# Simulation of Quasi-static Crack Propagation in Functionally Graded Materials 

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#### Abstract

In this chapter we present some ideas how quasi-static crack propagation in anisotropic functionally graded materials can be predicted using the Griffith' energy principle for plane problems. From a physical point of view the energy principle, already formulated by Griffith in 1921, can be applied in anisotropic and inhomogeneous materials to compute quasi-static crack propagation: A crack is growing in such a way that the total energy always is minimal. The total energy is composed from the surface energy and the potential energy, the latter is the difference of the elastic energy and the work performed by external forces. In linear-elastic plane structures the change of energy produced by a small elongation of the crack can be calculated asymptotically precise, if the material is homogeneous. Using methods of asymptotic analysis, the change of potential energy can be expressed in terms of the stress intensity factors and certain integral characteristics, depending on the geometry of the (small) crack elongation and the material properties. The main focus of this work is to show if and how these methods can be transferred to functionally graded materials. After presenting theoretical results, we setup a complete quasi-static framework in order to make these ideas applicable for the simulation of practical crack problems and discuss methods to calculate all required quantities numerically. Based on a dual-weighted-residual approach, integral characteristics can be calculated precisely by the finite element method. Finally, we present numerical results.


Key Words: quasi-static crack propagation, functionally graded materials, linear elasticity.

AMS Subject Classification: 65N30, 74B05, 74E05, 75E10, 74R10, 74S05..

## 1. Introduction

The growing application of non-homogeneous and anisotropic materials and especially functionally graded materials (FGMs), in order to fulfill the more and more specialized demands on structural components in modern engineering has given an impulse to the study of fracture mechanics in such structures. Till this day in particular crack propagation is a problem in many areas of aerospace, automotive and marine engineering. Cracks in structural components can be formed by many different influences and even at the production process already. Especially for aspects of safety the essential question is, can a crack be detected and if not, how will the crack grow till the next service? Can it become critical and result a break-down of the component? For means of a reliable fracture mechanical assessment the simulation of crack propagation processes is necessary.

This chapter shows ideas how quasi-static crack propagation in anisotropic functionally graded materials can be predicted using the energy principle for plane problems. FGM especially means, that the

[^0]material shows an inhomogeneous behavior and the elastic properties can change. From a physical point of view the energy principle, already formulated by Griffith in 1921 [Gri21], can be applied in anisotropic and inhomogeneous materials to compute quasi-static crack propagation:

## A crack is growing in such a way that the total energy always is minimal.

The total energy $\Pi$ is composed from the surface energy $\mathbf{S}$ and the potential energy $\mathbf{U}$, the latter is the difference of the elastic energy and the work performed by external forces.

For homogeneous solids composed of anisotropic, linear elastic materials, recent mathematical investigations showed the following [AN02]: Suppose the crack is increased by a (small) crack elongation of length $h$, then the change of the potential energy can be calculated asymptotically to

$$
\begin{equation*}
\Delta \mathbf{U}=-\frac{1}{2} \mathbf{K}^{\top} \cdot \mathbb{M}(h) \cdot \mathbf{K}+\mathcal{O}\left(h^{(N+2) / 2}\right), \quad h \rightarrow 0 . \tag{1}
\end{equation*}
$$

Thereby $\mathbf{K}$ denotes the vector of stress intensity factors (SIFs), $N$ is the number of terms used in the asymptotic decomposition of the displacement field near the crack tip and $\mathbb{M}(h)$ is a symmetric matrix, the so called energy release matrix (ERM). For a straight crack shoot, this formula is also well-known as Irwin-Rice-formula. The ERM contains certain integral characteristics depending on the geometry of the specimen and the crack elongation as well as the elastic properties of the material.

The derivation of formula (1) requires the asymptotic (Westergaard/Williams) decomposition of the displacement field at the crack tip [Wes39], [Wil52]:

$$
u \sim r^{1 / 2}\left(K_{I} \Phi^{1}(\varphi)+K_{I I} \Phi^{2}(\varphi)\right)+\ldots, \quad r \rightarrow 0
$$

The functions $r^{1 / 2} \Phi^{j}$, where $(r, \varphi)$ are plane polar coordinates, are power-law solutions or so-called eigenfunctions of the elasticity problem in the whole plane with a semi-infinite crack. The knowledge of the behavior of the displacement field near the crack tip is essential for the prediction of crack propagation.

In inhomogeneous materials, the structure of the asymptotic decomposition of the displacement field near the crack tip change. Additional so-called "shadow" terms arise from Taylor expansions of the elastic properties at the crack tip. In difference to the case of homogeneous materials, only the first three terms of the asymptotic expansion at the crack tip can be calculated explicitly. From this asymptotic expansion, also for inhomogeneous materials two terms of the expansion of the change of the potential energy can be constructed explicitly using methods of asymptotic analysis. These two terms take into account only the material properties frozen at the crack tip and for orthotropic FGMs this method is known as "local homogenization" and is widely used for FGMs [KP04a], [KP07].

With a representation for the change of potential energy at hand, crack propagation can be simulated approximating the path of the crack by a piece-wise linear polygon. Based in the Griffith' energy principle, the kink angle of these linear crack pieces can be found from the minimum of the total energy. But for determine the length of each crack piece, the question of the speed of the crack and thus time comes into play. Considering only fatigue crack growth and small deformations, a complete quasi-static framework can be build up on the linear elasticity equations for simulating crack propagation in practical applications. Modeling the energy principle with methods of asymptotic based on linear elasticity theory, crack speed can not be calculated from theoretical results and experimental data have to be used.

Considering a solid $\Omega$ composed of a linear elastic inhomogeneous material, the elliptic system of the elasticity equations,

$$
-\nabla \cdot \sigma=f \quad \text { in } \quad \Omega, \quad \sigma \cdot n=g \quad \text { on } \quad \partial \Omega
$$

defines the underlying partial differential equations, which have to be solved numerically, here with the finite element method. In order to calculate the change of energy, one is not interested in solutions of the elasticity system itself, but in certain functionals of numerical solutions, for example stress intensity factors. The precise-as-possible and efficient calculation of these functionals is till this day a numerical challenge. The "Dual-Weighed-Residual" method introduced by Rannacher and his co-workers [BR96] provides the construction of cell-wise error indicators which can be used for error bounds of numerical functional values and adaptive mesh refinement. Based on a solution of a so-called dual or conjugated problem, the numerical error of the functional of interest can be calculated in terms of cell-wise residuals, "weighted" with the dual solution. This method can be used very efficiently to calculate integral characteristics of interest in fracture mechanics.

Overview: This chapter is organized as follows:

In section 1 we introduce notations and a mathematical formulation of the problem. We show basic regularity results for the elasticity equations in usual Sobolev spaces.

In section 2 we give the asymptotic expansion of the displacement field at the crack tip in terms of power-law solutions of the elasticity problem in the whole plane with a semi-infinite crack as shown in [Kon67]. For homogeneous materials we discuss a special normalization of power-law solutions based on strains especially related to energy fracture criterion [Naz05] and give some further properties of this solutions. In the second part of this section we describe, how the asymptotic decomposition change, if the material is inhomogeneous. From expanding the elastic moduli near the crack tip, so-called "shadows" arise, which can be calculated from the power-solutions from the homogeneous case with material properties frozen at the crack tip by a recurrence relation [CD92]. Finally, we proof a formula for the computation of stress intensity factors in FGMs.

In section 3 we introduce the mathematical formulation of the energy principle based on methods of asymptotic analysis. For homogeneous materials, we give a sketch of the construction of an asymptotic decomposition of the change of potential energy and some further results [AN02], [Ste09]. After this, we show how this results can be transferred to inhomogeneous materials and especially the difference to the homogeneous case. The change of potential energy can be calculated in terms of local and global integral characteristics such as stress intensity factors. We show formulae for the practical calculation of all quantities needed for the prediction of crack propagation.

In section 4 we show ideas, how the obtained results can be used for practical applications. We introduce a quasi-static framework for the simulation of crack propagation based on the energy principle and solutions of linear elasticity problems. For numerical calculations we use a finite element approximation scheme and apply the dual-weighted-residual method for calculating numerical functional values for the different integral characteristics of interest.

In section 5 we present some numerical examples. We calculate stress intensity factors, integral characteristics and simulate a crack path in an isotropic material first, in order to compare with results from the literature, and in an anisotropic material, to see the influence of surface energy on the crack path. Finally, we show results for a functionally graded material. All numerical calculations presented in this chapter have been done using the package MCrack2D and the finite element library deal.II [BHK07] coupled with the mesh generator Cubit from Sandia National Laboratories.

### 1.1 The Problem of Elasticity in Functionally Graded Materials

We begin with the formulation of the problem. Let $\Omega$ be a domain in the plane $\mathbb{R}^{2}$ with compact closure $\bar{\Omega}$ and polygonal boundary $\Gamma$. We consider the problem of 2-dimensional linear elasticity theory in the domain $\Omega_{0}:=\Omega \backslash \Xi_{0}$, where $\Xi_{0}:=\left\{x \in \bar{\Omega}: x_{1} \leq 0, x_{2}=0\right\}$ is a rectilinear edge cut (see figure 1 ):

$$
\begin{align*}
-\nabla \cdot \sigma(u ; x)=f(x), & x \in \Omega_{0}, \\
\sigma^{(n)}(u ; x):=\sigma(u ; x) \cdot n(x)=p(x), & x \in \Gamma,  \tag{2}\\
\sigma^{(n)}(u ; x):=\sigma(u ; x) \cdot n(x)=0, & x \in \Xi_{0}^{+} \cup \Xi_{0}^{-} .
\end{align*}
$$

Here, $n=\left(n_{1}, n_{2}\right)^{\top}$ is the outward normal vector, $u=\left(u_{1}, u_{2}\right)^{\top}$ denotes the displacement field, $f=\left(f_{1}, f_{2}\right)^{\top}$ and $p=\left(p_{1}, p_{2}\right)^{\top}$ are the vectors of volume forces and surface loads, respectively, in the form of column vectors ( $T$ means transposition). With $\Xi_{0}^{+}$and $\Xi_{0}^{-}$we denote the upper and lower crack surfaces, considered to be traction-free, the term $u \cdot v=u_{i} v_{i}$ denotes the inner product in the Euclidean space (with sum convention). The coordinate system is centered at the crack tip $x_{0}=(0,0)^{\top}$. The strain tensor (in CARTESIAN coordinates, evaluated for the displacement field, at point $x) \varepsilon_{i j}(u ; x)=\frac{1}{2}\left(\partial_{i} u_{j}(x)+\partial_{j} u_{i}(x)\right), i, j=1,2$, is related to the stress tensor by Hooke's law:

$$
\sigma_{i j}(u ; x)=\sum_{k, l=1,2} a_{i j}^{k l}(x) \varepsilon_{k l}(u ; x), \quad i, j=1,2
$$

