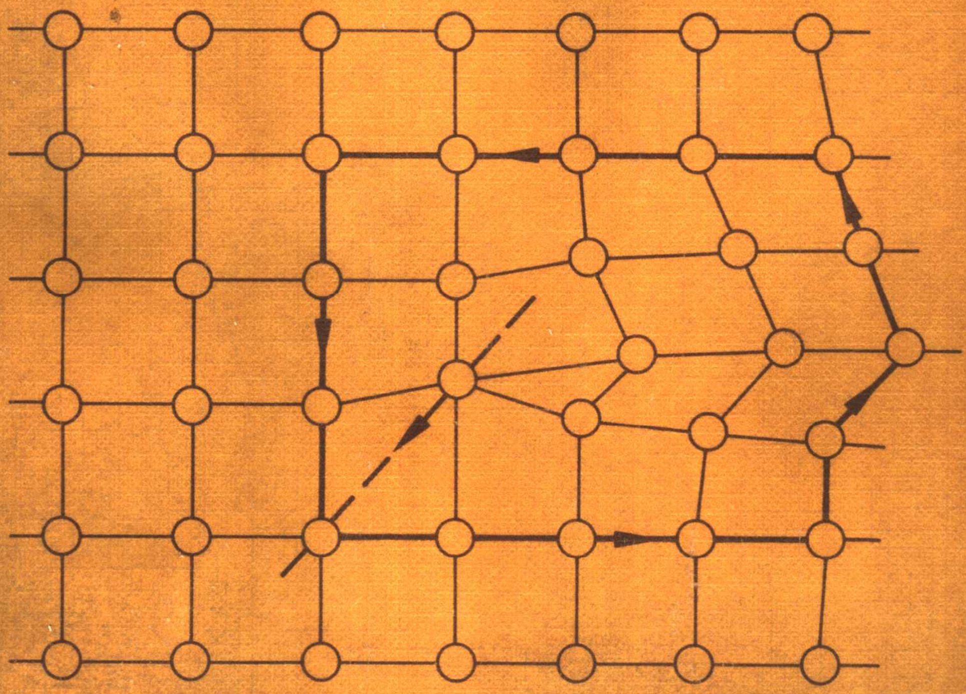
C. Teodosiu

Elastic Models of Crystal Defects



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Elastic Models of Crystal Defects

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PREFACE TO THE ENGLISH EDITION

This work deals with elastic models of crystal defects, a field situated at the boundary between continuum mechanics and solid state physics.

The understanding of the behaviour of crystal defects has become unavoidable for studying such processes as anelasticity, internal damping, plastic flow, rupture, fatigue, and radiation damage, which play a determining role in various fields of materials science and in top technological areas. On the other hand, the lattice distortion produced by a crystal defect can be calculated by means of elastic models, at least at sufficiently large distances from the defect. Furthermore, the interaction of a crystal defect with other defects and with applied loads is mainly due to the interaction of their elastic states. This explains the permanent endeavour to improve the elastic models of crystal defects, e.g. by taking into account anisotropic and non-linear elastic effects and by combining elastic with atomistic models in order to achieve a better description of the highly distorted regions near the defects.

This book has grown out of a two-semester course on "Continuum Mechanics with Applications to Solid State Physics" held by the author some ten years ago at the University of Stuttgart, which was an attempt to unify the topic with recent developments that have made continuum mechanics a highly deductive science. Since then, the extension of the application area and the development of new computing techniques have considerably enlarged the field and changed the plan of the work. However, the stress is still laid on theory and method: the problems solved are illustrative and intended to serve as background for approaching more complex or more specific applications. Moreover, their choice is inevitably influenced by the preference of the author for subjects to which personal contributions have been brought.

