

# Singularities in Elliptic Boundary Value Problems and Elasticity and Their Connection with Failure Initiation

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S.S. Antman  
Department of Mathematics  
*and*  
Institute for Physical Science  
and Technology  
University of Maryland  
College Park, MD 20742, USA  
[ssa@math.umd.edu](mailto:ssa@math.umd.edu)

L. Sirovich  
Department of Biomathematics  
Laboratory of Applied Mathematics  
Mt. Sinai School of Medicine  
Box 1012  
New York, NY 10029, USA  
[Lawrence.Sirovich@mssm.edu](mailto:Lawrence.Sirovich@mssm.edu)

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Princeton University  
215 Fine Hall  
Princeton, NJ 08544, USA  
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K. Sreenivasan  
Department of Physics  
New York University  
70 Washington Square South  
New York City, NY 10012, USA  
[katepalli.sreenivasan@nyu.edu](mailto:katepalli.sreenivasan@nyu.edu)

Zohar Yosibash

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 Springer

Zohar Yosibash  
Department of Mechanical Engineering  
Ben-Gurion University of the Negev  
PO Box 653  
84105 Beer-Sheva  
Israel

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*To my wife, Gila, and our children,  
Royee, Omer, and Inbar*



# Preface

Things in life break, and as my son used to say after being asked why he broke one of his toys, “*It happens.*” This monograph is mainly aimed at providing mathematical insight into why “it happens,” especially when brittle materials are of interest. We are interested also in investigating whether “nature is acquainted with the mathematical solution,” i.e., does the experimental evidence correspond to the mathematical predictions?

We are motivated by the theory of fracture mechanics, which has matured over the past half century and is able nowadays to predict failure incidents in mechanical components due to an existing *crack*. The classical approach to fracture mechanics is based on a simplified postulate, namely the correlation of a parameter characterizing the linear elastic solution in a neighborhood of the crack tip to experimental observations. It is well known that the linear elastic solution is singular at the crack tip, i.e., its gradient (associated with the stress field) tends to infinity. Thus, from an engineering viewpoint, the linear elastic solution is meaningless in the close vicinity of the crack tip, because of evident nonlinear effects such as large strains and plastic deformations.

Nevertheless, when the nonlinear behavior is confined entirely to some small region inside an elastic solution, then it can be determined through the solution of the linear elastic problem. Consequently, experimental observations on failure initiation and propagation in the neighborhood of a crack tip have been shown to correlate well with the linear elastic solution in many engineering applications.

Although attracting much attention, a crack tip is only a special, and rather simple case of singular points. In a solid body, singular solutions occur at reentrant corners, where material properties abruptly change along a free surface; at interior points where three or more zones of different materials intersect; or where an abrupt change in boundary conditions occurs. In the introduction we show some examples of the aforementioned singularities in “two-dimensional” domains.

From the mathematical viewpoint, the linear elastic solution in the vicinity of any of the above cases has the same characteristics as the solution in the neighborhood of a crack tip. Thus, an unavoidable question comes to mind: *Can one predict failure initiation at the singular points based on parameters of the elastic solution?*



The answer to this question is of major engineering importance due to its broad applicability to failures in electronic devices, composite materials and metallic structures. As in linear elasticity, the solution to heat-conduction problems has similar behavior near singularities, and the coupled thermo elastic response is crucial in understanding failure-initiation events in electronic components.

The first step toward a satisfactory answer is the capability to reliably compute the singular solution and/or functionals associated with it in the neighborhood of any singularity. This is one of the main motivations in writing this monograph. We also wanted to gather as many *explicit* mathematical results as possible on the linear elastic and heat-conduction solutions in the neighborhood of singular points, and present these in engineering terminology for practical usage. This means that we will rigorously treat the mathematical formulations from an engineering viewpoint. We present numerical algorithms for the computation of singular solutions in anisotropic materials and multi material interfaces, and advocate for the proper interpretation of the results in engineering practice, so that these can be correlated to experimental observations.

In the third part of the book, three-dimensional domains and singularities associated with edges and vertices are addressed. These have been mostly neglected in the mathematical analysis due to the tedious required treatment. In the past ten years, major achievements have been realized in the mathematical description of the singular solution in the vicinity of 3-D edges, with new insights into these realistic 3-D solutions. These are summarized herein together with new numerical methods for the extraction of so-called edge stress intensity functions and their relevance to fracture initiation. We also derive exact solutions in the vicinity of vertex singularities and extend the numerical methods for the computation of these solutions when analytical methods become too complex to be applied.

