Introduction to Elasticity Theory for Crystal Defects

An understanding of the elastic properties of crystal defects is of fundamental importance for materials scientists and engineers. This book presents a self-sufficient and user-friendly introduction to the anisotropic elasticity theory necessary to model a wide range of crystal defects.

With little prior knowledge of the subject assumed, the reader is first walked through the required basic mathematical techniques and methods. This is followed by treatments of point, line, planar, and volume type defects such as vacancies, dislocations, grain boundaries, inhomogeneities, and inclusions. Included are analyses of their elastic fields, interactions with imposed stresses and image stresses, and interactions between defects, all employing the basic methods introduced earlier. This step-by-step approach, aided by numerous exercises with solutions provided, strengthens the reader's understanding of the principles involved, extending it well beyond the immediate scope of the book.

As the first comprehensive review of anisotropic elasticity theory for crystal defects, this text is ideal for both graduate students and professional researchers.

R. W. Balluffi is Emeritus Professor of Physical Metallurgy at Massachusetts Institute of Technology. He has previously published two books and more than 200 articles in the field. He is a member of the National Academy of Sciences and has received numerous awards, including the Von Hippel Award, the highest honor of the Materials Research Society.

"This is a very nice, self-contained and inclusive book. It should provide a foundation for the anisotropic elastic theory of defects and their interactions for years to come."
John Hirth, Ohio State University

"This is a wonderful book on the elastic foundations of point, line and surface defects in crystals. It is well written by a master experimental and theoretical craftsman who has spent a long professional life in this field. The mathematical coverage of crystal defects and their interactions unfolds in classic style."
Johannes Weertman, Northwestern University

"Professor Balluffi has had a long and distinguished career in physics and materials science as a researcher and educator and made numerous landmark contributions to the theory of crystal defects and diffusion mechanisms. He taught discipline oriented graduate lecture courses on these subjects at both Cornell University and at MIT. In his present book he provides a detailed and comprehensive presentation of the Elasticity Theory of Crystal Defects in full anisotropic form. While mechanistic understanding of complex mechanical phenomena in crystalline solids can generally be had with isotropic elasticity, a full understanding of the ranges of applicability of mechanisms often necessitates the use of anisotropic elasticity employing advanced mathematical methodology. Such methodology is presently available only in scattered journal publications going back many years or in special treatises using advanced mathematical language of a large variety of forms and often involving frustrating statements of "it can be shown that". In his book Balluffi provides detailed and compassionate developments, that skip little detail, permitting the reader to obtain a rare and penetrating view into complex methodology with a uniform mathematical language that is familiar to most advanced students and professionals. This is certain to make this book a standard reference for years to come to physicists, materials scientists and practitioners in applied mechanics."
Ali Argon, MIT

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Preface

A unified introduction to the theory of anisotropic elasticity for static defects in crystals is presented. The term "defects" is interpreted broadly to include defects of zero, one, two, and three dimensionality: included are

- Point defects (vacancies, self-interstitials, solute atoms, and small clusters of these species),
- Line defects (dislocations),
- Planar defects (homophase and heterophase interfaces),
- Volume defects (inhomogeneities and inclusions).

The book is an outgrowth of a graduate course on "Defects in Crystals" offered by the author for many years at the Massachusetts Institute of Technology, and its purpose is to provide an introduction to current methods of solving defect elasticity problems through the use of anisotropic linear elasticity theory. Emphasis is put on methods rather than a wide range of applications and results. The theory generally allows multiple approaches to a given problem, and a particular effort is made to formulate and compare alternative treatments.

Anisotropic linear elasticity is employed throughout. This is now practicable because of significant advances in the theory of anisotropic elasticity for crystal defects that have been made over the last 35 years or so, including the development of Green's functions for unit point forces in infinite anisotropic spaces, half-spaces and joined dissimilar half-spaces. The use of anisotropic theory (rather than the simpler isotropic theory) is important, since, even though the results obtained by employing the two approaches often agree to within 25%, or so, there are many phenomena that depend entirely on elastic anisotropy. Unfortunately, however, the results obtained with the anisotropic theory are usually in the form of lengthy integrals that can be evaluated only using numerical methods and so lack transparency. To assist with this difficulty, isotropic elasticity is employed in parallel treatments of many problems where sufficiently simple conditions are assumed so that tractable analytic solutions can be obtained that are more transparent physically. Sections in the book where isotropic elasticity is employed are clearly distinguished to avoid confusion.

