

Micromechanics of defects in solids

Second, revised edition

Toshio Mura

Department of Civil Engineering

Northwestern University, Evanston, IL, U.S.A.

Micromechanics of defects in solids

Second, revised edition

Toshio Mura

Department of Civil Engineering

Northwestern University, Evanston, IL, U.S.A.



Distributors

for the United States and Canada: Kluwer Academic Publishers, P.O. Box 358, Accord Station, Hingham, MA 02018-0358, USA

for the UK and Ireland: Kluwer Academic Publishers, MTP Press Limited, Falcon House, Queen Square, Lancaster LA1 1RN, UK

for all other countries: Kluwer Academic Publishers Group, Distribution Center, P.O. Box 322, 3300 AH Dordrecht, The Netherlands

Library of Congress Cataloging in Publication Data

Mura, Toshio, 1925-
Micromechanics of defects in solids.

(Mechanics of elastic and inelastic solids : 3)

Bibliography: p.

Includes indexes.

1. Micromechanics. 2. Solids. 3. Crystals--Defects.

I. Title. II. Series.

QC176.8.M5M87 1986 620.11'05

85-29652

ISBN 90-247-3256-5

ISBN 90-247-3256-5 (paperback)

ISBN 90-247-3343-X (hardback)

Book Information

First edition 1982.

Copyright

© 1987 by Martinus Nijhoff Publishers, Dordrecht.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publishers,

Martinus Nijhoff Publishers, P.O. Box 163, 3300 AD Dordrecht,
The Netherlands.

PRINTED IN THE NETHERLANDS

Preface

This book stems from a course on Micromechanics that I started about fifteen years ago at Northwestern University. At that time, micromechanics was a rather unfamiliar subject. Although I repeated the course every year, I was never convinced that my notes have quite developed into a final manuscript because new topics emerged constantly requiring revisions, and additions. I finally came to realize that if this is continued, then I will never complete the book to my total satisfaction. Meanwhile, T. Mori and I had coauthored a book in Japanese, entitled *Micromechanics*, published by Baifu-kan, Tokyo, in 1975. It received an extremely favorable response from students and researchers in Japan. This encouraged me to go ahead and publish my course notes in their latest version, as this book, which contains further development of the subject and is more comprehensive than the one published in Japanese.

Micromechanics encompasses mechanics related to microstructures of materials. The method employed is a continuum theory of elasticity yet its applications cover a broad area relating to the mechanical behavior of materials: plasticity, fracture and fatigue, constitutive equations, composite materials, polycrystals, etc. These subjects are treated in this book by means of a powerful and unified method which is called the 'eigenstrain method.' In particular, problems relating to inclusions and dislocations are most effectively analyzed by this method, and therefore, special emphasis is placed on these topics. When this book is used as a text for a graduate course, Sections 3, 11, and 22 should be emphasized.

Eigenstrain is a generic name given by the author to such nonelastic strains as thermal expansion, phase transformation, and misfit strains. J.D. Eshelby, who is a pioneer in this area, refers to eigenstrains as stress-free transformation strains in his celebrated papers (1957, 1959). The term eigenstrain should not be confused with the term 'eigenvalue' which occurs in mathematical physics, and relates to an entirely different concept.

No particular background is required of readers of this book because necessary mathematics and physics are explained in the text and Appendix.

Although I have tried to be fair in citing literature, I have to apologize if some papers do not receive proper credit or are not cited.

The sections and subsections marked with an asterisk (*), can be skipped in the first reading, since the subjects discussed there are peripheral to the main theme.

I wish to express my thanks to all the people who have helped me during the course of the preparation of the manuscript: my previous graduate students, Zissis A. Moschovidis, Minoru Taya, Carl R. Vilmann, and Ronald B. Castles, as well as my friends R. Furuhashi, N. Kinoshita, T. Morita, M. Inokuti, and T. Mori. Mori receives my special thanks for having advised me on the subject matter, for discussing with me whole chapters, and for helping me to write Chapter 7. The manuscript reached the final form in his hands. I also wish to thank S. Nemat-Naser who has read through the manuscript and has given valuable comments.