I have tried to make this book introductory in nature and as much as possible self-contained, and much effort has been invested to make the text uniform in its form and notation. Nevertheless, some preliminary knowledge of the finite element method is advised (see, e.g., [178]) but not mandatory, because we use the method for the solution of example problems (a short chapter is devoted to finite element fundamentals). It is aimed at the postgraduate level and to practitioners (engineers and applied mathematicians) who are working in the field of failure initiation and propagation. *Many examples of engineering relevance are provided and solved in detail.* We apologize to authors of relevant works that have not been cited; this is the result of my ignorance rather than my judgment.

The book is divided into fourteen chapters, each containing several sections. Most of it (the first nine chapters) addresses two-dimensional domains, where only singular *points* exist. The thermo elastic system and the feasibility of using the eigen pairs and GSIFs for predicting failure initiation in brittle material in engineering practice are addressed. Several failure laws for two-dimensional domains with V-notches and multi material interfaces are presented, and their validity is examined by comparison to experimental observation. A sufficient simple and reliable condition for predicting failure initiation (crack formation) in micron-level electronic devices, involving singular points, is still a topic of active research and interest, and

we address it herein. Three-dimensional problems are addressed in the next five chapters, discussing the singular solution decomposition into edge, vertex, and edge-vertex singular solutions. I conclude with circular edges in 3-D domains and some remarks on open questions.

I have the pleasure of thanking many of my colleagues and friends who have assisted in various ways toward the successful completion of this manuscript and with whom I have had the privilege to collaborate over the past two decades: Prof. Barna Szabó (Washington University, St. Louis, MO, USA) for the motivation to write the monograph (he is a coauthor of papers based on which Chapters 3-6 are developed), Profs. Monique Dauge and Martin Costabel (University of Rennes 1, Rennes, France) for stimulating discussions and acute contributions to the understanding of edge flux/stress intensity functions (parts of Chapters 10, 13, and 14 are based on joint papers), Prof. George Karniadakis (Brown University, Providence, RI, USA) for the connection to the publisher and the encouragement to write the book. The first five chapters of the monograph were composed for the special course “Singularities in elliptic problems and their treatment by high-order finite element methods” taught in the Division of Applied Mathematics at Brown University in spring 2003 while I was on a sabbatical stay in Prof. Karniadakis’s group. Many thanks are also extended to Prof. Dominique Leguillon (University of Paris 6, Paris, France) for inspiring discussions on failure laws and singularities, Prof. Ernst Rank (Technical University of Munich, Munich, Germany) for many interesting and stimulating discussions on  $p$ -finite element methods. I would like to thank Profs. Sue Brenner (Louisiana State University, Baton Rouge, LA, USA), Ivo Babuška (University of Texas, Austin, TX USA); and Christoph Schwab (ETH, Zurich, Switzerland) for interesting discussions on a variety of topics associated with singularities, and Dr. Tatianna Zaltzman (Sapir College, Sderot, Israel) for her help with vertex singularities (she is a coauthor on a paper based on which Chapter 12 is developed). Thanks are extended to some of my graduate students who read parts of the manuscript and provided me with their comments and insights, and especially to Dr. Netta Omer; the chapters discussing edge flux/stress intensity functions are based her doctoral dissertation, and Mr. Samuel Shannon - the last chapter is based on his MSc dissertation.

