of an original approach of the solid lattices deformation using the Euler coordinates, and which introduces in details the concept of tensor dislocation charges and tensor disclination charges within a lattice. This new concept allows one to quantify the topological singularities which can appear at the microscopic scale of a solid lattice. On the basis of this original approach of the solid lattices and their topological singularities, one can deduce a set of fundamental and phenomenological equations allowing to treat rigorously the macroscopic spatiotemporal evolution of a newtonian solid lattice which deforms in the absolute space of an external observer laboratory.

Motivation and genesis of this book

When one desires to study the solid deformation, one generally uses lagrangian coordinates to describe the evolution of the deformations, and diverse differential geometries to describe the topological defects contained in the solid.

The use of lagrangian coordinates presents a number of inherent difficulties. From the mathematical point of view, the tensors describing the continuous solid deformation are always of order higher than one concerning the spatial derivatives of the displacement field components, which leads to a very complicated mathematical formalism when the solid presents strong distortions (deformations and rotations). To these mathematical difficulties are added physical difficulties when one has to introduce some known properties of solids. Indeed, the lagrangian coordinates become practically unusable, for example when one has to describe the temporal evolution of the microscopic structure of a solid lattice (phase transitions) and of its structural defects (point defects, dislocations, disclinations, boundaries, etc.), or when it is necessary to introduce some physical properties of the medium (thermal, electrical, magnetic or chemical properties) leading to scalar, vectorial or tensorial fields in the real space.

The use of differential geometries in order to introduce topological defects as dislocations in a deformable continuous medium has been initiated by the work of Nye[2] (1953), who showed for the first time the link between the dislocation density tensor and the lattice curvature. On the other hand, Kondo[3] (1952) and Bilby[4] (1954) showed independently that the dislocations can be

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[1] *Théorie eulérienne des milieux déformables, charges de dislocation et de désinclinaison dans les solides, G. Gremaud, Presses polytechniques et universitaires romandes, Lausanne, Suisse, 2013, 750 pages (ISBN 978-2-88074-964-4)*

[2] *J.F. Nye, Acta Metall.,vol. 1, p.153, 1953*

[3] *K. Kondo, RAAG Memoirs of the unifying study of the basic problems in physics and engineering science by means of geometry, volume 1. Gakujutsu Bunken Fukyu- Kay, Tokyo, 1952*

[4] *B. A. Bilby , R. Bullough and E. Smith, «Continuous distributions of dislocations: a new application of the methods of non-riemannian geometry», Proc. Roy. Soc. London, Ser. A 231, p. 263–273, 1955*

identified as a crystalline version of the Cartan's concept[5] of torsion of a continuum. This approach was generalized in details by Kröner[6] (1960). However, the use of differential geometries in order to describe the deformable media leads very quickly to difficulties similar to those of the lagrangian coordinates system. A first difficulty arises from the complexity of the mathematical formalism which is similar to the formalism of general relativity, what makes very difficult to handle and to interpret the obtained general field equations. A second difficulty arises with the differential geometries when one has to introduce topological defects other than dislocations. For example, Kröner[7] (1980) has proposed that the existence of extrinsic point defects could be considered as extra-matter and introduced in the same manner that matter in general relativity under the form of Einstein equations, which would lead to a pure riemannian differential geometry in the absence of dislocations. He has also proposed that the intrinsic point defects (vacancies and interstitials) could be approached as a non-metric part of an affine connection. Finally, he has also envisaged introducing other topological defects, as disclinations for example, by using higher order geometries much more complex, as Finsler or Kawaguchi geometries. In fact, the introduction of differential geometries implies generally a heavy mathematical artillery (metric tensor and Christoffel symbols) in order to describe the spatiotemporal evolution in infinitesimal local referentials, as shown for example in the mathematical theory of dislocations of Zorawski[8] (1967).

In view of the complexity of calculations in the case of lagrangian coordinates as well as in the case of differential geometries, it seemed to me that it would be better to develop a much simpler approach of deformable solids, but at least equally rigorous, which has been finally published in a first book[1] during year 2013: *la théorie eulérienne des milieux déformables*.