Chapter I concerns the basic concepts and laws of the kinematics, dynamics, and thermodynamics of deformable continuous media, the linear and non-linear elastic constitutive equations, as well as the formulation and solving of the boundary-value problems of linear elastostatics. Special attention is given to anisotropic elasticity, to the accurate formulation of boundary-value problems involving infinite domains and concentrated forces, and to the determination of Green's tensor function, in view of the importance of these topics for the simulation of crystal defects.

Chapter II contains a systematic study of the elastic states of single straight or curvilinear dislocations, of the elastic interactions between single dislocations, and of moving dislocations. The emphasis lies on the anisotropic elasticity theory of dislocations, especially on the powerful methods developed during the last ten years *for the computation of the elastic states of dislocation loops by means of straight dislocation data.*

Chapter III presents the main results obtained so far in describing non-linear effects in the elastic field of straight dislocations, as well as in the study of the core configuration of dislocations by using semidiscrete methods.

Chapter IV is devoted to the linear and non-linear theory of continuous distributions of dislocations and to its application to investigating the influence of dislocations on crystal density and on the low-temperature thermal conductivity of crystals.

Chapter V deals with the modelling of point defects as rigid or elastic inclusions in an elastic matrix, or as force multipoles. Finally, some of the results available on the interactions between point defects and other crystal defects are briefly reviewed.

Although the material in the text covers mainly the mathematical theory of crystal defects, the author has been constantly concerned with emphasizing the physical significance of the results and some of their possible applications. The reader can easily enlarge his information in these directions by reference to the standard books on crystal defects by Cottrell [84], Read [275], Friedel [124], Kröner [190], van Bueren [365], Indenbom [167], Nabarro [258], Hirth and Lothe [162], or to the review articles by Seeger [286], Eshelby [111], de Wit [385], and Bullough [50].

Printed jointly with Springer-Verlag, the English edition is a revised and up-dated version of the Romanian book "Modele elastice ale defectelor cristaline", published in 1977 by Editura Academiei. The present edition is supplemented by several subsections concerning the simulation of crystal dislocations by means of Volterra and Somigliana dislocations, the dislocation loops in anisotropic media, the interaction of crystal defects, and the flexible-boundary semidiscrete methods, as well as by a review of the main results published in the last four years.

The author expresses his deep gratitude to Prof. A. Seeger and Prof. E. Kröner for continuous encouragement to writing this book and for numerous discussions on the application of continuum mechanics to the simulation of crystal defects. The author is also greatly indebted to Dr. E. Soós for his valuable detailed criticism of the manuscript.

CHAPTER I

FUNDAMENTALS OF THE THEORY OF ELASTICITY

Before broaching the very subject of this chapter, we shall review briefly the basic elements of vector and tensor calculus that are necessary in the present work. This will also allow the reader to become familiar with the system of notation used in the following.

1. Vectors and tensors

1.1. Elements of vector and tensor algebra

We denote by $\mathscr{E}$ the three-dimensional Euclidean space; its elements $P, Q, \ldots$ are called *points*. The *translation vector space* associated with $\mathscr{E}$ is denoted by $\mathscr{V}$ and its elements $\mathbf{u}, \mathbf{v}, \ldots$ are called *vectors*.

The *scalar product* of the vectors $\mathbf{u}$ and $\mathbf{v}$ is denoted by $\mathbf{u}\cdot\mathbf{v}$. The magnitude of the vector $\mathbf{u}$ is the non-negative real number

$$\|\mathbf{u}\| = \sqrt{\mathbf{u}\cdot\mathbf{u}}. \tag{1.1}$$

Since $\mathscr{V}$ is also three-dimensional, any triplet of non-coplanar vectors is a *basis* of $\mathscr{V}$, and any vector of $\mathscr{V}$ can be written as a linear combination of the basis vectors. A *Cartesian co-ordinate frame* consists of an orthonormal basis $\{\mathbf{e}_k\} = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and a point O called the *origin*. Then