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# List of Main Symbols

|                            |   |
|----------------------------|---|
| $\mathbf{a}$               | Denotes a tensor.   |
| $\approx$                  |   |
| $\mathbf{a}$               | Denotes a vector.   |
| $[\mathbf{a}]$             | Denotes a matrix.   |
| $f_{,x}$                   | Denotes $\frac{\partial f}{\partial x}$ .   |
| $f'(x)$                    | Denotes $\frac{df}{dx}$ .   |
| $\mathcal{E}(\Omega)$      | The energy space of functions over the domain $\Omega$ . A function belongs to $\mathcal{E}(\Omega)$ if it has finite “strain energy.”  |
| $\mathcal{E}_c(\Omega)$    | The complementary energy space of fluxes/stresses over the domain $\Omega$ . A flux vector/stress tensor belongs to $\mathcal{E}_c(\Omega)$ if it satisfies the heat equation/equilibrium equation. |
| $\mathcal{E}_{ij}$         | Edge between vertices $V_i$ and $V_j$ in a 3-D domain.  |
| $\mathcal{G}$              | The energy release rate (ERR).  |
| $\mathcal{G}_c$            | Fracture energy, also known as critical energy release rate (ERR).  |
| $\mathcal{U}$              | Strain energy within an elastic domain.   |
| $\mathcal{B}(\tau, \chi)$  | The bilinear form of the weak formulation.  |
| $\mathcal{F}(\chi)$        | The linear form of the weak formulation.  |
| $\alpha, \beta$            | Elliptical coordinates.   |
| $\alpha_i$                 | The $i$ th singular exponent ( $i$ th eigenvalue). The $i$ th singular scalar solution is $\tau_i = r^{\alpha_i} s_i^+(\theta)$ .   |
| $\gamma_i$                 | The $i$ th singular exponent ( $i$ th eigenvalue) associated with a vertex singularity. The $i$ th singular scalar solution is $\tau_i = \rho^{\gamma_i} s_i^+(\theta, \varphi)$ .                  |
| $\partial_\beta$           | Derivative operator $\frac{\partial}{\partial x_\beta}$ .   |
| $\boldsymbol{\varepsilon}$ | The strain tensor.  |
| $\approx$                  |   |
| $\Gamma_1, \Gamma_2$       | Boundaries intersecting at the singular point.  |
| $\Gamma_R, \Gamma_{R^*}$   | Circular boundary around the singular point having a radius of $R$ (resp. $R^*$ ).  |

|  |   |
|--|---|
| $\Phi_i(\xi, \eta)$                        | The $i$ th shape function over the standard finite element.   |
| $\Phi_i^{(\alpha_j)}, \Phi_i^{(\alpha_j)}$ | The edge heat conduction/elasticity eigenfunction (for $i = 0$ ) primal or shadow function (for $i \geq 1$ ) associated with the $\alpha_j$ eigenvalue. $\Phi_i^{(\alpha_j)}(r, \theta) = r^{\alpha_j+i} \varphi_i(\theta)$ .   |
| $\Psi_i^{(\alpha_j)}, \Psi_i^{(\alpha_j)}$ | The edge dual heat conduction/elasticity eigenfunction (for $i = 0$ ) or dual shadow function (for $i \geq 1$ ) associated with the $\alpha_j$ eigenvalue. $\Psi_i^{(\alpha_j)}(r, \theta) = r^{-\alpha_j+i} \psi_i(\theta)$ .  |
| $\kappa$                                   | Kolosov constant: $(3 - \nu)/(1 + \nu)$ for plane-stress, $(3 - 4\nu)$ for plane-strain.  |
| $\lambda$                                  | One of the two Lamé constants.  |
| $\mu$                                      | Shear modulus $E/(2(1 + \nu))$ (one of the two Lamé constants). Also the normalized crack length associated with Leguillon's failure criteria at the rounded V-notch tip ( $\mu_0$ is normalized crack length for $\ell_0$ ).   |
| $\nu$                                      | Poisson ratio.  |
| $\omega$                                   | Rigid V-notch angle.  |
| $\Omega$                                   | 2-D or 3-D domain of interest.  |
| $\partial\Omega$                           | The boundary of $\Omega$ .  |
| $\rho$                                     | V-notch tip radius, or the radius vector of the spherical coordinate system.  |
| $\sigma$                                   | The elastic stress vector $(\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12})^T$ .  |
| $\tilde{\sigma}$                           | The elastic stress vector expressed in cylindrical/spherical coordinates, $(\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{zz}, \sigma_{\theta z}, \sigma_{rz}, \sigma_{r\theta})^T$ , or $(\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{\phi\phi}, \sigma_{\theta\phi}, \sigma_{r\phi}, \sigma_{r\theta})^T$ .                                       |
| $\sigma$                                   | The stress tensor.  |
| $\approx$                                  |   |
| $\sigma_c$                                 | Tensile strength.   |
| $\tau(\mathbf{x})$                         | Temperature field - the solution to the heat conduction equation (scalar elliptic equation).  |
| $\theta$                                   | Polar coordinate. In some chapters it is measured from one of the V-notch/crack edge and in others from the bisector of the solid angle.  |
| $(\xi, \eta)$                              | The coordinates of the standard finite element, $-1 \leq \xi, \eta \leq 1$ .  |
| $A_i$                                      | The $i$ th generalized flux/stress intensity factor or function (for edges).  |
| $A_{Ic}^{\text{blunt}}$                    | Critical mode I GSIF for rounded V-notches.   |
| $B_m(x_3), JB_m(x_3)$                      | Extraction polynomial and the Jacobi extraction polynomial of order $m$ , that depends on the coordinate $x_3$ along the edge.  |
| $[D]$                                      | Differential operator. In 3-D $[D]^T = \begin{bmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{bmatrix}$ and<br>in 2-D $[D]^T = \begin{bmatrix} \partial_1 & 0 & \partial_2 \\ 0 & \partial_2 & \partial_1 \end{bmatrix}$ . |