The rank- 4 tensor $a=\left(a_{i j}^{k l}\right)_{i, j, k, l=1,2}$ contains the elastic moduli and is symmetric and positive in any point. For the strain tensor, we also use the vector or Voigt notation

$$
\varepsilon(u ; x):=\left(\varepsilon_{11}(u ; x), \varepsilon_{22}(u ; x), \sqrt{2} \varepsilon_{12}(u ; x)\right)^{\top}=\mathscr{D}(\nabla) u(x)
$$

with the $3 \times 2$ matrix differential operator

$$
\mathscr{D}^{\top}(\nabla)=\left(\begin{array}{ccc}
\partial_{x_{1}} & 0 & \frac{1}{\sqrt{2}} \partial_{x_{2}}  \tag{3}\\
0 & \partial_{x_{2}} & \frac{1}{\sqrt{2}} \partial_{x_{1}}
\end{array}\right), \quad \nabla=\left(\partial_{x_{1}}, \partial_{x_{2}}\right), \quad \partial_{x_{j}}=\frac{\partial}{\partial x_{j}}, \quad j=1,2
$$

Then, for the stress tensor (in vector notation) the relation holds

$$
\sigma(u ; x)=A(x) \mathscr{D}(\nabla) u(x)=\left(\sigma_{11}(u ; x), \sigma_{22}(u ; x), \sqrt{2} \sigma_{12}(u ; x)\right)^{\top}
$$

with the matrix function

$$
A(x)=\left(\begin{array}{ccc}
a_{11}(x) & a_{21}(x) & \sqrt{2} a_{31}(x)  \tag{4}\\
a_{21}(x) & a_{22}(x) & \sqrt{2} a_{32}(x) \\
\sqrt{2} a_{31}(x) & \sqrt{2} a_{32}(x) & 2 a_{33}(x)
\end{array}\right)
$$

containing the elastic moduli, symmetric and uniformly positive definite:

$$
\xi^{\top} \cdot A(x) \cdot \xi \geq c_{A}|\xi|^{2} \quad \text { for all } \quad \xi \in \mathbb{R}^{3}, \quad x \in \Omega_{0}
$$

The matrix (function) $A$ is called the mathematical Hooke tensor or Hooke matrix. Because of the symmetry of the HoOke tensor, there are only six different elastic moduli. The factor $\sqrt{2}$ ensures, that strains (and stresses) have the same Euclidean norm, in vector and in tensor notation. We always assume, that $A$ is smooth in any point $x \in \Omega_{0}$ and from a physical point of view it is no restriction to assume, that $A$ is uniformly bounded.

In the following, the vector notation is more convenient to represent formulae, which are really complicated otherwise. With this intention also, we introduce the following notation for the partial differential operators in (2):

$$
\begin{array}{ll}
\mathscr{L}(x, \nabla) u(x):=\mathscr{D}(-\nabla)^{\top} A(x) \mathscr{D}(\nabla) u(x)=-\nabla \cdot \sigma(u ; x), & x \in \Omega_{0} \\
\mathscr{N}(x, \nabla) u(x):=\mathscr{D}(n(x))^{\top} A(x) \mathscr{D}(\nabla) u(x)=\sigma^{(n)}(u ; x), & x \in \partial \Omega_{0}
\end{array}
$$



Figure 1: Elastic solid $\Omega_{0}$ with edge cut $\Xi_{0}$.

### 1.2 Basic Regularity Results and Energy Solutions

We summarize basic existence and uniqueness results for finite energy solutions to problem (2). With $H^{m}(\Omega)$ we denote the usual SobOLEV space of integer order $m$ with the norm

$$
\left\|u ; H^{m}(\Omega)\right\|:=\left(\sum_{k=0}^{m}\left\|\nabla^{k} u ; L^{2}(\Omega)\right\|^{2}\right)^{1 / 2}
$$

here we use the notation

$$
\left\|\nabla^{k} u ; L^{2}(\Omega)\right\|^{2}:=\sum_{|\alpha|=k} \int_{\Omega}\left|\partial^{\alpha} u(x)\right|^{2} d x, \quad \quad \partial^{\alpha}=\frac{\partial^{|\alpha|}}{\partial_{x_{1}}^{\alpha_{1}} \partial_{x_{2}}^{\alpha_{2}}}
$$

where $\alpha$ is a multi-index. The expression $(u, v)_{\Omega}:=\int_{\Omega} u \cdot v d x$ indicates the inner-product of the Lebesgue space $L^{2}(\Omega)$ and $H^{1 / 2}(\partial \Omega)$ denotes the space of traces equipped with the norm

$$
\left\|u ; H^{1 / 2}(\partial \Omega)\right\|:=\inf \left\{\left\|v ; H^{1}(\Omega)\right\|: v \in H^{1}(\Omega) \text { and } u=v \text { on } \partial \Omega\right\}
$$

In our notation, we do not distinguish between scalar and vector-valued functions. The space of rigid motions is defined by

$$
\mathcal{R}:=\left\{\left(c_{1}-c_{0} x_{2}, c_{2}+c_{0} x_{1}\right)^{\top}: c_{q} \in \mathbb{R}\right\}
$$

On a polygonal domain $\Omega_{0}$ with an edge crack $\Xi_{0}$ for fields $u \in H^{2}\left(\Omega_{0}\right)$ and $v \in H^{1}\left(\Omega_{0}\right)$ we have GREEN's formula:

$$
(\mathscr{L} u, v)_{\Omega_{0}}+(\mathscr{N} u, v)_{\partial \Omega_{0}}=a\left(u, v ; \Omega_{0}\right)
$$

with

$$
a\left(u, v ; \Omega_{0}\right):=\int_{\Omega_{0}} \sigma(u ; x): \varepsilon(v ; x) d s=\int_{\Omega_{0}} A(x) \mathscr{D}(\nabla) u(x) \cdot \mathscr{D}(\nabla) v(x) d x .
$$

Note that $\frac{1}{2} a\left(u, v ; \Omega_{0}\right)$ is the elastic energy and the last relation is also known as ClAPEYRON's theorem. If $v \in H^{2}\left(\Omega_{0}\right)$, the second Green's formula (also called Betti identity) follows immediately from the symmetry of the Hooke matrix:

$$
(\mathscr{L} u, v)_{\Omega_{0}}+(\mathscr{N} u, v)_{\partial \Omega_{0}}=(u, \mathscr{L} v)_{\Omega_{0}}+(u, \mathscr{N} v)_{\partial \Omega_{0}} .
$$

We come back to the elasticity problem (2) and impose the following integrability conditions on the load vectors:

$$
f \in L^{2}\left(\Omega_{0}\right), \quad g \in L^{2}\left(\partial \Omega_{0}\right)
$$

together with the necessary compatibility conditions (self-equilibrium of the loading)

$$
\begin{equation*}
\int_{\Omega_{0}} f(x) \cdot v(x) d x+\int_{\partial \Omega_{0}} g(x) \cdot v(x) d s=0 \quad \text { for all } \quad v \in \mathcal{R} \tag{5}
\end{equation*}
$$

For (self-balanced) load vectors $\{f, g\} \in L^{2}\left(\Omega_{0}\right) \times L^{2}\left(\partial \Omega_{0}\right)$ we call $u \in H^{1}\left(\Omega_{0}\right)$ an energy or a weak solution, if $u$ fulfills the variational problem

$$
a\left(u, v ; \Omega_{0}\right)=(f, v)_{\Omega_{0}}+(g, v)_{\partial \Omega_{0}} \quad \text { for all } \quad v \in H^{1}\left(\Omega_{0}\right)
$$

Clearly, because of $\mathcal{R} \subset H^{1}\left(\Omega_{0}\right)$ there holds $a\left(u, v ; \Omega_{0}\right)=0$ for all $u \in H^{1}\left(\Omega_{0}\right)$, if $v \in \mathcal{R}$ and a solution $u$ exists only, if the compatibility conditions (5) are fulfilled. On the other hand, if $a\left(u, v ; \Omega_{0}\right)=0$ for all $v \in H^{1}\left(\Omega_{0}\right)$, then $a\left(u, u ; \Omega_{0}\right)=0$, hence $\varepsilon(u)=0$, which implies $u \in \mathcal{R}$ and thus a weak solution is determined up to a rigid motion only. A weak solution can always be fixed if we look for $u \in H_{\mathcal{R}}\left(\Omega_{0}\right)$, where $H_{\mathcal{R}}\left(\Omega_{0}\right)$ is a complement of the three dimensional space $\mathcal{R}$ in $H^{1}\left(\Omega_{0}\right)$. A choice is

$$
H_{\mathcal{R}}\left(\Omega_{0}\right):=\left\{u \in H^{1}\left(\Omega_{0}\right):(u, v)_{\Omega_{0}}=0 \text { for all } v \in \mathcal{R}\right\}
$$

By Korn's inequality [KO88], there exist a constant $c>0$ with

$$
\left\|\varepsilon(u) ; L^{1}\left(\Omega_{0}\right)\right\| \geq c\left\|u ; H^{1}\left(\Omega_{0}\right)\right\| \quad \text { for all } \quad u \in H_{\mathcal{R}}\left(\Omega_{0}\right)
$$

and the existence of a unique solution in $H_{\mathcal{R}}\left(\Omega_{0}\right)$ follows in a standard way from the Lax-Milgram theorem. Moreover, the following estimate can be verified:

$$
\left\|u ; H^{1}\left(\Omega_{0}\right)\right\| \leq c\left(\left\|f ; L^{2}\left(\Omega_{0}\right)\right\|+\left\|g ; L^{2}\left(\partial \Omega_{0}\right)\right\|\right), \quad c>0
$$

For more details see e.g. [BS02] and [SF07].