$$\mathbf{e}_k\cdot\mathbf{e}_m = \delta_{km}, \quad k, m = 1, 2, 3, \tag{1.2}$$

where

$$\delta_{km} = \begin{cases} 1 & \text{for} \quad k = m \\ 0 & \text{for} \quad k \neq m \end{cases} \tag{1.3}$$

is the *Kronecker delta*. The vector $\overrightarrow{OP} = \mathbf{x}$ is called the *position vector* of the point $P \in \mathscr{E}$. Clearly, the correspondence between points and their position vectors is one-to-one. Therefore, we shall sometimes label points by their position vectors, referring for conciseness to the point P whose position vector is $\mathbf{x}$ as "the point $\mathbf{x}$".

The real numbers u_1, u_2, u_3, uniquely defined by the relation

$$\mathbf{u} = u_1\mathbf{e}_1 + u_2\mathbf{e}_2 + u_3\mathbf{e}_3 \tag{1.4}$$

are called the *Cartesian components* of the vector $\mathbf{u}$.

Both *direct notation*, using only vector and tensor symbols, and *indicial notation*, making use of vector and tensor components, will be employed throughout. Whenever indicial notation is used, the subscripts are assumed to range over the integers 1, 2, 3, and summation over twice repeated subscripts is implied, e.g.

$$\mathbf{u}\cdot\mathbf{v} = u_k v_k = u_1 v_1 + u_2 v_2 + u_3 v_3. \tag{1.5}$$

From (1.4) and (1.2) we see that the Cartesian components of $\mathbf{u}$ can be also defined by

$$u_k = \mathbf{u}\cdot\mathbf{e}_k. \tag{1.6}$$

The *vector product* of two vectors $\mathbf{u}$ and $\mathbf{v}$ is denoted by $\mathbf{u}\times\mathbf{v}$. In view of (1.4) we can write

$$\mathbf{e}_k \times \mathbf{e}_l = \epsilon_{klm}\mathbf{e}_m, \tag{1.7}$$

where ϵ_{klm} is the *alternator symbol*. A direct proof shows that

$$\epsilon_{klm} = \begin{cases} 1 \text{ for } klm = 123, 231, 312 \\ 1 \text{ for } klm = 132, 213, 321 \\ 0 \text{ for any other values of } klm. \end{cases} \tag{1.8}$$

From (1.4) and (1.7) it follows that

$$\mathbf{u} \times \mathbf{v} = \epsilon_{klm} u_l v_m \mathbf{e}_k. \tag{1.9}$$

We notice that the symbols ϵ_{klm} satisfy the identities

$$\epsilon_{ikl}\epsilon_{jmn} = \begin{vmatrix} \delta_{ij} & \delta_{im} & \delta_{in} \\ \delta_{kj} & \delta_{km} & \delta_{kn} \\ \delta_{lj} & \delta_{lm} & \delta_{ln} \end{vmatrix}, \tag{1.10}$$

$$\epsilon_{ikl}\epsilon_{imn} = \delta_{km}\delta_{ln} - \delta_{kn}\delta_{lm}. \tag{1.11}$$

A *second-order tensor* $\mathbf{A}$ is a linear mapping[1] that assigns to each vector $\mathbf{u}$ a vector

$$\mathbf{v} = \mathbf{A}\mathbf{u}. \tag{1.12}$$

We denote by $\mathscr{L}$ the set of all second-order tensors defined on $\mathscr{V}$. The *sum* $\mathbf{A} + \mathbf{B}$ of two tensors $\mathbf{A}, \mathbf{B} \in \mathscr{L}$ is defined by

$$(\mathbf{A} + \mathbf{B})\,\mathbf{u} = \mathbf{A}\mathbf{u} + \mathbf{B}\mathbf{u}, \tag{1.13}$$

and the *product of a tensor* $\mathbf{A} \in \mathscr{L}$ *and a real number* α by

$$(\alpha\mathbf{A})\mathbf{u} = \alpha(\mathbf{A}\mathbf{u}). \tag{1.14}$$

The space $\mathscr{L}$ endowed with the composition rules (1.13) and (1.14) is also a vector space.

