Micromechanics of defects in solids

Second, revised edition

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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

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

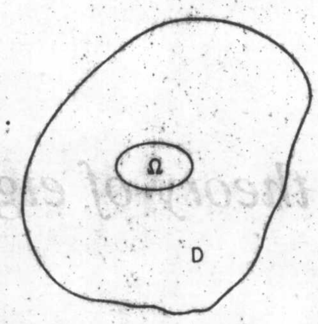

Fig. 1.1. Inclusion Ω

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,

$$\epsilon^*_{ij} = \delta_{ij}\alpha T, \tag{1.1}$$

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-Ω, 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},

$$\epsilon_{ij} = e_{ij} + \epsilon^*_{ij}. \tag{2.1}$$

The total strain must be compatible,

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

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

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

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

or

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

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 ($C_{ijlk} = C_{ijkl}$), we have $C_{ijkl}u_{l,k} = C_{ijkl}u_{k,l}$. In the domain where $\epsilon^*_{ij} = 0$, (2.4) becomes

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} = C_{ijkl}u_{k,l}. \tag{2.5}$$

The inverse expression of (2.3) is

$$\epsilon_{ij} - \epsilon^*_{ij} = C^{-1}_{ijkl}\sigma_{kl}, \tag{2.6}$$

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

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

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

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

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

and

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

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

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

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

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

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

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