I give my thanks to Vera Fisher for her skillful typing and her great patience with me, to the secretaries whom I involved in various aspects of the work over the years: Erika Ivansons, Miriam Littell, Masa Sumikura, and Carolyn Andrews, and to my family for their patience and understanding.

Finally, I acknowledge the National Science Foundation and the U.S. Army Research Office for their support of my research in the area of micromechanics.

November 13, 1980

T.M.

Contents

Preface	v
Chapter 1. General theory of eigenstrains	1
1. Definition of eigenstrains	1
2. Fundamental equations of elasticity	3
Hooke's law	3
Equilibrium conditions	5
Compatibility conditions	6
3. General expressions of elastic fields for given eigenstrain distributions	7
Periodic solutions	7
Method of Fourier series and Fourier integrals	9
Method of Green's functions	11
Isotropic materials	13
Cubic crystals	14
Hexagonal crystals (transversely isotropic)	14
4. Exercises of general formulae	15
A straight screw dislocation	15
A straight edge dislocation	18
Periodic distribution of cuboidal precipitates	20
5. Static Green's functions	21
Isotropic materials	22
* Anisotropic materials	25
* Transversely isotropic materials	26
* Kröner's formula	31
* Derivatives of Green's functions	32
* Two-dimensional Green's function	34
6. Inclusions and inhomogeneities	38
Inclusions	38
Inhomogeneities	40
* Effect of isotropic elastic moduli on stress	42

7. Dislocations	44
Volterra and Mura formulas	45
* The Indenbom and Orlov formula	48
* Disclinations	49
8. Dynamic solutions	53
Uniformly moving edge dislocation	55
Uniformly moving screw dislocation	57*
*9. Dynamic Green's functions	57
Isotropic materials	61
Steady State	64
*10. Incompatibility	65
* Riemann-Christoffel curvature tensor	71
Chapter 2. Isotropic inclusions	74
11. Eshelby's solution	74
Interior points	75
Sphere	79
Elliptic cylinder	80
Penny-shape	81
Flat ellipsoid	83
Oblate spheroid	84
Prolate spheroid	84
Exterior points	84
Thermal expansion with central symmetry	88
*12. Ellipsoidal inclusions with polynomial eigenstrains	89
* The I-integrals	92
* Sphere	93
* Elliptic cylinder	94
* Oblate spheroid	94
* Prolate spheroid	94
* Elliptical plate	95
* The Ferrers and Dyson formula	95
13. Energies of inclusions	97
Elastic strain energy	97
Interaction energy	99
Strain energy due to a spherical inclusion	101
Elliptic cylinder	101
Penny-shaped flat ellipsoid	101
Spheroid	102
*14. Cuboidal inclusions	104

15. Inclusions in a half space	110
Green's functions	110
Ellipsoidal inclusion with a uniform dilatational eigenstrain	114
* Cuboidal inclusion with uniform eigenstrains	121
* Periodic distribution of eigenstrains	121
Joined half-spaces	123
Chapter 3. Anisotropic inclusions	129
16. Elastic field of an ellipsoidal inclusion	129
17. Formulae for interior points	133
Uniform eigenstrains	134
Spheroid	137
Cylinder (elliptic inclusion)	141
Flat ellipsoid	143
Eigenstrains with polynomial variation	144
Eigenstrains with a periodic form	144
*18. Formulae for exterior points	149
Examples	156
19. Ellipsoidal inclusions with polynomial eigenstrains in anisotropic media	158
Special cases	160
*20. Harmonic eigenstrains	161
21. Periodic distribution of spherical inclusions	165
Chapter 4. Ellipsoidal inhomogeneities	177
22. Equivalent inclusion method	178
Isotropic materials	181
Sphere	183
Penny shape	184
Rod	185
Anisotropic inhomogeneities in isotropic matrices	187
Stress field for exterior points	187
23. Numerical calculations	188
Two ellipsoidal inhomogeneities	192
*24. Impotent eigenstrains	198
25. Energies of inhomogeneities	204
Elastic strain energy	204
Interaction energy	208
Colunneti's theorem	211
Uniform plastic deformation in a matrix	213
Energy balance	215