|                          |   |
|--------------------------|---|
| $[D^{(r,\theta)}]$       | $[D]$ operator in cylindrical coordinates.  |
| $e$ or $\mathbf{e}$      | Error between the exact and FE solutions. $e = \tau - \tau_{\text{FE}}$ , $\mathbf{e} = \mathbf{u} - \mathbf{u}_{\text{FE}}$ .  |
| $E$                      | Young's modulus.  |
| $[E]$                    | Elastic material matrix with elements denoted by $E_{ij}$ .   |
| $H_{11}$                 | A function that associates the small virtual crack increment at the V-notch tip and ERR - it depends on the V-notch tip geometry and boundary conditions $\Delta H_{11}$ is the change in $H_{11}$ between cracked and uncracked rounded notch tip. |
| $[k], k_{ij}$            | The thermal conductivity matrix and the coefficient of thermal conductivity in the $x_i$ and $x_j$ directions.  |
| $[K]$                    | The stiffness matrix with elements denoted by $K_{ij}$ .  |
| $k_c$                    | Critical material-dependent parameter at failure initiation at a V-notch tip $k_c = A_1 S_{\theta\theta}^{(1)}(0)$ .  |
| $K_I, K_{II}$            | Mode I and mode II stress intensity factors for cracks ( $K_I = \sqrt{2\pi} A_1$ , $K_{II} = \sqrt{2\pi} A_2$ ).  |
| $K_{Ic}$                 | Fracture toughness.   |
| $K_m^{(\alpha_i)} [B]$   | Quasidual singular function.  |
| $[M_R]$                  | The mass matrix associated with $\Gamma_R$ edge with $(M_R)_{ij}$ its $i, j$ element.   |
| $\ell_0$                 | Characteristic length.  |
| $\mathbf{n}$             | Outer normal unit vector to the surface $(n_1, n_2, n_3)^T$ .   |
| $n_g$                    | Gauss quadrature order.   |
| $N$                      | Number of degrees of freedom (DOFs), also number of terms in the singular asymptotic expansion.   |
| $r, \theta$              | Cylindrical coordinates.  |
| $s_i^+(\theta)$          | The $i$ th angular part of the primal singular function ( $i$ th eigenfunction) of the temperature/displacement.  |
| $s_i^-(\theta)$          | The $i$ th angular part of the dual singular function ( $i$ th dual eigenfunction) of the temperature/displacement.   |
| $S_i^+(\theta)$          | The $i$ th angular part of the primal eigenstress tensor.   |
| $S_i^-(\theta)$          | The $i$ th angular part of the dual eigenstress tensor.   |
| $\mathbf{t}$             | Tangential unit vector to the surface $(t_1, t_2, t_3)^T$ .   |
| $T$                      | T-stress in the vicinity of a crack tip.  |
| $\mathbf{T}$             | Traction vector to the surface $T_i = \sigma_{ji} n_j$ .  |
| $\mathbf{q}(\mathbf{x})$ | The flux vector. It is connected to the heat conduction solution by $\mathbf{q} = (q_1, q_1, q_3)^T = [k]\nabla\tau$ .  |
| $\mathbf{u}$             | The elastic displacements (solution of the Navier-Lamé elasticity system) $(u_1, u_2, u_3)^T$ .   |
| $\tilde{\mathbf{u}}$     | The elastic solution (displacements) expressed in cylindrical/spherical coordinates: $(u_r, u_\theta, u_z)^T$ , or $(u_\rho, u_\theta, u_\phi)^T$ .   |
| $V_i$                    | A vertex in a 3-D domain.   |
| $\mathbf{x}$             | Cartesian coordinates $(x_1, x_2, x_3)^T$ .   |