The results for the various defects are developed in a sequence of increasing complexity starting with their behavior in isolation in infinite homogeneous regions, where their elastic fields are derived, along with, in many cases, corresponding elastic strain energies and induced volume changes. The treatment then progresses to interactions between the defects and imposed applied and internal stresses as well as the image stresses that arise when the defects are in finite homogeneous regions in the vicinity of interfaces. Finally, elastic interactions between the defects themselves are considered in terms of interaction energies and corresponding forces. Owing to the breadth of the subject and the impossibility of including all important topics in detail, a selection is made of representative material. This should provide the reader with the background to master omitted topics.

The book is designed to be self-sufficient. Included is a preliminary chapter on the basic elements of linear elasticity that includes essentially all of the elements of anisotropic and isotropic theory necessary to master the material that follows. A number of appendices contain other essentials. A particular effort has been made to write the book in a pedagogical manner useful for graduate students and workers in the field of materials science and engineering. Essentially, all results are fully derived, and as many intermediate steps as practicable are written out in full, and the use of the phrase “it can be shown” is avoided. Numerous exercises, with solutions, are provided, which, in many cases, expand the scope of the subject matter.

Requirements for use of the book are a familiarity with undergraduate materials science, including the structural aspects of the various defects, and knowledge of linear algebra, vector calculus, and differential equations. To avoid long unwieldy expressions, the repeated index summation convention is employed. Consistent sign conventions are used, and introductory lists of the common symbols employed throughout the text are provided. To keep the notation as simple as possible, additional symbols are employed locally in various sections of the book and are identified in brief lists in the relevant chapters for the convenience of the reader.

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I am particularly indebted to Professor David M. Barnett for permission to include his previously unpublished derivations of the anisotropic Green's functions for unit point forces in infinite spaces, half-spaces, and joined dissimilar half-spaces and for providing other valuable assistance. Professor Adrian Sutton offered encouragement and advice, and Professor John Hirth assisted with several questions. I am grateful to the Dept. of Materials Science and Engineering, Cornell University and its Director, Professor Emmanuel Giannelis, for hospitality and support during the writing of this book.

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Frequently used symbols

Roman

a: A	Scalar quantities (light face)
a^* : A^*	Complex conjugate of a or A
$\bar{a}$: $\bar{A}$	Fourier transform of a or A
$\mathbf{a}$: $\mathbf{A}$	Vectors (bold face)
a_i : A_i	Components of $\mathbf{a}$ or $\mathbf{A}$
$\hat{\mathbf{a}}$	Unit vector
$\lvert\mathbf{a}\rvert = a$	Magnitude of $\mathbf{a}$
$\underline{\mathbf{a}}$: $\underline{\mathbf{A}}$	Second-rank tensors (bold face, underlined)
a_{ij} : A_{ij}	Components of $\underline{\mathbf{a}}$ or $\underline{\mathbf{A}}$
$\underline{\underline{\mathbf{a}}}$: $\underline{\underline{\mathbf{A}}}$	Fourth-rank tensors (bold face and double underlined)
a_{ijkl} : A_{ijkl}	Components of fourth-rank tensor $\underline{\underline{\mathbf{a}}}$ or $\underline{\underline{\mathbf{A}}}$
$[a]$: $[A]$	Matrices
a_i : A_i	Elements of $[a]$ or $[A]$ if 1×3 or 3×1 matrix
a_{ij} : A_{ij}	Elements of $[a]$ or $[A]$ if 3×3 matrix
a_{ijkl} : A_{ijkl}	Elements of $[a]$ or $[A]$ if 9×9 matrix
$(aa)_{jk}$	Notation used for element of matrix representing Christoffel tensor: defined by $(aa)_{jk} \equiv a_i C_{ijkl} a_l$ (employs curved brackets rather than the square brackets used for matrices elsewhere throughout book)
(aa)	Matrix representing Christoffel tensor
$[A]^{-1}$	Inverse of $[A]$
$[A]^{\mathrm{T}}$	Transpose of $[A]$
$\mathbf{b}$	Burgers vector of dislocation
$\underline{\underline{\mathbf{C}}}$: C_{ijkl}	Elastic stiffness tensor
e_{ijk}	Alternator symbol: $e_{ijk} \equiv \hat{\mathbf{e}}_i \cdot (\hat{\mathbf{e}}_j \times \hat{\mathbf{e}}_k)$
$\hat{\mathbf{e}}_i$	Base unit vector of Cartesian, right-handed, orthogonal coordinate system
e	Dilatation: (sum of the normal elastic strain components: $e = \varepsilon_{mm}$)
E	Modulus of elasticity (or Young's modulus)
E	Total elasto-mechanical energy, i.e., elastic strain energy plus potential energy of applied forces
$\mathbf{F}$	Force
f	Force per unit length