26.	Precipitates and martensites	218
	Isotropic precipitates	219
	Anisotropic precipitates	220
	Incoherent precipitates	226
	Martensitic transformation	229
	Stress orienting precipitation	237
Chapter 5. Cracks		240
27.	Critical stresses of cracks in isotropic media	240
	Penny-shaped cracks	240
	Slit-like cracks	242
	Flat ellipsoidal cracks	244
	Crack opening displacement	247
28.	Critical stresses of cracks in anisotropic media	248
	Uniform applied stress	248
	Non-uniform applied stress	253
	* II integrals for a penny-shaped crack	255
	* II integrals for cubic crystals	255
	* II integrals for transversely isotropic materials	257
29.	Stress intensity factor for a flat ellipsoidal crack	260
	Uniform applied stresses	264
	Non-uniform applied stresses	268
30.	Stress intensity factor for a slit-like crack	271
	Uniform applied stresses	272
	Non-uniform applied stresses	274
	Isotropic materials	274
31.	Stress concentration factors	277
	Simple tension	278
	Pure shear	279
32.	Dugdale-Barenblatt cracks	280
	BCS model	288
	Penny shaped crack	292
*33.	Stress intensity factor for an arbitrarily shaped plane crack	297
	* Numerical examples	305
34.	Crack growth	307
	Energy release rate	307
	The J-integral	311
	Fatigue	314
	Dynamic crack growth	319

Chapter 6. Dislocations	324
35. Displacement fields	324
Parallel dislocations	325
A straight dislocation	327
36. Stress fields	327
Dislocation segments	328
Willis' formula	333
The Asaro et al. formula	334
Dislocation loops	335
37. Dislocation density tensor	338
Surface dislocation density	341
Impotent distribution of dislocations	343
38. Dislocation flux tensor	345
Line integral expression of displacement and plastic distortion fields	348
The elastic field of moving dislocations wave equations of tensor potentials.	351
Wave equations of tensor potentials	352
39. Energies and forces	353
Dynamic consideration	354
40. Plasticity	361
Mathematical theory of plasticity	361
Dislocation theory	363
Plane strain problems	365
Beams and cylinders	373
41. Dislocation model for fatigue crack initiation	379
Chapter 7. Material properties and related topics	388
42. Macroscopic average	388
Average of internal stresses	388
Macroscopic strains	389
Tanaka-Mori's theorem	390
Image stress	393
Random distribution of inclusions-Mori and Tanaka's theory	394
43. Work-hardening of dispersion hardened alloys	398
Work-hardening in simple shear	398
Dislocations around an inclusion	402
Uniformity of plastic deformation	405
44. Diffusional relaxation of internal and external stresses	406
Relaxation of the internal stress in a plastically deformed dispersion strengthened alloy	407

	Diffusional relaxation process, climb rate of an Orowan loop	408
	Recovery creep of a dispersion strengthened alloy	412
	Interfacial diffusional relaxation	414
45.	Average elastic moduli of composite materials	421
	The Voigt approximation	421
	The Reuss approximation	424
	Hill's theory	426
	Eshelby's method	428
	Self-consistent method	430
	Upper and lower bounds	433
	Other related works	437
46.	Plastic behavior of polycrystalline metals and composites	439
	Taylor's analysis	439
	Self-consistent method	443
	Embedded weakened zone	448
47.	Viscoelasticity of composite materials	449
	Homogeneous inclusions	449
	Inhomogeneous inclusions	452
	Waves in an infinite medium	453
48.	Elastic wave scattering	455
	Dynamic equivalent inclusion method	459
	Green's formula	460
49.	Interaction between dislocations and inclusions	463
	Inclusions and dislocations	463
	Cracks in two-phase materials	471
50.	Eigenstrains in lattice theory	477
	A uniformly moving screw dislocation	480
51.	Sliding inclusions	484
	Shearing Eigenstrains	486
	Spheroidal inhomogeneous inclusions	488
52.	Recent developments	492
	Inclusions, precipitates, and composites	492
	Half-spaces	494
	Non-elastic matrices	494
	Cracks and inclusions	495
	Sliding and debonding inclusions	497
	Dynamic cases	497
	Miscellaneous	498