Regarding *the description of defects (topological singularities)* which can appear within a solid, as dislocations and disclinations, it is a domain of physics initiated principally by the idea of macroscopic defects of Volterra[9] (1907). This domain experienced a fulgurant development during the twentieth century, as well illustrated by Hirth[10] (1985). The lattice dislocation theory started up in 1934, when Orowan[11], Polanyi[12] and Taylor[13] published independently papers describing the edge dislocation. In 1939, Burgers[14] described the screw and mixed dislocations. And finally in 1956, Hirsch, Horne et Whelan[15] and Bollmann[16] observed independently dislocations in me-

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[5] *E. Cartan, C.R. Akad. Sci., 174, p. 593, 1922 & C.R. Akad. Sci., 174, p.734, 1922*

[6] *E. Kröner, «Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen», Arch. Rat. Mech. Anal., 4, p. 273-313, 1960*

[7] *E. Kröner, «Continuum theory of defects», in «physics of defects», ed. by R. Balian et al., Les Houches, Session 35, p. 215–315. North Holland, Amsterdam, 1980.*

[8] *M. Zorawski, «Théorie mathématique des dislocations», Dunod, Paris, 1967.*

[9] *V. Volterra, «L'équilibre des corps élastiques», Ann. Ec. Norm. (3), XXIV, Paris, 1907*

[10] *J.-P. Hirth, «A Brief History of Dislocation Theory», Metallurgical Transactions A, vol. 16A, p. 2085, 1985*

[11] *E. Orowan, Z. Phys., vol. 89, p. 605,614 et 634, 1934*

[12] *M. Polanyi, Z. Phys., vol.89, p. 660, 1934*

[13] *G. I. Taylor, Proc. Roy. Soc. London, vol. A145, p. 362, 1934*

[14] *J. M. Burgers, Proc. Kon. Ned. Akad. Weten schap., vol.42, p. 293, 378, 1939*

[15] *P. B. Hirsch, R. W. Horne, M. J. Whelan, Phil. Mag., vol. 1, p. 667, 1956*

[16] *W. Bollmann, Phys. Rev., vol. 103, p. 1588, 1956*

tals by using electronic microscopes. Concerning the disclinations, it is in 1904 that Lehmann[17] observed them in molecular crystals, and in 1922 that Friedel[18] gave them a physical explanation. From the second part of the century, the physics of lattice defects has grown considerably.

In the first part of this essay, the dislocations and the disclinations are approached by introducing intuitively the concept of dislocation charges by using the famous Volterra pipes[19] (1907) and an analogy with the electrical charges. With Euler coordinates, the concept of dislocation charge density appears then in an equation of geometro-compatibility of the solid, when the concept of flux of charges is introduced in an equation of geometro-kinetics of the solid.

The *rigorous formulation of the charge concept* in the solids makes the essential originality of this approach of the topological singularities. The detailed development of this concept leads to the appearance of tensorial charges of first order, *the dislocation charges*, associated with *the plastic distortions* of the solid (plastic deformations and rotations), and of tensorial charges of second order, *the disclination charges*, associated with *the plastic contortions* of the solid (plastic flexions and torsions). It appears that these topological singularities are quantified in a solid lattice and that they have to appear as *strings (thin tubes)* which can be modelized as unidimensional lines of dislocation or disclination, or as *membranes (thin sheets)* which can be modelized as two-dimensional boundaries of flexion, torsion or accommodation.

The concept of dislocation and disclination charges allows one to find rigorously the main results obtained by the classical dislocation theory. But it allows above all to define a tensor $\vec{\Lambda}_i$ of *linear dislocation charge*, from which one deduces a scalar Λ of *linear rotation charge*, which is associated with the screw part of the dislocation, and a vector $\vec{\Lambda}$ of *linear flexion charge*, which is associated with the edge part of the dislocation. For a given dislocation, both charges Λ and $\vec{\Lambda}$ are perfectly defined without needing a convention at the contrary of the classical definition of a dislocation with its Burger vector! On the other hand, the description of the dislocations in the eulerian coordinate system by the concept of dislocation charges allows one to treat exactly the evolution of the charges and the deformations during very strong volumetric contractions and expansions of a solid medium.

Content of the book

This book is composed of four sections which summarize autonomously the eulerian theory of deformation introduced in my first book[1] published in 2013.