## 2. Asymptotic Behavior of the Displacement Field Near the Crack Tip

For the prediction of crack propagation, the behavior of the solid under consideration near the crack tip is of importance. Since the work of Wieghardt [Wie07] the displacement field was approximated near the crack tip by an asymptotic expansion of square-root type

$$
u \sim r^{1 / 2} \sum_{q \in \mathbb{N}} c_{q}(\log (r))^{q} \Phi_{q}(\varphi)
$$

Later, this idea was used by Westergaard [Wes39], Williams [Wil52] and Irwin [Irw57] to formulate a fracture criterion for isotropic linear elastic solids based on the coefficients in the asymptotic expansion. In a fundamental work Kondrat'ev [Kon67] justified the correctness of the asymptotic expansion for weak solutions of elliptic partial differential equations near conical points. Based on this results the nowadays classical Kondrat'ev theory for elliptic problems was expanded to various different problems in singular perturbed domains.
Regularity results for such a type of problems can be obtained in weighted Sobolev spaces. The asymptotic expansion near the perturbed part of the boundary, and especially the number of terms that can be written explicitly, depend on the structure and smoothness of the differential operators and the regularity of the right-hand sides. For more details we refer to the literature of Maz'ya, Plamenevsky, Nazarov e.g. [MNP91] and Grisvard [Gri85].

For homogeneous and inhomogeneous materials the asymptotic decomposition consists of special solutions of the homogeneous elasticity problem with constant material properties in the whole plane with a semi-infinite cut. This so-called eigenfunctions or power-law solutions can be calculated explicitly for isotropic, but only numerically for general anisotropic materials. In order to establish a fracture criterion, a "mechanical" normalization of power-law solutions is needed. In the following, we discuss two possible normalization based on stresses and on strains and show further properties. Because we do not want to discuss regularity results in weighted Sobolev spaces, we always assume, that the volume load $f$ vanishes near the crack tip. In this case, arbitrary many terms in the asymptotic expansion at the crack tip can be written explicitly in homogeneous materials. On the basis of this results we show, how the asymptotic decomposition change and can be calculated, if the material is inhomogeneous.

### 2.1 The Case of Homogeneous Materials

In any anisotropic homogeneous solid, the displacement field $u \in H^{1}\left(\Omega_{0}\right)$ has an asymptotic expansion of well-known square-root type at the crack tip:

$$
\begin{equation*}
u(x)=K_{I} U^{1,1}(x)+K_{I I} U^{2,1}(x)+K_{T} U^{1,2}(x)+k_{1,3} U^{1,3}(x)+k_{2,3} U^{2,3}(x)+\ldots, \quad|x| \rightarrow 0 . \tag{6}
\end{equation*}
$$

The coefficients $K_{I}, K_{I I}$ are called main stress intensity factors (SIFs), $K_{T}$ is the $T$-stress intensity factor and all remaining coefficients are called junior stress intensity factors. As we have seen in the previous section, a weak solution is unique only up to a rigid motion. We can always fix a solution in such a way, that the asymptotic expansion at the crack tip does not contain any rigid motion. This solution is of course unique. The functions

$$
U^{j, k}(x)=r^{k / 2} \Phi^{j, k}(\varphi), \quad j=1,2, \quad k=1,2, \ldots,
$$

where $(r, \varphi)$ are plane polar coordinates, are power-law solutions of the homogeneous elasticity problem in the whole plane with a semi-infinite cut:

$$
\begin{align*}
-\nabla \cdot \sigma\left(U^{j, k} ; x\right) & =0, \\
\sigma_{2 i}\left(U^{j, k} ; x\right) & =0, \tag{7}
\end{align*} \quad x \in \mathbb{R}^{2} \backslash \Xi_{\infty}:=\left\{x: x_{1} \leq 0, x_{2}=0\right\}, \quad i=1,2 .
$$

Power-law solutions, also called generalized eigenfunctions of the elasticity operator, are known explicitly for isotropic materials and some classes of anisotropic ones [SNS08]. In general, they can be computed numerically with arbitrary precision using the approach in [Lek63] (also known as Stroh formalism [Str62], see also [SPI65], [KP07]) or by solving a system of ordinary differential equations [SNS08]).

Groups of power-law solutions and normalization. In accordance with the mechanical interpretation power-law solutions can be divided into four groups. The first group of solutions,

$$
U^{j, 2 m+1}(x)=r^{m+1 / 2} \Phi^{j, 2 m+1}(\varphi), \quad m=0,1, \ldots, \quad j=1,2
$$

possess finite elastic energy in any area around the crack tip, but generate singularities in the stresses or their derivatives at the crack tip. The second group consists of polynomials in the variables $x_{1}$ and $x_{2}$ :

$$
U^{j, 2 m}(x)=r^{m} \Phi^{j, 2 m}(\varphi), \quad m=0,1, \ldots, \quad j=1,2
$$

We see, that the angular parts $\Phi^{j, k}(\varphi)$ of the power-law solutions are not uniquely determined, any linear combination of angular parts leads again to a power-law solution. Using the asymptotic expansion (6) to establish a physical reasonable fracture criterion, a (mechanical) normalization of the powerlaw solutions is necessary. According to the classical definition of stress intensity factors for isotropic materials,

$$
\begin{equation*}
K_{I}=\lim _{x_{1} \rightarrow+0}(2 \pi r)^{1 / 2} \sigma_{2,2}\left(u ; x_{1}, 0\right), \quad K_{I I}=\lim _{x_{1} \rightarrow+0}(2 \pi r)^{1 / 2} \sigma_{1,2}\left(u ; x_{1}, 0\right) \tag{8}
\end{equation*}
$$

a basis of these power-law solutions $U_{\sigma}^{j, k}, k \in 0,1,2, \ldots$, can be chosen according to the normalizing (stress) conditions [GS01]

$$
\begin{aligned}
\sigma_{3-i, 2}\left(U_{\sigma}^{j, 2 m+1} ; x_{1}, 0\right) & =(2 \pi)^{-1 / 2} r^{n-1 / 2} \delta_{i, j}, & & x_{1}>0, \quad m=0,1, \ldots \\
\sigma_{11}\left(U_{\sigma}^{j, 2 m} ; x_{1}, 0\right) & =r^{n-1} \delta_{1, j}, & & x_{1}>0, \quad m=1,2, \ldots \\
\partial_{x_{2}} \sigma_{11}\left(U_{\sigma}^{j, 2 m} ; x_{1}, 0\right) & =-(n-1) r^{n-2} \delta_{2, j}, & & x_{1}>0, \quad m=2,3, \ldots
\end{aligned}
$$

where $i, j=1,2$ and $\delta_{i, j}$ denotes the Kronecker symbol. As proven in [AN02] also for anisotropic materials a basis of eigenfunctions matched to these conditions exists. A normalization adapted especially to energy and deformation fracture criteria is suggested in [Naz05], namely

$$
\begin{array}{rlr}
\frac{1}{2}\left[U_{\varepsilon, i}^{j, 2 m+1}\right]\left(-x_{1}\right) & =4(2 \pi)^{-1 / 2}\left(A^{-1}\right)_{11} r^{m+1 / 2} \delta_{3-i, j},  \tag{9}\\
U_{\varepsilon, i}^{j, 2 m}\left(x_{1}, 0\right) & =r^{m} \delta_{i, j}
\end{array}
$$

$i, j=1,2, m=0,1,2, \ldots$, where $[u]\left(x_{1}\right)=u\left(x_{1},+0\right)-u\left(x_{1},-0\right), x_{1}<0$, is the jump over the crack faces. Here, $A^{-1}$ denotes the compliance matrix hence $\left(A^{-1}\right)_{11}=2\left(a_{22} a_{33}-a_{32}^{2}\right) / \operatorname{det}(A)$. A basis adapted to (9) is called deformation or strain basis. But what does this normalization mean from a mechanical point of view? If we look at the asymptotic expansion at the crack tip

$$
u(x)=K_{I} U_{\varepsilon}^{1,1}(x)+K_{I I} U_{\varepsilon}^{2,1}(x)+\ldots, \quad|x| \rightarrow 0
$$

the jump of the displacement field over the crack near the tip can be calculated to

$$
[u]\left(-x_{1}\right)=\frac{8}{\sqrt{2 \pi}}\left(A^{-1}\right)_{11} r^{1 / 2}\left(K_{I}\binom{0}{1}+K_{I I}\binom{1}{0}\right)+\ldots, \quad|x| \rightarrow 0
$$

Defining the "strain" intensity factors by the limit

$$
\begin{equation*}
K_{I}=\frac{\sqrt{2 \pi}}{8}\left(A^{-1}\right)_{11} \lim _{x_{1} \rightarrow-0} r^{-1 / 2}\left[u_{2}\right]\left(x_{1}\right), \quad K_{I I}=\frac{\sqrt{2 \pi}}{8}\left(A^{-1}\right)_{11} \lim _{x_{1} \rightarrow-0} r^{-1 / 2}\left[u_{1}\right]\left(x_{1}\right) \tag{10}
\end{equation*}
$$

we see that $K_{I}$ and $K_{I I}$ are related directly to opening (Mode I) and sliding (Mode II) of the crack.
The connection between the strain basis and the classical stress basis is given by the following equation [Naz05]:

$$
U_{\sigma}^{j, k}(x)=T_{1, j}^{k} U_{\varepsilon}^{1, k}(x)+T_{2, j}^{k} U_{\varepsilon}^{2, k}(x), \quad j=1,2, \quad k=0,1,2, \ldots,
$$

where $T \in \mathbb{R}^{2 \times 2}$ is a matrix, which can be calculated exactly for isotropic materials to

$$
T^{k}=\left(\begin{array}{cc}
(-1)^{m}(2 m+1)^{-1} & 0 \\
0 & (-1)^{m}(2 m+1)^{-1}
\end{array}\right), \quad k=2 m+1 .
$$

For isotropic materials the normalizing factor is chosen in such a way, that the first basis functions coincide: $U_{\sigma}^{j, 1}=U_{\varepsilon}^{j, 1}, j=1,2$, but they differ for general anisotropic materials. In any case, the coefficients (SIFs) are related to the equation

$$
K_{I}^{\varepsilon}=K_{I}^{\sigma} T_{1,1}^{1}+K_{I I}^{\sigma} T_{1,2}^{1}, \quad K_{I I}^{\varepsilon}=K_{I}^{\sigma} T_{2,1}^{1}+K_{I I}^{\sigma} T_{2,2}^{1}
$$

Besides energy power-law solutions, there exist two groups consisting of singular solutions to problem (7):

$$
\begin{aligned}
V^{j, 2 m+1}(x) & =r^{-m-1 / 2} \Psi^{j, 2 m+1}(\varphi), \quad m=0,1, \ldots, \quad j=1,2, \\
V^{j, 0}(x) & =\psi^{j, 0}(\varphi) \log (r)+\Psi^{j, 0}(\varphi), \\
V^{j, 2 m}(x) & =r^{-m} \Psi^{j, 2 m}(\varphi), \quad m=1,2, \ldots, \quad j=1,2 .
\end{aligned}
$$