<i>Contents</i>	xiii
Appendix 1	499
Einstein summation convention	499
Kronecker delta	499
Permutation tensor	499
Appendix 2	501
The elastic moduli for isotropic materials	501
Appendix 3	505
Fourier series and integrals	505
Dirac's delta function and Heaviside's unit function	507
Laplace transform	508
Appendix 4	510
Dislocations pile-up	510
References	513
Author index	572
Subject index	582

General theory of eigenstrains

The definition of eigenstrains is given first. Then the associated general solutions for elastic fields for given eigenstrains are expressed by Fourier integrals and Green's functions. Some details of calculations for Green's functions are described for static and dynamic cases.

As fundamental formulae for the subsequent chapters, general expressions of elastic fields are given for inclusions, dislocations, and disclinations. The stress discontinuity on boundaries of inclusions and the incompatibility of eigenstrains are discussed as general theories.

Throughout this work, a fixed rectangular Cartesian coordinate system with coordinate axes x_i , $i = 1, 2, 3$, is used.

1. Definition of eigenstrains

'Eigenstrain' is a generic name given by the author to such nonelastic strains as thermal expansion, phase transformation, initial strains, plastic strains, and misfit strains. 'Eigenstress' is a generic name given to self-equilibrated internal stresses caused by one or several of these eigenstrains in bodies which are free from any other external force and surface constraint. The eigenstress fields are created by the incompatibility of the eigenstrains.

This new English terminology was adapted from the German 'Eigenspannungen und Eigenspannungsquellen,' which is the title of H. Reissner's paper (1931) on residual stresses. Eshelby (1957) referred to eigenstrains as stress-free transformation strains in his celebrated paper which has stimulated the present author to work on inclusion and dislocation problems. The term 'elastic polarization' was used by Kröner (1958) for eigenstrains in a slightly different context—when the nonhomogeneity of polycrystal deformation is under consideration.

Engineers have used the term 'residual stresses' for the self-equilibrated internal stresses when they remain in materials after fabrication or plastic deformation. Eigenstresses are called thermal stresses when thermal expansion

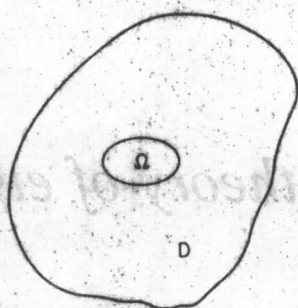


Fig. 1.1. Inclusion Ω

is a cause of the corresponding elastic fields. For example, when a part Ω of a material (Fig. 1.1) has its temperature raised by T , thermal stress σ_{ij} is induced in the material D by the constraint from the part which surrounds Ω . The thermal expansion αT , where α is the linear thermal expansion coefficient, constitutes the thermal expansion strain,

$$\epsilon_{ij}^* = \delta_{ij} \alpha T, \quad (1.1)$$

where δ_{ij} is the Kronecker delta (see Appendix 1). The thermal expansion strain is the strain caused when Ω can be expanded freely with the removal of the constraint from the surrounding part.

The actual strain is then the sum of the thermal and elastic strains. The elastic strain is related to the thermal stress by Hooke's law. The thermal expansion strain (1.1) is a typical example of an eigenstrain. In the elastic theory of eigenstrains and eigenstresses, however, it is not necessary to attribute ϵ_{ij}^* to any specific source. The source could be phase transformation, precipitation, plastic deformation or a fictitious source necessary for the equivalent inclusion method (to be discussed in Section 22).

When an eigenstrain ϵ_{ij}^* is prescribed in a finite subdomain Ω in a homogeneous material D (see Fig. 1.1) and it is zero in the matrix $D-\Omega$, then Ω is called an inclusion. The elastic moduli of the material are assumed to be homogeneous when inclusions are under consideration.

If a subdomain Ω in a material D has elastic moduli different from those of the matrix, then Ω is called an inhomogeneity. Applied stresses will be disturbed by the existence of the inhomogeneity. This disturbed stress field will be simulated by an eigenstress field by considering a fictitious eigenstrain ϵ_{ij}^* in Ω in a homogeneous material.