The *unit tensor* $\mathbf{1}$ and the *zero tensor* $\mathbf{0}$ are defined by the relations

$$\mathbf{1}\mathbf{u} = \mathbf{u}, \quad \mathbf{0}\mathbf{u} = \mathbf{0} \quad \text{for every } \mathbf{u} \in \mathscr{V}, \tag{1.15}$$

where $\mathbf{0}$ is the *zero vector.*

The *tensor product* $\mathbf{u}\mathbf{v}$ of two vectors $\mathbf{u}$ and $\mathbf{v}$ is the second-order tensor defined by

$$(\mathbf{u}\mathbf{v})\mathbf{w} = \mathbf{u}(\mathbf{v}\cdot\mathbf{w}) \text{ for every } \mathbf{w} \in \mathscr{V}. \tag{1.16}$$

It can be shown that if $\mathbf{f}_k$ and $\mathbf{g}_m$ are two arbitrary bases of $\mathscr{V}$, then the tensor products $\mathbf{f}_k\mathbf{g}_m$, $k, m = 1, 2, 3$, are a basis of $\mathscr{L}$, which is thus a nine-dimensional vector space. In particular, the tensor products $\mathbf{e}_k\mathbf{e}_m$, $k, m = 1, 2, 3$, are a basis of $\mathscr{L}$, and we can write for every $\mathbf{A} \in \mathscr{L}$

$$\mathbf{A} = A_{km}\mathbf{e}_k\mathbf{e}_m. \tag{1.17}$$

The nine real numbers A_{km}, uniquely defined by (1.17), are called the *Cartesian components* of the tensor $\mathbf{A}$. From (1.17), (1.16), and (1.2), we deduce the relation

$$A_{km} = \mathbf{e}_k\cdot(\mathbf{A}\mathbf{e}_m), \tag{1.18}$$

which can be considered as an equivalent definition of the tensor components. In particular, by applying this definition to the unit tensor and taking into account $(1.15)_1$ and (1.2), we infer that δ_{km} are the Cartesian components of the unit tensor, i.e.

$$\mathbf{1} = \delta_{km}\mathbf{e}_k\mathbf{e}_m.$$

---

[1] This definition can still be applied when $\mathscr{V}$ is an arbitrary vector space.

If $\mathbf{v} = \mathbf{Au}$, we also have by (1.17) and (1.16)

$$\mathbf{v} = (A_{km}\mathbf{e}_k\mathbf{e}_m)\,\mathbf{u} = A_{km}u_m\mathbf{e}_k,$$

and hence

$$v_k = A_{km}u_m. \tag{1.19}$$

The *product* **AB** *of two tensors* **A** *and* **B** is defined by the composition rule

$$(\mathbf{AB})\,\mathbf{u} = \mathbf{A}(\mathbf{Bu}) \text{ for every } \mathbf{u} \in \mathscr{V},$$

wherefrom it follows that

$$(\mathbf{AB})_{km} = A_{kp}B_{pm}. \tag{1.20}$$

The *transpose* of the tensor $\mathbf{A} = A_{km}\mathbf{e}_k\mathbf{e}_m$ is the tensor $\mathbf{A}^T = A_{mk}\mathbf{e}_k\mathbf{e}_m$. A second-order tensor **A** is called *symmetric* if $\mathbf{A}^T = \mathbf{A}$, and *skew* or *antisymmetric* if $\mathbf{A}^T = -\mathbf{A}$. By defining

$$\operatorname{sym}\mathbf{A} = \tfrac{1}{2}(\mathbf{A} + \mathbf{A}^T), \quad \operatorname{skw}\mathbf{A} = \tfrac{1}{2}(\mathbf{A} - \mathbf{A}^T)$$

as the *symmetric part* and the *skew part* of an arbitrary second-order tensor **A**, we can always write

$$\mathbf{A} = \operatorname{sym}\mathbf{A} + \operatorname{skw}\mathbf{A}.$$

Given any skew tensor $\mathbf{\Omega}$, there exists a unique vector $\boldsymbol{\omega}$ such that

$$\mathbf{\Omega u} = \boldsymbol{\omega} \times \mathbf{u} \text{ for every } \mathbf{u} \in \mathscr{V}. \tag{1.21}$$