These power-law solutions generate forces that are concentrated at the crack tip with infinite elastic energy. They can be normalized using path-independent integrals:

$$
\begin{equation*}
\int_{\gamma}\left(\sigma^{(n)}\left(U^{j, k}\right) \cdot V^{i, l}-\sigma^{(n)}\left(V^{i, l}\right) \cdot U^{j, k}\right) d s=\delta_{i, j} \delta_{k, l} \tag{11}
\end{equation*}
$$

for $i, j=1,2, k, l=1,2, \ldots$ (see e.g. [NP96]), where $\gamma$ is any simple closed curve around the crack tip, connecting the crack faces $\Xi_{\infty}^{ \pm}$. We remark, that the functions $V^{i, l}$ depend on the normalization of the functions $U^{j, k}$.
Depending on the normalization, power-law solutions have different useful properties. For example, differentiation of a power-law solution along the crack is again a power-law solution and for the strain basis we have [AN02]

$$
\begin{equation*}
\partial_{x_{1}} U^{j, 2 m+2}(x)=(m+1) U^{j, 2 m}(x), \quad \quad \partial_{x_{1}} U^{j, 2 m+3}(x)=\left(m+\frac{3}{2}\right) U^{j, 2 m+1}(x) \tag{12}
\end{equation*}
$$

for $j=1,2, m=0,1,2, \ldots$. An equivalent relation holds for the groups of singular power-law solutions:

$$
\partial_{x_{1}} V^{j, k}(x)=-\frac{k}{2} V^{j, k+2}(x), \quad k=0,1,2, \ldots,
$$

and also for "passing down" from energy to singular solutions by differentiation:

$$
-\partial_{x_{1}} U^{j, 1}(x)=M_{j, 1} V^{1,1}(x)+M_{j, 2} V^{2,1}(x), \quad j=1,2 .
$$

As proven in [Naz05], the first components of the first element of the strain basis are even and odd functions with respect to the crack:

$$
U_{1}^{1,1}\left(x_{1}, \pm 0\right)=0, \quad U_{1}^{2,1}\left(x_{1}+0\right)=-U_{1}^{2,1}\left(x_{1},-0\right), \quad x_{1}<0,
$$

and there holds

$$
\partial_{x_{2}} U^{1,1}(x)=-\partial_{x_{1}} U^{2,1}(x)
$$

In the following, we always assume that the power-law solutions are subjected to the strain normalization conditions (9) and (11). If the volume load $f$ vanishes near the crack tip, in homogeneous solids the SIFs defined in (10) can be calculated using singular power-law solutions (see e.g. [Bue70], [MP77]):

$$
\begin{equation*}
K_{j, k}=\int_{\gamma} \sigma^{(n)}(u) \cdot V^{j, k} d s-\int_{\gamma} u \cdot \sigma^{(n)}\left(V^{j, k}\right) d s, \quad j=1,2, \quad k=0,1,2, \ldots \tag{13}
\end{equation*}
$$

We also use the notation $K_{j, k}$ for the SIF corresponding to the power-law solution $U^{j, k}$ in expansion (6). Formula (13) can be derived from the normalization property (11) and we will show the idea in paragraph 2.3 generalized to functional graded materials.

We close this section with a comment on the calculation of power-law solutions. As mentioned, this kind of solutions of the elasticity problem can be calculated numerically with arbitrary precision by various methods. But only for isotropic materials all groups of power-law solutions can be found explicitly [NP96]. Up to now (to the best knowledge of the author) this is not possible for general anisotropic materials. Using the idea of algebraic equivalent materials, for some classes of anisotropic materials all power-law solutions are given explicitly in closed form in [SNS08]. Nevertheless, we can calculate the polynomial eigenfunctions using the properties of the strain basis. From the normalizing condition

$$
U_{i}^{j, 2 m}\left(x_{1}, 0\right)=r^{m} \Phi_{i}^{j, 2 m}(0)=\delta_{i, j}, \quad i, j=1,2, \quad m=0,1, \ldots
$$

we find (rigid motions)

$$
U^{1,0}(x)=\binom{1}{0}, \quad \quad U^{2,0}(x)=\binom{0}{1}
$$

Using the relation (12) we can calculate the power-law solution of order $2 m=1$ by integration, moreover, by the special structure of this functions we have

$$
U^{1,2}(x)=\binom{x_{1}}{0}+x_{2}\binom{c_{1}}{c_{2}}, \quad U^{2,2}(x)=\binom{0}{x_{1}}+x_{2}\binom{c_{3}}{c_{4}}
$$

The constants $c_{q}$ can be found from the equations

$$
-\nabla \cdot \sigma\left(U^{j, 2} ; x\right)=0, \quad x \in \mathbb{R}^{2} \backslash \Xi_{\infty}, \quad \sigma_{2 i}\left(U^{j, 2} ; x\right)=0, \quad x \in \Xi_{\infty}, \quad i, j=1,2
$$

to

$$
\binom{c_{1}}{c_{2}}=\frac{1}{a_{22} a_{33}-a_{32}^{2}}\binom{a_{21} a_{32}-a_{22} a_{31}}{a_{31} a_{32}-a_{21} a_{33}}, \quad\binom{c_{3}}{c_{4}}=\binom{-1}{0}
$$

As we expect, $U^{2,2}$ is a rotation. This argument can be iterated to find all polynomials explicitly [Ste09]. The same procedure also works for power-law solutions of square root type, but we need a solution to start the iteration and such a solution is not known explicitly up to now for general anisotropic materials.

### 2.2 The Case of Inhomogeneous Materials

We assume, that the Hooke matrix depends smoothly on the space coordinates and is bounded in the whole domain $\Omega_{0}$. We do not consider the case of discontinuous material properties as in composite materials or laminates. We only want to remark, that the asymptotic structure will change more significantly, if the elastic moduli are not continuous, this case is not included in the following considerations.

From the general Kondrat'ev theory [Kon67] it is known, that a solution of an elliptic problem as the elasticity equations can be decomposed near a crack tip in terms of solutions of the homogeneous problem in the whole plane with a semi-infinite cut:

$$
\mathscr{L}(x, \nabla) \mathscr{U}(x)=0, \quad \mathbb{R}^{2} \backslash \Xi_{\infty}^{ \pm}, \quad \mathscr{N}(x, \nabla) \mathscr{U}(x)=0, \quad x \in \Xi_{\infty}^{ \pm}
$$

This decomposition at the crack tip depends on the structure of the differential operators as well as on the smoothness of their coefficients. If the coefficients are constant and the operators do not contain derivatives of other order then two, the asymptotic decomposition is explicitly known, this we have seen in (6). If the coefficients are smooth but non-constant or if the differential operators contain lower order derivatives the structure of the asymptotic expansion change. In both cases additional so-called "shadow terms" can arise from the TAYLOR expansions of the coefficients near the crack tip. Except the order of decay near the crack tip, the structure of this additional terms is not known explicitly.
We remark that in the case of smooth and bounded coefficients the operators $\{\mathscr{L}, \mathscr{N}\}$ are $\delta$-admissible with $\delta=1$ [KMR97] and from general results it is known, that only the first two terms in the asymptotic decomposition can be calculated explicitly. For the elasticity problem, we will see this from direct calculations.

In the following, we use the more convenient operator notation. If the HoOKE matrix depends on the space variable $x$, we can decompose the operator $\mathscr{L}$ into two homogeneous operators with non-constant coefficients, of order one and two, respectively:

$$
\begin{align*}
& \mathscr{L}(x, \nabla)=\mathscr{D}(-\nabla) A(x) \mathscr{D}(\nabla)=\mathscr{L}_{2}(x, \nabla)+\mathscr{L}_{1}(x, \nabla)  \tag{14}\\
& \mathscr{N}(x, \nabla)=\mathscr{D}(n(x)) A(x) \mathscr{D}(\nabla) . \tag{15}
\end{align*}
$$

We introduce the notation

$$
\begin{equation*}
\mathscr{L}_{k}(x, \nabla)=\sum_{|\alpha|=k} l_{\alpha}(x) \partial_{x}^{\alpha}, \quad k=1,2 \tag{16}
\end{equation*}
$$

where the operator of order two is given by

$$
\begin{equation*}
\mathscr{L}_{2}(x, \nabla)=-\left(l_{20}(x) \partial_{x_{1} x_{1}}^{2}+l_{11}(x) \partial_{x_{1} x_{2}}^{2}+l_{02}(x) \partial_{x_{2} x_{2}}^{2}\right) \tag{17}
\end{equation*}
$$

with the matrix functions

$$
\begin{gathered}
l_{20}(x)=\left(\begin{array}{cc}
a_{11}(x) & a_{31}(x) \\
a_{31}(x) & a_{33}(x)
\end{array}\right), \\
l_{02}(x)=\left(\begin{array}{cc}
a_{33}(x) & a_{32}(x) \\
a_{32}(x) & a_{22}(x)
\end{array}\right), \\
l_{11}(x)=\left(\begin{array}{cc}
2 a_{31}(x) & a_{21}(x)+a_{33}(x) \\
a_{21}(x)+a_{33}(x) & 2 a_{32}(x)
\end{array}\right)
\end{gathered}
$$

The operator of order one can be presented as

$$
\mathscr{L}_{1}(x, \nabla)=-\left(l_{10}(x) \partial_{x_{1}}+l_{01}(x) \partial_{x_{2}}\right)
$$

with

$$
\begin{aligned}
& l_{10}(x)=\left(\begin{array}{ll}
\partial_{x_{1}} a_{11}(x)+\partial_{x_{2}} a_{31}(x) & \partial_{x_{1}} a_{31}(x)+\partial_{x_{2}} a_{33}(x) \\
\partial_{x_{1}} a_{31}(x)+\partial_{x_{2}} a_{21}(x) & \partial_{x_{1}} a_{33}(x)+\partial_{x_{2}} a_{32}(x)
\end{array}\right), \\
& l_{01}(x)=\left(\begin{array}{ll}
\partial_{x_{1}} a_{31}(x)+\partial_{x_{2}} a_{33}(x) & \partial_{x_{1}} a_{21}(x)+\partial_{x_{2}} a_{32}(x) \\
\partial_{x_{1}} a_{33}(x)+\partial_{x_{2}} a_{32}(x) & \partial_{x_{1}} a_{32}(x)+\partial_{x_{2}} a_{22}(x)
\end{array}\right) .
\end{aligned}
$$