$\mathcal{F}$	Force per unit area
$\mathbf{f}$	Force density
$H(x)$	Heaviside step function: $H(x) = 0$, when $x < 0$; $H(x) = 1$, when $x > 0$
K	Bulk elastic modulus
$\hat{\boldsymbol{l}}: \hat{l}_i$	Unit directional vector: component of $\boldsymbol{l}$ (direction cosine)
N	Number
n	Number per unit volume (density)
$\hat{\mathbf{n}}$	Unit vector normal to surface (taken to be positive for a closed surface when pointing outwards)
P	Hydrostatic pressure (positive when compressive)
$\mathbf{k}$	Fourier transform vector
r	Radius
$r,\ \theta,\ z$	Cylindrical coordinates (see Fig. A.1a)
$r,\ \theta,\ \phi$	Spherical coordinates (see Fig. A.1b)
R	Radius of curvature: distance between source point at $\mathbf{x}'$ and field point at $\mathbf{x}$
s	Arc length along line: distance
S^E_{ijkl}	Eshelby tensor
$\mathcal{S}$	Region of surface
S	Surface area
$\hat{S}$	Surface of unit sphere
$\underline{\underline{\mathbf{S}}} : S_{ijkl}$	Elastic compliance tensor
$\text{sgn}(x)$	$\text{sgn}(x) = 1$, if $x > 0$: $\text{sgn}(x) = -1$, if $x < 0$
$\hat{\mathbf{t}}$	Unit vector tangent to dislocation
$\mathbf{T}$	Traction
$\mathbf{u}$	Elastic displacement
$\mathbf{u}^{\mathrm{T}}$	Displacement associated with transformation strain
$\mathbf{u}^{\mathrm{tot}}$	Total displacement $((\mathbf{u}^{\mathrm{tot}} = \mathbf{u} + \mathbf{u}^{\mathrm{T}}))$
$\mathcal{V}$	Region of volume
V	Volume
W: w: $\mathcal{w}$	Elastic strain energy: elastic strain energy density: strain energy per unit length
$\mathcal{W}$	Work
x_1, x_2, x_3	Cartesian coordinates
$\mathbf{x}$: x_i: x	Field vector in Cartesian coordinates: component of $\mathbf{x}$: magnitude of $\mathbf{x}$, i.e., $x = \lvert\mathbf{x}\rvert = (x_1^2 + x_2^2 + x_3^2)^{1/2}$
$\mathbf{x}' : x'_1 : x'$	Source vector in Cartesian coordinates

Greek

δ_{ij}	Kronecker delta operator ($\delta_{ij} = 1$, when $i = j$: $\delta_{ij} = 0$, when $i \neq j$)
$\delta(\underline{\mathbf{x}} - \underline{\mathbf{x}}_{\mathrm{o}})$	Dirac delta function
$\underline{\boldsymbol{\varepsilon}} : \varepsilon_{ij}$	Elastic strain tensor: component of $\underline{\boldsymbol{\varepsilon}}$

$\varepsilon_{ij}^{\mathrm{T}}$	Transformation strain
$\varepsilon_{ij}^{\mathrm{T}^*}$	Transformation strain of equivalent homogeneous inclusion
$\varepsilon_{ij}^{\mathrm{tot}}$	Total strain ($\varepsilon_{ij}^{\mathrm{tot}} = \varepsilon_{ij} + \varepsilon_{ij}^{\mathrm{T}}$)
θ	Sum of the normal stress components: ($\theta \equiv \sigma_{mm}$)
r, θ, z	Cylindrical coordinates (see Fig. A.1a)
r, θ, ϕ	Spherical coordinates (see Fig. A.1b)
λ	Lamé elastic constant
μ	Lamé elastic constant (elastic shear modulus)
ν	Poisson's ratio
$\underline{\boldsymbol{\sigma}}$: σ_{ij}	Stress tensor: component of $\underline{\boldsymbol{\sigma}}$
Φ	Potential energy of forces applied to body
ϕ	Newtonian potential
ψ	Biharmonic potential
Ω	Atomic volume

Frequently used superscripts

D	Defect
DIS	Dislocation
IM	Image
INC	Inclusion
INH	Inhomogeneity
LF	Line force
M	Matrix