Indeed, from (1.21), (1.9), and (1.11), it results that

$$\omega_i = -\tfrac{1}{2}\epsilon_{ijk}\Omega_{jk}, \quad \Omega_{ij} = -\epsilon_{ijk}\omega_k. \tag{1.22}$$

The vector $\boldsymbol{\omega}$, uniquely defined by $(1.22)_1$, is called the *axial vector* of the skew tensor $\mathbf{\Omega}$.

The trace of $\mathbf{A} \in \mathscr{L}$ is the real number

$$\operatorname{tr}\mathbf{A} \doteq A_{mm}. \tag{1.23}$$

The passing from **A** to tr **A** is called (tensor) *contraction*. It is easily seen that

$$\operatorname{tr}\mathbf{A}^T = \operatorname{tr}\mathbf{A}, \qquad \operatorname{tr}(\mathbf{AB}) = \operatorname{tr}(\mathbf{BA}). \tag{1.24}$$

The *inner product* $\mathbf{A}\cdot\mathbf{B}$ of two second-order tensors **A** and **B** is the real number

$$\mathbf{A}\cdot\mathbf{B} = \operatorname{tr}(\mathbf{AB}^T) = A_{km}B_{km}, \tag{1.25}$$

while the *magnitude* of **A** is the real number

$$\|\mathbf{A}\| = \sqrt{\mathbf{A}\cdot\mathbf{A}} = \sqrt{A_{km}A_{km}}\,. \tag{1.26}$$

The *determinant* det **A** of the tensor **A** is defined by

$$\det \mathbf{A} = \det [A_{km}], \tag{1.27}$$

where $[A_{km}]$ denotes the matrix of the Cartesian components of **A**. From this definition and some well-known rules of matrix algebra, we see that for every $\mathbf{A}, \mathbf{B} \in \mathscr{L}$:

$$\det \mathbf{A}^T = \det \mathbf{A}, \quad \det(\mathbf{AB}) = (\det \mathbf{A})(\det \mathbf{B}). \tag{1.28}$$

If $\det \mathbf{A} \neq 0$, there exists a unique inverse linear transformation $\mathbf{A}^{-1}$ of $\mathscr{V}$ on $\mathscr{V}$ such that if $\mathbf{v} = \mathbf{Au}$ then $\mathbf{u} = \mathbf{A}^{-1}\mathbf{v}$ for every $\mathbf{u}, \mathbf{v} \in \mathscr{V}$. From these two equations and $(1.15)_1$ it follows that

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{1}. \tag{1.29}$$

The tensor $\mathbf{A}^{-1}$ is called the *inverse* tensor of **A**.

A tensor **Q** is said to be *orthogonal* if

$$\mathbf{QQ}^T = 1, \quad Q_{kp}Q_{mp} = \delta_{km}. \tag{1.30}$$

By (1.30) and (1.28) we have $(\det \mathbf{Q})^2 = 1$, $\det \mathbf{Q} = \pm 1$. Hence, every orthogonal tensor admits an inverse and, by $(1.30)_1$, $\mathbf{Q}^{-1} = \mathbf{Q}^T$. The set of all orthogonal tensors forms a group, called the *orthogonal group;* the set of all orthogonal tensors with determinant equal to $+1$ forms a subgroup of the orthogonal group, called the *proper orthogonal group*.