# Chapter 1

## Introduction

The point of departure is the motivation to write this monograph, and the assumptions under which linear theories predict well failure initiation and propagation effects. Thereafter, a layout of the book is provided, after which a rather simplified model problem presents the notation adopted.

The main goal of this book is to provide a unified approach for the analysis of singular points, both analytically and numerically, and the subsequent use of the computed data in engineering practice for predicting and eventually preventing failures in structural mechanics. We also summarize recent new insights on the solutions of realistic three-dimensional domains in the vicinity of singular edges and vertices. We strive to provide a rigorous mathematical framework for singularities in two- and three-dimensional domains in a systematic and simple manner. We then turn to numerical methods, specifically high-order finite element analysis, and summarize advanced methods for the computation of the necessary mathematical quantities for realistic problems too complex to be tackled analytically. Failure criteria based on the generated data are being proposed and supported by experimental observations.

### 1.1 What Is It All About?

During the last two decades, several books on singular solutions of elliptic boundary value problems have been published, among them [49, 72, 73, 97, 98, 109, 123, 127]. A comprehensive, rigorous, and up-to-date mathematical treatment of corner singularities and analytic regularity for linear elliptic systems is about to be published in a new monograph [45], which may serve as a reference to more mathematically oriented readers. Singularities of elliptic equations in polyhedra domains are rigorously covered from the mathematical viewpoint in a recent book [117]. These books provide an excellent mathematical foundation on singular solutions of linear elliptic boundary value problems. However, most of them require highly mathematical



proficiency and are not aimed at practical applications to failure initiation and propagation in real-life structures (except [109]). At the same time, high-order finite element methods (FEMs), namely the  $p$ - and  $hp$ -versions of the FEM, were developed and proved to be very efficient for approximating the solutions of elliptic boundary value problems with singular points on the boundary [9–11]. The use of these  $p$ -FEMs together with new extraction methods enables the computation of special singular solutions [12, 13, 177] elegantly and very efficiently suitable for use in engineering practice. Furthermore, three-dimensional explicit solutions for edge and vertex singularities are seldom provided, and their connection to two dimensional approximation is not well documented. Because of a growing demand for efficient and reliable means for predicting and eventually preventing failure initiation and propagation in multi-chip modules (MCM), electronic packages, and composite materials subjected to mechanical and thermal loads, there is a need to clearly address these singular solutions and utilize them in engineering practice. Thermal, elastic, and thermoelastic problems associated with large-scale integrated circuits, electronic packaging, and composites increase in complexity and importance. These components are assemblages of dissimilar materials with different thermal and mechanical properties. The mismatch of the physical properties causes flux and stress intensification at the corners of interfaces and can lead to mechanical failures. For example, in a conference paper on electronic components [119] the following was stated: *“The catastrophic effects of the residual stresses in electronic devices has been very well documented...”* However, no appropriate solutions are available yet: *“Most of these analyses though, have been based on elementary strength of materials concepts such as beam theory and proved inadequate to predict the shear stress magnitude at material interfaces.”*

The traditional finite element analysis of stresses is also considered inadequate [81]: *“Since the stress and displacement fields near a bonding edge show singularity behavior, the adhesive strength evaluation method, using maximum stresses calculated by a numerical stress analysis, such as the finite element method, is generally not valid.”*

These material interfaces, as well as crack tips, are called singular points because the temperature fluxes are infinite in the linear theory of steady-state heat conduction, and so are the stresses in the linear theory of elasticity. For example, typical singular points where failures initiate and propagate in an electronic device are illustrated in Figure 1.1.

Typical cracks can be observed by sectioning a VLSI device followed by a scanning electron microscope inspection, as shown in Figure 1.2. As observed, the failure initiates at the vertex of a reentrant V-notch.