When Ω in Fig. 1.1 is a plane embedded in a three-dimensional material D and ϵ_{ij}^* is given on Ω as a plastic strain caused by a finite slip b , the boundary

of Ω is called a dislocation loop. If ϵ_{ij}^* is created by a rigid rotation of plane Ω by ω , the boundary of Ω is called a disclination loop.

2. Fundamental equations of elasticity

In this section the field equations for the elasticity theory will be reviewed with particular reference to solving eigenstrain problems. These problems consist of finding displacement u_i , strain ϵ_{ij} , and stress σ_{ij} at an arbitrary point $x(x_1, x_2, x_3)$ when a free body D is subjected to a given distribution of eigenstrain ϵ_{ij}^* . A free body is one which is free from any external surface or body force.

Hooke's law

For infinitesimal deformations considered in this book, the total strain ϵ_{ij} is regarded as the sum of elastic strain e_{ij} and eigenstrain ϵ_{ij}^* ,

$$\epsilon_{ij} = e_{ij} + \epsilon_{ij}^* \quad (2.1)$$

The total strain must be compatible,

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad (2.2)$$

where $u_{i,j} = \partial u_i / \partial x_j$.

The elastic strain is related to stress σ_{ij} by Hooke's law;

$$\sigma_{ij} = C_{ijkl} e_{kl} = C_{ijkl} (\epsilon_{kl} - \epsilon_{kl}^*) \quad (2.3)$$

or

$$\sigma_{ij} = C_{ijkl} (u_{k,l} - \epsilon_{kl}^*), \quad (2.4)$$

where C_{ijkl} are the elastic moduli (constants) (see Appendix 2), and the summation convention for the repeated indices is employed (see Appendix 1). Since C_{ijkl} is symmetric ($C_{ijkl} = C_{jilk}$), we have $C_{ijkl} u_{l,k} = C_{ijkl} u_{k,j}$. In the domain where $\epsilon_{ij}^* = 0$, (2.4) becomes

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl} = C_{ijkl} u_{k,l} \quad (2.5)$$

The inverse expression of (2.3) is

$$\epsilon_{ij} - \epsilon_{ij}^* = C_{ijkl}^{-1} \sigma_{kl}, \quad (2.6)$$

where C_{ijkl}^{-1} is the elastic compliance.

For isotropic materials, (2.3) and (2.6) can be written as

$$\begin{aligned}\sigma_{ij} &= 2\mu(\epsilon_{ij} - \epsilon_{ij}^*) + \lambda\delta_{ij}(\epsilon_{kk} - \epsilon_{kk}^*), \\ \epsilon_{ij} - \epsilon_{ij}^* &= \{\sigma_{ij} - \delta_{ij}\sigma_{kk}\nu/(1+\nu)\}/2\mu,\end{aligned}\quad (2.7)$$

where λ and μ are the Lamé constants, and ν is Poisson's ratio. Young's modulus E , the shear modulus μ , and the bulk modulus K are connected by $2\mu = E/(1+\nu)$, $K = E/3(1-2\nu)$, and $\lambda = 2\mu\nu/(1-2\nu)$. The alternative expressions for (2.7) are

$$\begin{aligned}\sigma_x &= \frac{E}{1+\nu} \left\{ (\epsilon_x - \epsilon_x^*) + \frac{\nu}{1-2\nu} (\epsilon_{kk} - \epsilon_{kk}^*) \right\}, \\ \sigma_y &= \frac{E}{1+\nu} \left\{ (\epsilon_y - \epsilon_y^*) + \frac{\nu}{1-2\nu} (\epsilon_{kk} - \epsilon_{kk}^*) \right\}, \\ \sigma_z &= \frac{E}{1+\nu} \left\{ (\epsilon_z - \epsilon_z^*) + \frac{\nu}{1-2\nu} (\epsilon_{kk} - \epsilon_{kk}^*) \right\}, \\ \sigma_{xy} &= \frac{E}{1+\nu} (\epsilon_{xy} - \epsilon_{xy}^*), \\ \sigma_{yz} &= \frac{E}{1+\nu} (\epsilon_{yz} - \epsilon_{yz}^*), \\ \sigma_{zx} &= \frac{E}{1+\nu} (\epsilon_{zx} - \epsilon_{zx}^*),\end{aligned}\quad (2.8)$$