A *tensor of n'th order* is a linear mapping that assigns to each vector $\mathbf{u} \in \mathscr{V}$ a tensor of $(n-1)$'st order, $n \geqslant 3$. Combining this definition with that of a second-order tensor given above allows the iterative introduction of tensors of an arbitrary order. We denote by $\mathscr{L}_n$ the space of all tensors of order n.

The tensor product $\mathbf{u}_1\mathbf{u}_2 \ldots \mathbf{u}_n$ is a tensor of n'th order defined as a linear mapping of $\mathscr{V}$ in $\mathscr{L}_{n-1}$ by the relation

$$(\mathbf{u}_1\mathbf{u}_2 \ldots \mathbf{u}_{n-1}\mathbf{u}_n)\,\mathbf{v} = \mathbf{u}_1\mathbf{u}_2 \ldots \mathbf{u}_{n-1}(\mathbf{u}_n\cdot\mathbf{v}) \text{ for every } \mathbf{v} \in \mathscr{V}.$$

It can be shown that the tensor products $\mathbf{e}_{k_1} \ldots \mathbf{e}_{k_n}$, $k_1, \ldots, k_n = 1, 2, 3$, form a basis of $\mathscr{L}_n$. Hence $\mathscr{L}_n$ is 3^n-dimensional, and every tensor $\mathbf{\Phi} \in \mathscr{L}_n$ can be written uniquely in the form

$$\mathbf{\Phi} = \Phi_{k_1\ldots k_n}\mathbf{e}_{k_1} \ldots \mathbf{e}_{k_n}, \tag{1.31}$$

where $\Phi_{k_1\ldots k_n}$ are the Cartesian components of $\mathbf{\Phi}$. Moreover, if $\mathbf{\Psi} = \mathbf{\Phi u}$, the n

$$\Psi_{k_1\ldots k_{n-1}} = \Phi_{k_1\ldots k_{n-1}k_n}u_{k_n}.$$

Let us consider now the transformation rules of vector and tensor components when passing from the orthonormal basis $\{\mathbf{e}_k\}$ to another orthonormal basis $\{\mathbf{e}'_r\}$. Denote by

$$q_{kr} = \mathbf{e}_k \cdot \mathbf{e}'_r = \cos(\mathbf{e}_k, \mathbf{e}'_r), \qquad k, r = 1, 2, 3, \tag{1.32}$$

the direction cosines of the unit vectors $\mathbf{e}_k$ with respect to the unit vectors $\mathbf{e}'_r$. By (1.4) and (1.6), we obviously have

$$\mathbf{e}_k = q_{kr}\mathbf{e}'_r, \quad \mathbf{e}'_r = q_{kr}\mathbf{e}_k, \tag{1.33}$$

wherefrom

$$q_{kr}q_{ks} = \delta_{rs}, \quad q_{kr}q_{lr} = \delta_{kl}.$$

Substituting successively (1.33) into the relation

$$\mathbf{u} = u_k\mathbf{e}_k = u'_r\mathbf{e}'_r,$$

and taking into account the unicity of Cartesian components, we obtain the transformation rule of the vector components

$$u_k = q_{kr}u'_r, \qquad u'_r = q_{kr}u_k. \tag{1.34}$$

In a similar way, the transformation rule of the components of a second-order tensor $\mathbf{A}$ reads

$$A_{km} = q_{kr}q_{ms}A'_{rs}, \quad A'_{rs} = q_{kr}q_{ms}A_{km}, \tag{1.35}$$

the generalization for higher-order tensors being evident.

A real number λ is said to be a *principal* or *characteristic value* of a second-order tensor $\mathbf{A}$ if there exists a unit vector $\mathbf{n}$ such that

$$\mathbf{A}\mathbf{n} = \lambda\mathbf{n}; \tag{1.36}$$

in this case $\mathbf{n}$ is called a *principal direction* corresponding to λ.