It has been known for several decades that in large metallic structures, cracks may cause catastrophic failures. One of the recent and well-documented events of a structural failure in a civil airplane is the Aloha Airlines Flight 243 accident on April 28, 1988. A section of the upper fuselage was torn away in flight at 24,000 ft in a Boeing B-777-200 due to cracks originating in multiple places around riveted holes; see Figure 1.3. The airplane had flown 89,680 flights over its 19-year lifetime. Aircraft bulkheads can also break due to fatigue cracks, as did the F-16 bulkhead shown in Figure 1.4. There are many other examples of failed structures

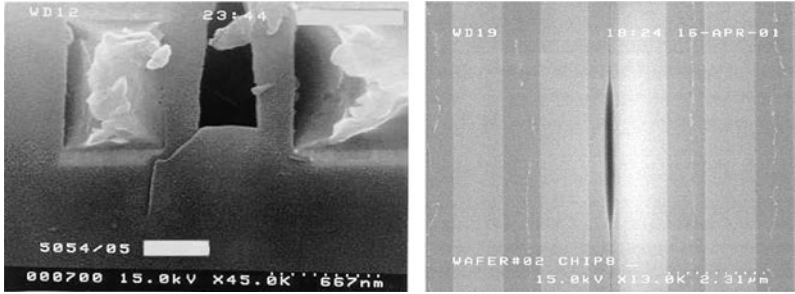


Fig. 1.1 Typical sites of failure initiation in an electronic device.

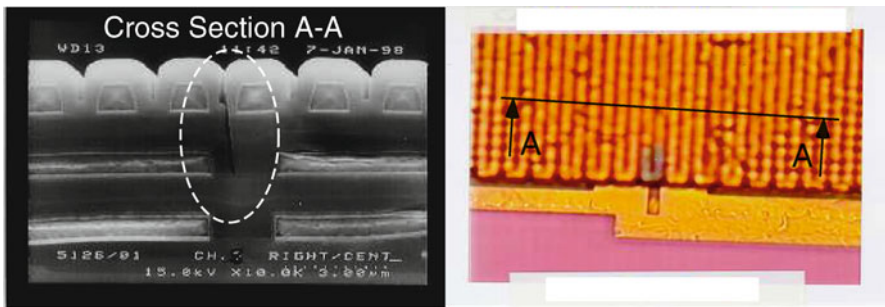


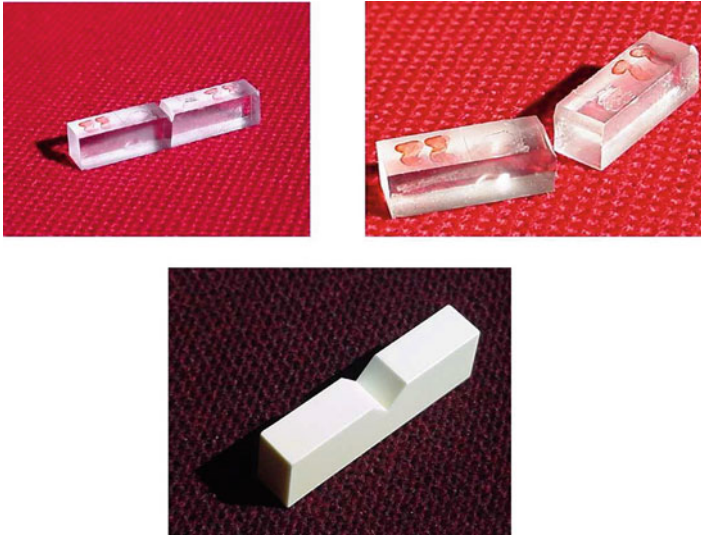
Fig. 1.2 Cracks in the passivation layer of a VLSI device: on the right a top view of the wafer, on the left a scanning electron microscope image showing the cross-section.



Fig. 1.3 The Aloha Airline Boeing 777 immediately after landing, April 1988.