The first section (A) introduces *the eulerian deformation theory of newtonian lattices.*

The deformation of a lattice is characterized by *distortions and contortions (chap. 1 to 3)*. A vectorial representation of the tensors, presenting undeniable advantages over purely tensorial representation thanks the possibility to use the powerful formalism of the vectorial analysis, allows to obtain *the geometro-compatibility equations* of the lattice which insure its solidity, and *the geometro-kinetics equations* of the lattice, which allow one to describe the deformation kinetics.

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[17] *O. Lehmann, «Flussige Kristalle», Engelman, Leibzig, 1904*

[18] *G. Friedel, Ann. Physique, vol. 18, p. 273, 1922*

[19] *V. Volterra, «L'équilibre des corps élastiques», Ann. Ec. Norm. (3), XXIV, Paris, 1907*

One introduces then the physics in this topological context *(chap. 4)*, namely *the newtonian dynamics* and *the eulerian thermo-kinetics* (based on the first and second principles of thermodynamics). With all these ingredients, it becomes possible to describe the particular behaviors of a solid lattice *(chap. 5)*, as *the elasticity, the anelasticity, the plasticity* and *the self-diffusion*. This first section ends with the establishment of the complete set of evolution equations of a lattice in the Euler coordinate system *(chap. 6)*.

The second section (B) is dedicated to *the applications of the eulerian theory (chap. 7).*

It presents very succinctly some examples of *phenomenologies of everyday solids*. One shows how to obtain the functions and equations of state of an isotropic solid, what are the elastic and thermal properties which can appear, how waves propagate and why there exist thermoelastic relaxations, what are the mass transport phenomena and why it could appear inertial relaxations, what are the common phenomenologies of anelasticity and plasticity, and finally how it can appear structural transitions of first and second order in a solid lattice.

The third section (C) is dedicated to the introduction of *dislocation charges* and *disclination charges* in the eulerian lattices.

After the analytical introduction of the concepts of density and flux of dislocation and disclination charges in the lattices *(chap. 8)*, one presents a detailed review of *the lattice macroscopic and microscopic topological singularities* which can be associated to the dislocation and disclination charges *(chap. 9)*.

Then one discusses the motion of dislocation charges within the lattice by introducing *the dislocation charges flux of the dislocation charges* and *the Orowan relations (chap. 10)*. Finally, one deduces the Peach and Koehler force which acts on the dislocations, and one establishes the new set of evolution equations of a lattice in the Euler coordinate system *(chap. 11)*, which takes into account the existence of topological singularities within the lattice.

The fourth section (C) is dedicated to *the applications of the charge concept* within the eulerian solid lattice *(chap. 12)*.

It shows the elements of the dislocation theory in the everyday solids. One begins to show that, in the particular case of the deformation of isotropic lattices by pure shears, one can replace the shear strain tensor by the rotation vector, which allows one to find a set of equations which corresponds strictly *to all the Maxwell equations of electromagnetism*! One shows then how to calculate the fields and energies of the screw and edge dislocations in an isotropic lattice, just as the interactions which can occur between dislocations. One finishes this section of applications by presenting *the string model* of dislocations, which is the fundamental model allowing one to explain most of the macroscopic behaviors of anelasticity and plasticity of crystalline solids.

An other application of the theory

In this book, the reader will see numerous analogies between the eulerian theory of deformable media and the theories of electromagnetism, gravitation, special relativity and general relativity. These analogies are sufficiently surprising and remarkable to alert any open and curious scientific spirit! But it is also clear that these analogies are, by far, not perfect in this book. It is then tantalizing to analyze much more carefully these analogies and to try to find how to perfect them. That is done in an other book[20],[21], which is entirely allotted to the deepening, the improvement and the understanding of these analogies.

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[20] Gérard Gremaud, "Universe and Matter conjectured as a 3-dimensional Lattice with Topological Singularities", Amazon company, Lausanne, 2016, 646 pages, ISBN 978-2-8399-1934-0

[21] Gérard Gremaud, "Univers et Matière conjecturés comme un Réseau Tridimensionnel avec des Singularités Topologiques", Amazon company, Lausanne, 2016, 660 pages, ISBN 978-2-8399-1940-1