Normal stresses on the crack surfaces $\Xi_{\infty}^{+}$and $\Xi_{\infty}^{-}$are given by

$$
\left.\mathscr{N}(x, \nabla)\right|_{\Xi \pm} ^{ \pm}=\mathscr{D}\left(\mp \mathbf{e}_{2}\right)^{\top} A(x) \mathscr{D}(\nabla)=\mp b_{10}(x) \partial_{x_{1}} \mp b_{01}(x) \partial_{x_{2}}
$$

with $\mathbf{e}_{2}=(0,1)^{\top}$ and the coefficient matrices

$$
b_{10}(x)=\left(\begin{array}{cc}
a_{31}(x) & a_{33}(x) \\
a_{21}(x) & a_{32}(x)
\end{array}\right), \quad \quad b_{01}(x)=\left(\begin{array}{cc}
a_{33}(x) & a_{32}(x) \\
a_{32}(x) & a_{22}(x)
\end{array}\right)
$$

As in the case of homogeneous materials, we look for solutions of the elasticity problem in the whole plane with a semi-infinite crack with zero right-hand sides:

$$
\mathscr{L}(x, \nabla) \mathscr{U}(x)=0, \quad \mathbb{R}^{2} \backslash \Xi_{\infty}^{ \pm}, \quad \mathscr{N}(x, \nabla) \mathscr{U}(x)=0, \quad x \in \Xi_{\infty}^{ \pm}
$$

Solutions of this problem are perturbations of the ones from the case with constant coefficients frozen at the crack tip [Kon67], [NP94]. They have asymptotic expansions of the form [CD92]

$$
\mathscr{U} \sim \sum_{p=0}^{\infty} U_{p}, \quad U_{p}=r^{\lambda+p} \sum_{q=0}^{Q}(\log (r))^{q} \Phi_{q}(\varphi), \quad Q \in \mathbb{N}
$$

with smooth functions $\Phi_{q}$. In order to describe these expansions more precisely, we expand the coefficients of the operators $\{\mathscr{L}, \mathscr{N}\}$ at the crack tip $x_{0}$ into a TAYLOR series:

$$
\mathscr{L}=\mathscr{L}^{(0)}+\mathscr{L}^{(1)}+\mathscr{L}^{(2)}+\ldots, \quad \quad \mathscr{N}=\mathscr{N}^{(0)}+\mathscr{N}^{(1)}+\mathscr{N}^{(2)}+\ldots
$$

If the coefficients are smooth and bounded, asymptotically there holds [CD92]

$$
\{\mathscr{L}, \mathscr{N}\} \mathscr{U} \sim \sum_{q=0}^{\infty}\left\{\mathscr{L}^{(q)}, \mathscr{N}^{(q)}\right\} \mathscr{U}, \quad|x| \rightarrow 0
$$

with

$$
\begin{align*}
& \mathscr{L}^{(0)}(\nabla)=\mathscr{L}_{2}^{(0)}(\nabla), \\
& \mathscr{L}^{(1)}(\nabla)=\mathscr{L}_{2}^{(1)}(\nabla)+\mathscr{L}_{1}^{(0)}(\nabla),  \tag{18}\\
& \mathscr{L}^{(2)}(\nabla)=\mathscr{L}_{2}^{(2)}(\nabla)+\mathscr{L}_{1}^{(1)}(\nabla), \quad \ldots
\end{align*}
$$

The operators are given by

$$
\begin{equation*}
\mathscr{L}_{k}^{(q)}(\nabla)=\sum_{|\beta|=q} \sum_{|\alpha|=k} \frac{x^{\beta}}{\beta!} \partial_{x}^{\beta} l_{\alpha}\left(x_{0}\right) \partial_{x}^{\alpha}, \quad \quad \mathscr{N}^{(q)}(\nabla)=\sum_{|\beta|=q} \sum_{|\alpha|=1} \frac{x^{\beta}}{\beta!} \partial_{x}^{\beta} b_{\alpha}\left(x_{0}\right) \partial_{x}^{\alpha} \tag{19}
\end{equation*}
$$

Beginning with a solution $U_{0}$ of the problem with constant coefficients frozen at the crack tip $x_{0}$, the functions $U_{p}$ can be found in terms of CAUCHY integrals from the recurrence relation [CD92]

$$
\begin{equation*}
\left\{\mathscr{L}^{(0)}, \mathscr{N}^{(0)}\right\} U_{p}=-\sum_{q=0}^{p-1}\left\{\mathscr{L}^{(p-q)}, \mathscr{N}^{(p-q)}\right\} U_{q} \tag{20}
\end{equation*}
$$

Solutions of the problem

$$
\mathscr{L}^{(0)}(\nabla) U_{0}(x)=0, \quad \mathbb{R}^{2} \backslash \Xi_{\infty}^{ \pm}, \quad \mathscr{N}^{(0)}(\nabla) U_{0}(x)=0, \quad x \in \Xi_{\infty}^{ \pm}
$$

with constant coefficients frozen at the crack tip are the power-law solutions $U_{0}^{j, k}=r^{k / 2} \Phi_{0}^{j, k}(\varphi)$ discussed in the previous section. From (20) we see, that the next functions have the form

$$
U_{p}^{j, k}(x)=r^{k / 2+p} \Phi_{p}^{j, k}(\log (r), \varphi), \quad k=1,2,3, \ldots
$$

The asymptotic expansion at the crack tip can be written as

$$
\begin{align*}
u(x)= & K_{I}\left(U_{0}^{1,1}(x)+U_{1}^{1,1}(x)+U_{2}^{1,1}(x)+\ldots\right) \\
& +K_{I I}\left(U_{0}^{2,1}(x)+U_{1}^{2,1}(x)+U_{2}^{2,1}(x)+\ldots\right)+K_{T}\left(U_{0}^{1,2}(x)+U_{1}^{1,2}(x)+\ldots\right)  \tag{21}\\
& +k_{1,3}\left(U_{0}^{1,3}(x)+U_{1}^{1,3}(x)+\ldots\right)+k_{2,3}\left(U_{0}^{2,3}(x)+U_{2}^{2,3}(x)+\ldots\right) \\
= & K_{I} U_{0}^{1,1}(x)+K_{I I} U_{0}^{2,1}(x)+K_{T} U_{0}^{1,2}(x) \\
& +\left(K_{I} U_{1}^{1,1}(x)+K_{I I} U_{1}^{2,1}(x)+k_{1,3} U_{0}^{1,3}(x)+k_{2,3} U_{0}^{2,3}(x)\right)+\ldots, \quad|x| \rightarrow 0 \tag{22}
\end{align*}
$$

with

$$
\left(K_{I} U_{1}^{1,1}(x)+K_{I I} U_{1}^{2,1}(x)+k_{1,3} U_{0}^{1,3}(x)+k_{2,3} U_{0}^{2,3}(x)\right) \sim r^{3 / 2} \Phi(\log (r), \varphi), \quad r \rightarrow 0
$$

where $\Phi$ is a polynomial of $\log (r)$ with smooth coefficients in the variable $\varphi$. But here is a difference to the case of homogeneous materials. We do not have any more information about the structure of the shadows and especially we can not calculate higher order stress intensity factors $k_{13}, k_{23}, k_{14}, \ldots$ There is no information about normalization. The first terms are the solutions of the homogeneous problem with coefficients frozen at the crack tip. We will see in the next section, how we can calculate the first SIFs $K_{I}, K_{I I}, K_{T}$, but not any other of the coefficients $k_{1,3}, k_{2,3}, \ldots$.

### 2.3 Calculation of Stress Intensity Factors

Especially for practical applications, we need a method to calculate SIFs in FGMs. We assume that the crack tip is the origin $x_{0}=(0,0)^{\top}$ and in order to simplify notations we always consider indices $j=1,2$ and $k=1,2$ with $(j, k) \neq(2,2)$. Let $G \subset \Omega$ be an arbitrary small polygonal domain with the crack tip inside and $G_{0}:=\Omega_{0} \cap G$ (figure 2). With

$$
\begin{equation*}
V_{0}^{1,1}=r^{-1 / 2} \Psi_{0}^{1,1}(\varphi), \quad V_{0}^{2,1}=r^{-1 / 2} \Psi_{0}^{2,1}(\varphi), \quad V_{0}^{1,2}=r^{-1} \Psi_{0}^{1,2}(\varphi) \tag{23}
\end{equation*}
$$

we denote the singular power-law solutions related to the elasticity problem (7) with constant Hooke matrix $A\left(x_{0}\right)$. Then the following integral representation for the stress intensity factors holds:

$$
\begin{equation*}
K_{j, k}=\int_{\partial G_{0}}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s+\int_{G_{0}}\left(f \cdot V_{0}^{j, k}-u \cdot \mathscr{L} V_{0}^{j, k}\right) d x \tag{24}
\end{equation*}
$$

where $u$ is the displacement field of $\Omega_{0}$. This formula is an extension of the (classical) representation (13) to FGMs and can be easily adapted also to more complicated geometries and especially kinked cracks with obvious changes.
Formula (24) is only valid for such domains $G$, that the part of the crack inside of $G$ is a straight line. This is based on the following fact. At least one component of the power-law solutions $V_{0}^{j, k}$ has a jump over the semi-infinite crack $\Xi_{\infty}$. Therefore, if the line $\left\{x \in G: x_{1} \leq 0, x_{2}=0\right\}$ is not part of the boundary, applying Green's formula and especially the operator $\mathscr{L}$ on $V_{0}^{j, k}$ will cause a delta distribution. If the crack is not straight, one has to choose a suitable domain $G$ or one has to introduce cut-off functions.