**Fig. 1.4** A broken bulkhead from a F-16 aircraft due to a small surface crack.

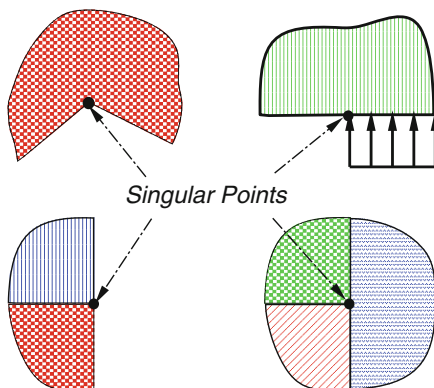


**Fig. 1.5** PMMA and Alumina-7%Zirconia specimens that break due to failures starting at V-notch tips.

such as those shown in Figure 1.5; where the failure starts at the V-notch tip in a PMMA polymer, or an Alumina-7%Zirconia ceramic. Such failures and their possible prediction will be discussed in this monograph.

New approaches to predicting the initiation and extension of delaminations in plastic-encapsulated LSI (large scale integrated circuit) devices, for example, are based on the computation of certain functionals, called the generalized flux/stress intensity factors (GFIFs/GSIFs); the strength of the stress singularity; and in thermoelastic problems, the thermal stress intensity factors (TSIFs). These are defined in the sequel, and they apply to many types of singular points, such as reentrant corners, abrupt change in boundary conditions, multimaterial interfaces, and at an internal intersection point of several materials. We show in Figure 1.6 some examples of the aforementioned singularities in two-dimensional domains.

**Fig. 1.6** Typical singular points in two-dimensional domains.



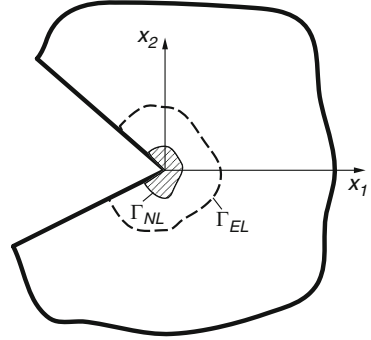
Some may claim that failure initiation and crack propagation are inherently non-linear processes, and the linear elastic solution may not be of practical application. However, when the nonlinear behavior is confined entirely to some small region inside an elastic solution, then it can be determined through the solution of the linear elastic problem. Consequently, experimental observations on failure initiation and propagation in the neighborhood of a crack tip have been shown to correlate well with the linear elastic solution in many engineering applications. An overview of the mechanical problems in electronic devices supports the new trend [85]. *“The author has organized the research committee on the mechanical problems in electron devices, which consists of the members from Japanese universities and private industries. The committee examined the research results on the mechanical problems in electron devices... The intensity and the order of the stress singularity are the main parameters to determine the (failure) criterion...”*

The approach of correlating the GFIFs/GSIFs or TSIFs (determined through an elastic analysis) to experimental observations for establishing failure laws seems to be *the right approach*, as shown by several recent publications [58, 59, 77, 81, 143, 206]. Quoting from [81], for example: *“... in the case of plastic encapsulated LSI (Large Scale Integrated Circuit) devices, the thermal-expansion mismatch of utilized materials causes thermal stresses... these thermal stresses could cause serious reliability problems, such as interface debonding, resin cracking... A new method for evaluating adhesive strength was developed which uses two-stress-singularity parameters... this method was applied to estimate delamination behavior of plastic encapsulated LSI models, and these estimated results coincide well with the observed results using scanning acoustic tomography”*.

## 1.2 Principles and Assumptions

It is assumed throughout the monograph that the principles of continuum mechanics remain valid everywhere within the body. Let us describe the various assumptions shown experimentally to be valid for brittle materials, on the basis of a two-

**Fig. 1.7** Definition of  $\Gamma_{NL}$  and  $\Gamma_{EL}$ .



dimensional domain containing a singular point. Let  $\mathbf{u}_{NL} = \{u_1, u_2\}_{NL}$  be the displacement vector (in  $x_1$  and  $x_2$  directions) that is the solution to the fully solid mechanics nonlinear problem. It is expected that failure initiation will depend on  $\mathbf{u}_{NL}$ , or some functionals computed from it, in the strongly nonlinear region of the singular point bounded by a boundary  $\Gamma_{NL}$ , as shown in Figure 1.7. This region is called the *process zone*. Let  $\Gamma_{EL}$  be a curve outside of  $\Gamma_{NL}$ , with  $\mathbf{u}_{NL}|_{\Gamma_{EL}}$  the trace of  $\mathbf{u}_{NL}$  on this curve. Denoting the solution of the linear elastic problem by  $\mathbf{u}_{EL}$ , then the following reasonable assumptions hold for brittle materials:

**Assumption 1.1** *Inside of  $\Gamma_{EL}$  the error  $\mathbf{u}_{NL}|_{\Gamma_{EL}} - \mathbf{u}_{EL}|_{\Gamma_{EL}}$  is so small that conclusions based on  $\mathbf{u}_{EL}|_{\Gamma_{EL}}$  are sufficiently close to conclusions based on  $\mathbf{u}_{NL}|_{\Gamma_{NL}}$  for practical purposes.*

This assumption is valid whenever the nonlinear behavior is confined entirely to some small region inside  $\Gamma_{EL}$  (a typical situation for brittle metals and ceramic materials). Assumption 1.1 leads to the important conclusion that failure initiation, which depends on the solution of the nonlinear problem inside of  $\Gamma_{NL}$ , can be determined through a solution of the linear elastic problem, even though all basic assumptions of the linear theory may be violated inside  $\Gamma_{NL}$ . Consequently, failure initiation in the neighborhood of a singular point can be predicted on the basis of the theory of linear elasticity.

**Assumption 1.2** *There exists a physical principle that establishes the relationship between crack initiation and the stress field on the basis of information obtained from the linear solution  $\mathbf{u}_{EL}$  only.*

The theory of linear elastic fracture mechanics, having been used successfully in engineering practice for over half a century, is a typical application of Assumption 1.2, where not the total elastic solution is of interest, but a specific parameter characterizing its behavior in the vicinity of the singular point. In general, the linear solution  $\mathbf{u}_{EL}$  is not known, and only an approximation to it, obtained by finite element methods, for example, and denoted by  $\mathbf{u}_{FE}$  is known. Therefore the following assumption is necessary:

**Assumption 1.3** *There exists a norm  $\|\bullet\|$  such that when  $\|\mathbf{u}_{\text{EL}} - \mathbf{u}_{\text{FE}}\|$  is sufficiently small, then the physical principle of Assumption 1.2 is not sensitive to replacement of  $\mathbf{u}_{\text{EL}}$  with  $\mathbf{u}_{\text{FE}}$ .*

Of course, the specific norm is expected to depend on the physical principle of Assumption 1.2, which is material-dependent.

Based on these assumptions, linear elastic computations can be used for prediction of failure initiation and propagation even though failure processes are nonlinear in nature. There are two essential elements of failure initiation analysis:

1. A hypothesis concerning the relationship between certain parameters of the stress/strain field and observed failure initiation or crack propagation events.
2. Convincing experimental confirmation that the hypothesis holds independently of variations in geometric attributes, loading, and constraints.

It would not be sensible to perform failure initiation analysis unless a detailed understanding of  $\mathbf{u}_{\text{EL}}$  is achieved, and an accurate estimate of  $\mathbf{u}_{\text{FE}}$  is obtained. Thus it is our aim in this book to explore the solution in the vicinity of singularities and its approximation by FE methods.

## 1.3 Layout

The book is divided into fourteen chapters, each containing several sections. The first nine chapters address two-dimensional domains, where only singular *points* exist. Thermoelastic singularities, failure laws and their application for predicting failure initiation in electronic devices are presented in Chapters 7–9. We then proceed to three-dimensional problems addressed in Chapters 10–13. We conclude with circular 3-D edges and remarks on open questions.

In the introduction the notation and problems of interest are presented. We formulate mathematically the problems of heat conduction and linear elasticity in two and three dimensions and present the general functional representation of the singular solutions. Based on the simple Laplace equation, we derive explicitly the singular solution in the vicinity of a reentrant corner. Chapter 2 provides a short introduction to the finite element method (FEM), especially the p-version of the FEM. The singular solutions have a strong impact on the rates of convergence of the finite element approximations: thus these are discussed also. Chapters 3 and 4 are devoted to two-dimensional heat conduction singular solutions. Basic ideas are presented and computation of so-called eigenpairs by the modified Steklov weak formulation is performed in Chapter 3. The modified Steklov weak eigenproblem is derived for a general scalar elliptic equation representing heat conduction in anisotropic domains and multimaterial interfaces. In the case of an isotropic domain, the weak eigenproblem is simplified and corresponds to the Laplace equation, for which the explicit solution has been given in the introduction. In Chapter 4