It can be shown (see, e.g. Halmos [151], Sect. 79) that if $\mathbf{A}$ is a symmetric second-order tensor, then there exists an orthonormal basis $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ and three (not necessarily distinct) principal values $\lambda_1, \lambda_2, \lambda_3$ of $\mathbf{A}$ such that

$$\mathbf{A} = \sum_{k=1}^{3} \lambda_k\mathbf{n}_k\mathbf{n}_k. \tag{1.37}$$

If $\lambda_1 = \lambda_2$, equation (1.37) reduces to

$$\mathbf{A} = \lambda_1\mathbf{n}_1\mathbf{n}_1 + \lambda_2(\mathbf{1} - \mathbf{n}_1\mathbf{n}_1). \tag{1.37a}$$

Finally, if $\lambda_1 = \lambda_2 = \lambda_3$, then

$$\mathbf{A} = \lambda_1\mathbf{1}. \tag{1.37b}$$

This theorem, called the *spectral theorem*, is of great importance for the elasticity theory. For instance, it implies the existence of the principal values of the strain tensor and of the Cauchy stress tensor for these are symmetric second-order tensors.

1.2. Elements of vector and tensor analysis

In this section we choose a *fixed* Cartesian co-ordinate frame in $\mathscr{E}$, with origin O and orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. Let (x_1, x_2, x_3) denote the Cartesian co-ordinates of a point $P \in \mathscr{E}$ with respect to this frame. The position vector $\overrightarrow{OP} = \mathbf{x}$ can be written as

$$\mathbf{x} = x_k \mathbf{e}_k.$$

For the sake of simplicity we denote the partial derivative $\partial(.)/\partial x_k$ by $(.)_{,k}$.

Let D be an open set in $\mathscr{E}$. A function $\mathbf{\Phi}$ that assigns to each point $P \in D$ a scalar, vector, or tensor $\mathbf{\Phi}(P)$ is called *scalar, vector*, or *tensor field* on D, respectively. A vector or tensor field is said to be of class C^n on D if its components with respect to the fixed co-ordinate frame are continuous on D together with their partial derivatives up to the n'th order.

Let $\mathbf{\Phi}$ be a scalar, vector, or tensor field on $\mathscr{E}$. Denoting $\|\overrightarrow{OP}\| = r$, we shall write $\mathbf{\Phi}(P) = O(r^n)$ as $r \to \infty$, or $\mathbf{\Phi}(P) = o(r^n)$ as $r \to \infty$, according to whether the expression $\|r^{-n}\mathbf{\Phi}(P)\|$ is bounded or tends to zero as $r \to \infty$. The same system of notation will be used to describe analogous properties for $r \to 0$.

Consider a scalar field F of class C^1. The *gradient* of F is the vector field

$$\operatorname{grad} F = F_{,m}\, \mathbf{e}_m. \tag{1.38}$$

Let $\mathbf{u}$ be a vector field of class C^1 on D. The *gradient* of $\mathbf{u}$ is the second-order tensor field [1]

$$\operatorname{grad} \mathbf{u} = u_{k,m}\, \mathbf{e}_k \mathbf{e}_m, \tag{1.39}$$

the *curl* of $\mathbf{u}$ is the vector field

$$\operatorname{curl} \mathbf{u} = \epsilon_{mrs} u_{r,s} \mathbf{e}_m, \tag{1.40}$$

and the *divergence* of $\mathbf{u}$ is the scalar field

$$\operatorname{div} \mathbf{u} = \operatorname{tr}(\operatorname{grad} \mathbf{u}) = u_{m,m}. \tag{1.41}$$

These operators, as well as those subsequently introduced in this section, can be also defined as linear mappings between scalar, vector, or tensor spaces (see, e.g. Gurtin [150], Sect. 4), and hence they are independent of the co-ordinate system.

[1] Note that we use throughout the so-called right-hand gradients, curls, and divergences of vector and tensor fields (cf. Malvern [227], Sect. 2.5, Jaunzemis [433], p. 88).