Justification. In order to justify (24), we cut out a circle of radius $0<\varepsilon \ll 1$ around the crack tip and apply Clapeyron's theorem in the domain $G(\varepsilon):=G_{0} \backslash\{x:|x| \leq \varepsilon\}$ :

$$
\int_{G(\varepsilon)} \mathscr{L} u \cdot V_{0}^{j, k} d x+\int_{\partial G(\varepsilon)} \mathscr{N} u \cdot V_{0}^{j, k} d s=\int_{G(\varepsilon)} u \cdot \mathscr{L} V_{0}^{j, k} d x+\int_{\partial G(\varepsilon)} u \cdot \mathscr{N} V_{0}^{j, k} d s
$$

Rearranging both sides, we find

$$
\begin{aligned}
\int_{\gamma_{\varepsilon}}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s & =\sum_{ \pm} \int_{\Xi^{ \pm}(\varepsilon)}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s \\
& +\int_{G(\varepsilon)}\left(\mathscr{L} u \cdot V_{0}^{j, k}-u \cdot \mathscr{L} V_{0}^{j, k}\right) d x+\int_{\partial G}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s .
\end{aligned}
$$

Here, $\Xi^{ \pm}(\varepsilon)$ are the parts of the crack faces inside of $G(\varepsilon)$ and $\gamma_{\varepsilon}=\{x:|x|=\varepsilon\}$ is the inner part of the boundary of $G(\varepsilon)$ (figure 2). To evaluate the integrals on the left, we use the Taylor expansion of the elasticity operator (18), (19) at the crack tip,

$$
\mathscr{L}=\mathscr{L}^{(0)}+\mathscr{L}^{(1)}+\ldots, \quad \mathscr{N}=\mathscr{N}^{(0)}+\mathscr{N}^{(1)}+\ldots, \quad|x| \rightarrow 0
$$

and for $\varepsilon$ small enough, we can use the asymptotic expansion of the displacement field:

$$
\begin{aligned}
& \int_{\gamma_{\varepsilon}}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s \\
&=\sum_{q \in \mathbb{N}_{0}} \sum_{i, l=1,2} K_{i, l}\left(\int_{\gamma_{\varepsilon}}\left(\mathscr{N}^{(q)} U_{0}^{i, l} \cdot V_{0}^{j, k}-U_{0}^{i, l} \cdot \mathscr{N}^{(q)} V_{0}^{j, k}\right) d s\right)+\mathcal{O}\left(\varepsilon^{1 / 2}\right) .
\end{aligned}
$$

Taking into account the properties (11) of singular power-law solutions, the first summand in the last expression simplifies to

$$
\sum_{i, l=1,2} K_{i, l}\left(\int_{\gamma_{\varepsilon}}\left(\mathscr{N}^{(0)} U_{0}^{i, l} \cdot V_{0}^{j, k}-U_{0}^{i, l} \cdot \mathscr{N}^{(0)} V_{0}^{j, k}\right) d s\right)=\sum_{i, l=1,2} K_{i, l} \delta_{i, j} \delta_{k, l}=K_{j, k} .
$$

Using the representation (18) and transforming into polar coordinates, we find for $q \geq 1$ :

$$
\begin{aligned}
\int_{\gamma_{\varepsilon}}\left(\mathscr{N}^{(q)} U_{0}^{i, l}\right. & \left.\cdot V_{0}^{j, k}-U_{0}^{i, l} \cdot \mathscr{N}^{(q)} V_{0}^{j, k}\right) d s \\
& =\left.\sum_{|\beta|=q|\alpha|=1} \sum_{x} \frac{\partial_{x}^{\beta} b_{\alpha}\left(x_{0}\right)}{\beta!} \int_{-\pi}^{\pi}\left(\widetilde{\Phi}_{\alpha}^{i, l}(\varphi) \cdot \Psi_{0}^{j, k}(\varphi)-\Phi_{0}^{i, l}(\varphi) \cdot \widetilde{\Psi}_{\alpha}^{j, k}(\varphi)\right) r^{q}\right|_{r=\varepsilon} d \varphi=\mathcal{O}\left(\varepsilon^{q}\right) .
\end{aligned}
$$



Figure 2: Domain $G$ around the crack tip.

Note that the Hooke matrix is considered to be smooth and bounded. All derivatives of order $|\alpha|$ of $\Phi_{0}^{i, l}$ and $\Psi_{0}^{j, k}$ rewritten in polar coordinates are collected in the terms $\widetilde{\Phi}_{\alpha}^{i, l}$ and $\widetilde{\Psi}_{\alpha}^{j, k}$. Because of $\mathscr{L}^{(0)} V_{0}^{j, k}=0$, similar calculations show

$$
\int_{\{x:|x|<\varepsilon\}} u \cdot \mathscr{L} V_{0}^{j, k} d x=\mathcal{O}(\varepsilon) .
$$

If we assume, that the volume force $f$ vanishes near the crack tip, we also find

$$
\int_{\{x:|x|<\varepsilon\}} f \cdot V_{0}^{j, k} d x=\mathcal{O}(\varepsilon)
$$

Because the part of the crack in $G$ is a linear polygonal, the integrals over the crack faces can be calculated to

$$
\sum_{i=1}^{2}\left(\int_{-\varepsilon}^{0} u_{i}\left(x_{1}, \pm 0\right) \sigma_{2 i}\left(V_{0}^{j, k} ; x_{1}, \pm 0\right) d x_{1}\right)=\mathcal{O}\left(\varepsilon^{1 / 2}\right)
$$

Taking into account the relations in (2), we finally get

$$
K_{j, k}=\int_{\partial G_{0}}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s+\int_{G_{0}}\left(f \cdot V_{0}^{j, k}-u \cdot \mathscr{L} V_{0}^{j, k}\right) d x+\mathcal{O}\left(\varepsilon^{1 / 2}\right)
$$

Sending $\varepsilon \rightarrow 0$ completes the proof of (24).

From the main idea of the proof of the integral representation we can see immediately, why higher-order SIFs in (21) can not be calculated this way. For example, calculating $k_{1,5}$ integrals over the singular power-law solution $V_{0}^{1,5} \sim r^{-5 / 2}$ and $U_{1}^{1,1} \sim r^{3 / 2}$ arise:

$$
\int_{\gamma_{\varepsilon}}\left(\mathscr{N}^{(0)} U_{1}^{1,1} \cdot V_{0}^{1,5}-U_{1}^{1,1} \cdot \mathscr{N}^{(0)} V_{0}^{1,5}\right) d s \sim \varepsilon^{-1}
$$

this integral is not finite for $\varepsilon \rightarrow 0$. In the case of homogeneous materials the normalization condition (11) ensures, that integrals of the type

$$
\int_{\gamma_{\varepsilon}}\left(\mathscr{N}^{(0)} U^{j, k} \cdot V^{i, l}-U^{j, k} \cdot \mathscr{N}^{(0)} V^{i, l}\right) d s
$$

vanish for any $\varepsilon>0$ if $i \neq j$ or $k \neq l$. For shadow terms we do not have such a normalization condition.

## 3. Fracture Criterion - the Energy Principle

In this section we show ideas, how quasi-static crack propagation can be modeled using methods of asymptotic analysis. Based on the equations of linear elasticity the displacement field (and stresses) of the solid under volume and surface loads can be calculated. But the displacement field itself does not provide direct information about crack propagation. The displacement field is continuous and the boundary of the solid is mapped to (displaced) boundary, no new crack surface is formed. For the prediction of crack propagates an additional fracture criterion is needed.

It is a practical experience, that a specimen under simple loading with a crack will either collapse or not. Especially in metals there can occur large plastic deformations before a specimen finally breaks down. The final breaking of a solid is to fast, no calculations are possible and at this point, of course simulations are not needed anymore. Quasi-static crack propagation describes another phenomenon. Consider a specimen under cyclic loading, not high enough to break down the solid in one step, the material will fatigue with increasing number of load cycles and the crack can start to propagate. In such scenarios, also in metals, the zone of plastic deformation at the crack tip is small and in a first step the material can be assumed to be linearly elastic. The region where the displacement field can be described by an asymptotic expansion as in (6) is much larger then the zone of plastic deformation.

From a physical point of view, the energy principle can be used to calculate quasi-static crack propagation, also in anisotropic and inhomogeneous materials. As already formulated, a crack is growing in such a way, that the total energy is always minimal [Gri24]. A crack can only propagate, if energy is released. The total energy $\Pi$ is the sum of the surface energy $\mathbf{S}$ (also called fracture toughness) and the potential energy $\mathbf{U}$ :

$$
\Pi=\mathbf{S}+\mathbf{U}=\mathbf{S}+\frac{1}{2} \int_{\Omega_{0}} \sigma_{i j}(u) \varepsilon_{i j}(u) d x-\int_{\Gamma} p \cdot u d s=\mathbf{S}-\frac{1}{2} \int_{\Gamma} p \cdot u d s
$$

Here, we use the sum convention, the last equation follows from Clapeyron's theorem.

Asymptotic Analysis. First, we need a mathematical formulation for a growing crack. Let $u^{h}$ be the displacement field to problem (2) in the solid $\Omega_{h}$, where the crack has propagated along a small elongation $\Upsilon_{h}$ of (small) length $0<h<h_{0} \ll 1$. For practical (numerical) applications it is no restriction to suppose that $\Upsilon_{h}$ is a linear polygon, starting from the tip of the crack $\Xi_{0}$ directed at an angle $\theta \in(-\pi, \pi)$ (see figure 3 ):

$$
\Upsilon_{h}(\theta):=\left\{x \in \Omega: 0 \leq x_{1} \leq h \cos (\theta), x_{2}=x_{1} \tan (\theta)\right\}
$$



Figure 3: Linear crack elongation.

The elongated crack is denoted by $\Xi_{h}:=\Xi_{0} \cup \Upsilon_{h}$ and $\Omega_{h}:=\Omega_{0} \backslash \Xi_{h}$. In the case of small deformations, we can assume that the outer part of the boundary $\Gamma$ is not highly deformed and for simplicity we
assume, that $\Gamma^{h}=\Gamma$ for all $h \geq 0$. The new part of the crack is also assumed to be traction-free and we define

$$
\left.g^{h}\right|_{\Gamma}:=p,\left.\quad \quad g^{h}\right|_{\Xi_{h}}:=0, \quad h \geq 0
$$

The total energy $\Pi$ in $\Omega_{h}$ with respect to $u^{h}$ and the loading $F^{h}:=\left\{f, g^{h}\right\}$ is defined as

$$
\Pi\left(\Omega_{h}, u^{h}, F^{h}\right):=\mathbf{U}\left(\Omega_{h}, u^{h}, F^{h}\right)+\mathbf{S}\left(\Omega_{h}\right)=\mathbf{E}\left(\Omega_{h}, u^{h}, F^{h}\right)-\mathbf{W}\left(\Omega_{h}, u^{h}, F^{h}\right)+\mathbf{S}\left(\Omega_{h}\right)
$$

Here, $\mathbf{U}$ is the potential energy as the difference of the elastic deformation energy

$$
\mathbf{E}\left(\Omega_{h}, u^{h}, F^{h}\right):=\frac{1}{2} \int_{\Omega_{h}} \sigma_{i j}\left(u^{h} ; x\right) \varepsilon_{i j}\left(u^{h} ; x\right) d x
$$

(with sum convention), and the work of external forces:

$$
\mathbf{W}\left(\Omega_{h}, u^{h}, F^{h}\right):=\int_{\Omega_{h}} f(x) \cdot u^{h}(x) d x+\int_{\Gamma} p(x) \cdot u^{h}(x) d s
$$