and

$$\begin{aligned}\epsilon_x - \epsilon_x^* &= \{\sigma_x - \nu(\sigma_y + \sigma_z)\}/E, \\ \epsilon_y - \epsilon_y^* &= \{\sigma_y - \nu(\sigma_z + \sigma_x)\}/E, \\ \epsilon_z - \epsilon_z^* &= \{\sigma_z - \nu(\sigma_x + \sigma_y)\}/E, \\ \epsilon_{xy} - \epsilon_{xy}^* &= \frac{1+\nu}{E} \sigma_{xy}, \\ \epsilon_{yz} - \epsilon_{yz}^* &= \frac{1+\nu}{E} \sigma_{yz}, \\ \epsilon_{zx} - \epsilon_{zx}^* &= \frac{1+\nu}{E} \sigma_{zx},\end{aligned}\quad (2.9)$$

where $\epsilon_{kk} = \epsilon_x + \epsilon_y + \epsilon_z$ and $\epsilon_{kk}^* = \epsilon_x^* + \epsilon_y^* + \epsilon_z^*$. It is convenient to use (2.8) for the plane strain case where $\epsilon_z = 0$. Expression (2.9) is recommended for the plane stress case where $\sigma_z = \sigma_{zx} = \sigma_{zy} = 0$. It should be noted that solutions for the plane stress can be obtained directly from those for the plane strain by replacing $E/(1-\nu^2)$ with E and $\nu/(1-\nu)$ with ν .

When Hooke's law (2.8) is rewritten for the two-dimensional case, we have

$$\begin{aligned}\sigma_x &= \frac{\mu}{\kappa-1} \left\{ (\kappa+1)(\epsilon_x - \epsilon_x^*) + (3-\kappa)(\epsilon_y - \epsilon_y^*) \right\}, \\ \sigma_y &= \frac{\mu}{\kappa-1} \left\{ (\kappa+1)(\epsilon_y - \epsilon_y^*) + (3-\kappa)(\epsilon_x - \epsilon_x^*) \right\}, \\ \sigma_{xy} &= 2\mu(\epsilon_{xy} - \epsilon_{xy}^*), \\ \sigma_z = \sigma_{zx} = \sigma_{zy} &= 0,\end{aligned}\tag{2.9.1}$$

for the plane stress and $\kappa = (3-\nu)/(1+\nu)$. For the plane strain, we have

$$\begin{aligned}\sigma_x &= \frac{\mu}{\kappa-1} \left\{ (\kappa+1)(\epsilon_x - \epsilon_x^* - \nu\epsilon_z^*) + (3-\kappa)(\epsilon_y - \epsilon_y^* - \nu\epsilon_z^*) \right\}, \\ \sigma_y &= \frac{\mu}{\kappa-1} \left\{ (\kappa+1)(\epsilon_y - \epsilon_y^* - \nu\epsilon_z^*) + (3-\kappa)(\epsilon_x - \epsilon_x^* - \nu\epsilon_z^*) \right\}, \\ \sigma_{xy} &= 2\mu(\epsilon_{xy} - \epsilon_{xy}^*), \\ \sigma_z &= -\frac{\kappa+1}{\kappa-1}\mu\epsilon_z^* + \frac{3-\kappa}{\kappa-1}\mu(\epsilon_x + \epsilon_y - \epsilon_x^* - \epsilon_y^*), \\ \sigma_{zx} = \sigma_{zy} &= 0,\end{aligned}\tag{2.9.2}$$

where $\kappa = 3 - 4\nu$.

Equilibrium conditions

When eigenstresses are calculated, material domain D is assumed to be free from any external force and any surface constraint (if these conditions for the free body are not satisfied, the stress field can be constructed from the superposition of the eigenstress of the free body and the solution of a proper boundary value problem).

The equations of equilibrium are

$$\sigma_{i,j,j} = 0 \quad (i = 1, 2, 3).\tag{2.10}$$