The term $\mathbf{S}$ describes a dissipative energy, which is released if the material breaks and the crack propagates. From the macroscopic point of view of continuum mechanics, all these processes, cracking of the micro structure, forming of micro cracks, are collected in the expression surface energy [GS01]. In general, the surface energy can be described by an integral expression and especially for linear elastic, homogeneous solids it can be assumed to be proportional to the crack length:

$$
\mathbf{S}\left(\Omega_{h}\right)=2\left(\gamma\left(\Xi_{0}\right) a+\gamma\left(\Upsilon_{h}(\theta)\right) h\right)=2\left(\gamma\left(\Xi_{0}\right) a+\gamma(\theta) h\right)
$$

The factor 2 occurs, because we have two crack faces and $a$ denotes the length of the initial crack $\Xi_{0}$. Because we assume, that the crack shoot is a linear polygon, surface energy of the shoot depends only on the direction $\theta$ and the length $h$. In isotropic materials, $\gamma$ is a material constant, but in general depends also on the crack direction. By Clapeyron's theorem there holds

$$
\mathbf{E}\left(\Omega_{h}, u^{h}, F^{h}\right)=\frac{1}{2} \mathbf{W}\left(\Omega_{h}, u^{h}, F^{h}\right)
$$

Using the foregoing notations, the energy criterion reads as follows: A crack grows in such a way, that

$$
\Pi\left(\Omega_{h}, u^{h}, F^{h}\right)=\min
$$

where the minimum is taken over all $h>0$ and all directions $\theta$. A crack can only grow along the shoot $\Upsilon_{h}(\theta)$ if energy is released:

$$
\Pi\left(\Omega_{0}, u^{0}, F^{0}\right)>\Pi\left(\Omega_{h}, u^{h}, F^{h}\right), \quad h>0
$$

A new crack surface of length $h$ to direction $\theta$ can be formed only, if the surface energy can be overcome:

$$
\mathbf{U}\left(\Omega_{0}, u^{0}, F\right)-\mathbf{U}\left(\Omega_{h}, u^{h}, F\right)>\mathbf{S}\left(\Omega_{h}\right)-\mathbf{S}\left(\Omega_{0}\right)=2 \gamma(\theta) h, \quad h>0
$$

According to this, the virtual energy release rate is defined as

$$
\mathscr{G}_{0}(\theta):=\lim _{h \rightarrow 0+} \frac{\mathbf{U}\left(\Omega_{0}, u^{0}, F\right)-\mathbf{U}\left(\Omega_{h}, u^{h}, F\right)}{h}=-\left.\frac{\mathrm{d}}{\mathrm{~d} h} \mathbf{U}\left(\Omega_{h}, u^{h}, F\right)\right|_{h=0+}
$$

Here we assume, that the crack has propagated along a virtual crack shoot to direction $\theta$. This is only possible, if $\mathbf{U}\left(\Omega_{0}, u^{0}, F\right)-\mathbf{U}\left(\Omega_{h}, u^{h}, F\right)>2 \gamma(\theta) h \geq 0$ and therefore $\mathscr{G}_{0}(\theta) \geq 0$. The crack can only start to propagate to direction $\theta$, if

$$
\begin{equation*}
\left.\frac{\mathrm{d}}{\mathrm{~d} h} \Pi\left(\Omega_{h}, u^{h}, F\right)\right|_{h=0+}=2 \gamma(\theta)-\mathscr{G}_{0}(\theta) \leq 0 \tag{25}
\end{equation*}
$$

This is a criterion for simulating crack paths. If the energy release rate can be calculated numerically for different directions $\theta$, the direction where the change of total energy has a minimum can be calculated also. The crack can start to propagate to this direction only, if this minimum is negative.

Asymptotic expansion of the change of potential energy. Using the energy principle for crack grow simulations, one has to know, how the potential change, if the crack propagates along a small kink $\Upsilon_{h}(\theta)$. We look for an asymptotic expansion in terms of the crack length $h$ :

$$
\Delta \mathbf{U}:=\mathbf{U}\left(\Omega_{h}, u^{h}, F\right)-\mathbf{U}\left(\Omega_{0}, u^{0}, F\right) \sim h^{\alpha}, \quad \alpha \geq 1 .
$$

With $\alpha \geq 1$ we implicitly assume, that the change of potential energy is continuous and differentiable in $h$. This is based on a more physical point of view. If the crack is not elongated (this means $h=0$ ) there should be no energy release, also there should be no jump of energy release if the crack starts to grow. Such kind of dynamical effects can not be considered with this mathematical model.

The general idea is the following. If we can approximate the displacement field $u^{h}$ by $u^{0}$ plus some terms depending on $h$, we can substitute $u^{h}$ in $\Delta \mathbf{U}$ by this approximation and the remaining expression will depend somehow on $h$. Sounding very simple, the construction of a "good" approximation of $u^{h}$ is far from being an elementary calculation. In [AN02] a method from asymptotic analysis ("Method of matched asymptotic expansions" (see e.g. [MNP91], [II'92], [NP96]) was used for the (formal) construction of an asymptotic approximation of $u^{h}$, if $h$ is small. The approximation is constructed from solutions of different limit problems in different areas of the domain. We give a sketch of the construction procedure.

Far away from the crack tip, the solution $u^{h}$ will not differ so much from the initial displacement field and we approximate $u^{h}$ in a distance from the crack tip in terms of solutions of the initial problem in $\Omega_{0}$ :

$$
u^{h}(x) \sim u^{0}(x)+a_{1}(h) v^{1}(h ; x)+a_{2}(h) v^{2}(h ; x)+\ldots, \quad|x| \geq c_{1}>h,
$$

with some coefficients $a_{j}(h)$. This is called an outer expansion and the initial problem is the first limit problem, because of the limit procedure $h \rightarrow 0$.

The influence of the crack shoot on $u^{h}$ will be significantly higher near the crack tip. In order to detect this influence, we change coordinates to $\xi=h^{-1} x$ to get a crack shoot with fixed length equal to one. Sending $h \rightarrow 0$, the outer boundary of the domain vanishes and we end up in an elasticity problem in the whole plane with a semi-infinite kinked crack, called second limit problem. The change of coordinates and sending $h \rightarrow 0$ can be seen as a kind of "zooming" into the domain or with a look throw a magnifying glass. We are interested only in the behavior at the tip of an infinitesimal small crack shoot and we enlarge exactly this part of the domain. Therefore, we approximate $u^{h}$ near the crack tip in terms of solutions of the problem in the whole plane with a crack shoot:

$$
u^{h}\left(h^{-1} x\right) \sim b_{1}(h) w^{1}(h ; \xi)+b_{2}(h) w^{2}(h ; \xi)+b_{3}(h) w^{3}(h ; \xi)+\ldots, \quad h \ll 1 .
$$

This is an inner expansion and the idea for calculating the coefficients $a_{j}(h)$ and $b_{j}(h)$ is the following: If inner and outer expansion should approximate the solution $u^{h}$, only in different areas of the domain $\Omega_{h}$, they must coincide in a region of the domain, where $|x|$ is small and $|\xi|$ is large. From this "matching procedure" we can obtain the coefficients $a_{j}(h)$ and $b_{j}$.

### 3.1 The Change of Potential Energy in Homogeneous Materials

We sketch the construction of an asymptotic approximation of $u^{h}$ for homogeneous materials. In order to simplify notations, we always consider only pairs of indices $\neq(2,2)$. As previously mentioned, we want to approximate $u^{h}$ in some distance of $\Upsilon_{h}(\theta)$ by an outer expansion

$$
u^{h}(x) \sim v(h ; x)=u^{0}(x)+v^{1}(h ; x)+v^{2}(h ; x)+v^{3}(h ; x)+\ldots,
$$

where $u^{0}$ is a solution of the initial problem. Because $u^{0}$ fulfills the boundary conditions, all other functions $v^{k}(h ; \cdot)$ should be solutions of the homogeneous problem

$$
\mathscr{L}(\nabla) v(x)=0, \quad x \in \Omega_{0}, \quad \mathscr{N}(\nabla) v(x)=0, \quad x \in \partial \Omega_{0}
$$

Solutions with finite energy are the rigid motions only and other solutions have singularities [Bue70], [MP77]:

There exist unique singular solutions

$$
\zeta^{j, k}(x):=V^{j, k}(x)+\widetilde{\zeta}^{j, k}(x), \quad j=1,2, \quad k=1,2,3, \ldots,
$$

of the homogeneous elasticity problem where $\widetilde{\zeta}^{j, k} \in H^{1}\left(\Omega_{0}\right)$ with asymptotic decomposition

$$
\widetilde{\zeta}^{j, k}(x)=m_{1,1}^{j, k} U^{1,1}(x)+m_{2,1}^{j, k} U^{2,1}(x)+m_{1,2}^{j, k} U^{1,2}(x)+\ldots, \quad|x| \rightarrow 0
$$

This singular solutions are also called weight functions and the classical formula for SIFs [Bue70], [MP77] can be verified with the same arguments as (24):

$$
K_{j, k}=\int_{\Omega_{0}} \zeta^{j, k}(x) \cdot f(x) d x+\int_{\Gamma} \zeta^{j, k}(x) \cdot p(x) d s
$$

The coefficients $m_{i, l}^{j, k}$ in the asymptotic decomposition of the functions $\widetilde{\zeta}^{j, k}$ can be collected in a $(2 N-1) \times(2 N-1)$ matrix $\mathbf{m}$ for any fixed $N \in \mathbb{N}$ :

$$
\mathbf{m}:=\left(\begin{array}{cccccccc}
m_{1,1}^{1,1} & m_{2,1}^{1,1} & m_{1,2}^{1,1} & m_{1,3}^{1,1} & m_{2,3}^{1,1} & \ldots & m_{1, N}^{1,1} & m_{2, N}^{1,1} \\
m_{1,1}^{2,1} & m_{2,1}^{2,1} & m_{1,2}^{2,1} & m_{1,3}^{2,1} & m_{2,3}^{2,1} & \ldots & m_{1, N}^{2,1} & m_{2,1}^{2,1} \\
m_{1,2}^{1,1} & m_{2,2}^{1,1} & m_{1,2}^{1,2} & m_{1,2}^{1,2} & m_{2,2}^{1,2} & \ldots & m_{1,2}^{1, N} & m_{2,2}^{1,2} \\
m_{1,3}^{1,3} & m_{2,3}^{1,3} & m_{1,3}^{1,3} & m_{1,3}^{1,3} & m_{2,3}^{1,3} & \ldots & m_{1, N}^{1,3} & m_{2, N}^{1,3} \\
m_{1,1}^{2,3} & m_{2,1}^{2,3} & m_{1,2}^{2,3} & m_{1,3}^{2,3} & m_{2,3}^{2,3} & \ldots & m_{1, N}^{2,3} & m_{2, N}^{2,3} \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
m_{1, N}^{1, N} & m_{2,1}^{1, N} & m_{1,2}^{1, N} & m_{1,3}^{1, N} & m_{2,3}^{1, N} & \ldots & m_{1, N}^{1, N} & m_{2, N}^{1, N} \\
m_{1,1}^{2, N} & m_{2,1}^{2, N} & m_{1,2}^{2, N} & m_{1,3}^{2, N} & m_{2,3}^{2, N} & \ldots & m_{1, N}^{2, N} & m_{2, N}^{2, N}
\end{array}\right)
$$

Matrix $\mathbf{m}$ is symmetric and there holds [MP77]

$$
\begin{equation*}
m_{i, l}^{j, k}=\int_{\Gamma} \mathscr{N}(\nabla) \widetilde{\zeta}^{j, k}(x) \cdot \zeta^{i, l}(x) d s, \quad i, j=1,2, \quad k, l=1,2,3, \ldots \tag{26}
\end{equation*}
$$

The coefficients $m_{i, l}^{j, k}$ and also the SIFs depend on the material properties and especially on the geometry of the domain $\Omega_{0}$. They are so-called global integral characteristics.

To figure out the influence of the crack shoot in detail, we zoom into the domain near the crack. Mathematically, this means a change of coordinates to

$$
\xi:=\frac{x}{h}, \quad \xi=(\rho \cos (\varphi), \rho \sin (\varphi))^{\top} \quad \text { for } \quad h \rightarrow 0
$$

The outer boundary vanishes and the crack shoot transforms to a shoot of fixed length one. For the unbounded domain we introduce the notation

$$
\Omega_{\infty}:=\mathbb{R}^{2} \backslash\left(\Xi_{\infty} \cup \Upsilon\right)
$$

with the semi-infinite kinked crack

$$
\Xi_{\infty}:=\left\{\xi: \xi_{1} \leq 0, \xi_{2}=0\right\}, \quad \Upsilon(\theta):=\left\{\xi: 0 \leq \xi_{1} \leq \cos (\theta), \xi_{2}=\xi_{1} \tan (\theta)\right\}
$$

Because the crack is assumed to be traction free, we approximate $u^{h}$ near the crack tip in stretched coordinates by an inner expansion

$$
u^{h}(h \xi) \sim w(h ; \xi)=w^{1}(h ; \xi)+w^{2}(h ; \xi)+w^{3}(h ; \xi)+\ldots
$$

where $w^{k}(h ; \cdot)$ are solutions of the homogeneous elasticity problem in the unbounded domain:

$$
\mathscr{L}\left(\nabla_{\xi}\right) w(\xi)=0, \quad \xi \in \Omega_{\infty}, \quad \mathscr{N}\left(\nabla_{\xi}\right) w(\xi)=0, \quad \xi \in \partial \Omega_{\infty}
$$

Solutions of this problem also have singularities and an asymptotic decomposition at infinity [NP96], [AN02], [Ste09]:

There exist singular solutions

$$
\eta^{j, k}(\xi)=U^{j, k}(\xi)+\widetilde{\eta}^{j, k}(\xi), \quad j=1,2, \quad k=1,2,3, \ldots
$$

of the homogeneous elasticity problem with the following decomposition at infinity:

$$
\widetilde{\eta}^{j, k}(\xi)=M_{1,1}^{j, k}(\theta) V^{1,1}(\xi)+M_{2,1}^{j, k}(\theta) V^{2,1}(\xi)+M_{1,2}^{j, k}(\theta) V^{1,2}(\xi)+\ldots, \quad|\xi| \rightarrow \infty
$$

Also the coefficients $M_{i, l}^{j, k}(\theta)$ can be collected into a $(2 N-1) \times(2 N-1)$ matrix $\mathbf{M}(\theta)$, this matrix is symmetric and there holds [NP96]

$$
\begin{equation*}
M_{i, l}^{j, k}(\theta)=\sum_{ \pm}\left(\int_{\Upsilon \pm(\theta)} \widetilde{\eta}^{i, l}(\xi) \cdot \mathscr{N}\left(\nabla_{\xi}\right) \widetilde{\eta}^{j, k}(\xi) d s\right), \quad i, j=1,2, \quad k, l=1,2,3, \ldots \tag{27}
\end{equation*}
$$

The coefficients $M_{i, l}^{j, k}(\theta)$ are so-called local integral characteristics. They depend on the material properties and the shape of the crack shoot, especially here on the kink angle $\theta$, but not on the initial configuration $\Omega_{0}$.

Construction of an inner and outer expansion. First, we rewrite the asymptotic expansion of the displacement field $u^{0}$ for $|x| \rightarrow 0$ in stretched coordinates:

$$
\begin{aligned}
u^{0}(x) & =K_{I} U^{1,1}(x)+K_{I I} U^{2,1}(x)+K_{T} U^{1,2}(x)+\ldots \\
& =h^{1 / 2}\left(K_{I} U^{1,1}(\xi)+K_{I I} U^{2,1}(\xi)\right)+h K_{T} U^{1,2}(\xi)+\ldots
\end{aligned}
$$

Therefore, the inner expansion has to include solutions with singular behavior $w^{k} \sim|\xi|^{k / 2}$ for $|\xi| \rightarrow \infty$ and we set

$$
w^{j, k}(\xi):=b_{j, k} h^{k / 2} \eta^{j, k}(\xi), \quad j=1,2, \quad k=1,2,3, \ldots
$$

with some coefficients $b_{j, k}$. If we transform the expansion of the solutions $\eta^{j, k}$ at infinity to $x$ coordinates, we get

$$
w\left(h ; h^{-1} x\right)=\sum_{(j, k)}\left(b_{j, k} U^{j, k}(x)+\sum_{(i, l)} h^{(k+l) / 2} b_{j, k} M_{i, l}^{j, k}(\theta) V^{i, l}(x)\right)+\ldots
$$

for $h^{-1} r \rightarrow \infty$ and the outer expansion has to contain terms with singularities at the crack tip:

$$
v^{k}(h ; x)=a_{j, k}(h) \zeta^{j, k}(x), \quad \quad \zeta^{j, k}(x) \sim V^{j, k}(x), \quad|x| \rightarrow 0 .
$$

We use the more comfortable notation

$$
\sum_{(j, k)}:=\sum_{j=1}^{2} \sum_{k=1}^{N} \quad \text { with } \quad(j, k) \neq(2,2) .
$$

If both expansions should approximate $u^{h}$, they have to coincide for $x$ small and $\xi$ large, for example if $r \sim h^{1 / 2}$. Choosing two constants $0<c_{1}<c_{2}$ with $\Upsilon_{h}(\theta)$ contained in the slitted annulus $\mathcal{K}=\{x \in$ $\left.\Omega_{h}: c_{1} h^{1 / 2}<|x|<c_{2} h^{1 / 2}\right\}$ we see, that both expansions coincide, if

$$
\mathbf{K}+\mathbf{m} \cdot \mathbf{a}(h)=\mathbf{b}, \quad \mathbf{a}(h)=\mathbf{M}(h ; \theta) \cdot \mathbf{b} .
$$

This is the case, if

$$
\mathbf{K}+\mathbf{m} \cdot \mathbf{M}(h ; \theta) \cdot \mathbf{b}=\mathbf{b}, \quad \text { hence } \quad \mathbf{b}=(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h ; \theta))^{-1} \cdot \mathbf{K},
$$

and

$$
\mathbf{a}(h)=\mathbf{M}(h ; \theta) \cdot \mathbf{b}=\mathbf{M}(h ; \theta) \cdot(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h ; \theta))^{-1} \cdot \mathbf{K}
$$

Here,

$$
\begin{aligned}
\mathbf{K} & =\left(K_{I}, K_{I I}, K_{T}, k_{13}, k_{23}, \ldots\right)^{\top}, \\
\mathbf{a}(h) & =\left(a_{1,1}(h), a_{2,1}(h), a_{1,2}(h), a_{1,3}(h), a_{2,3}(h), \ldots\right)^{\top}, \\
\mathbf{b} & =\left(b_{1,1}, b_{2,1}, b_{1,2}, b_{1,3}, b_{2,3}, \ldots\right)^{\top}
\end{aligned}
$$

are the vectors composed of the $(2 N-1)$ coefficients $a_{j, k}, b_{j, k}, K_{j, k}$ and $\mathbf{M}(h ; \theta)$ is the matrix with entries $M_{j, k}^{i, l}(h ; \theta):=h^{(k+l) / 2} M_{j, k}^{i, l}(\theta)$.

Because of $\operatorname{det}(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h ; \theta)) \approx 1+h$ for $h \ll 1$, the matrix $(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h ; \theta))$ is invertible and using the theorem on Neumann's series, we get

$$
(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h ; \theta))^{-1}=\sum_{q=0}^{\infty}(\mathbf{m} \cdot \mathbf{M}(h ; \theta))^{q}=\mathbb{I}+\mathbf{m} \cdot \mathbf{M}(h ; \theta)+\ldots .
$$

For $h \ll 1$ this series converges. Moreover, we find

$$
\mathbf{a}(h)=\mathbf{M}(h ; \theta) \cdot \mathbf{K}+\mathbf{M}(h ; \theta) \cdot \mathbf{m} \cdot \mathbf{M}(h ; \theta) \cdot \mathbf{K}+\ldots
$$

and because of $M_{i, l}^{j, k}(h)=h^{(k+l) / 2} M_{i, l}^{j, k}$, the coefficients have the representation

$$
a_{j, k}(h)=h^{(k+1) / 2} a_{j, k}+\mathcal{O}\left(h^{(k+2) / 2}\right) .
$$

Using this asymptotic approximation of the displacement field $u^{h}$, the following fundamental formula is established in [AN02]:

The change of potential energy with respect to the crack length $h$ has the asymptotic expansion

$$
\begin{equation*}
\Delta \mathbf{U}=-\frac{1}{2} \mathbf{K}^{\top} \cdot\left(\mathbf{M}(h) \cdot(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}(h))^{-1}\right) \cdot \mathbf{K}+\mathcal{O}\left(h^{(N+1) / 2+\varepsilon}\right), \quad h \rightarrow 0 \tag{28}
\end{equation*}
$$

with a number $\varepsilon \in(0,1 / 2)$.

We see that

$$
\Delta \mathbf{U}=-\frac{1}{2}\left(h \mathbf{U}_{0}+h^{3 / 2} \mathbf{U}_{1}+h^{2} \mathbf{U}_{2}+\ldots\right)
$$

with

$$
\begin{aligned}
\mathbf{U}_{0}= & K_{I}^{2} M_{1,1}^{1,1}+2 K_{I} K_{I I} M_{2,1}^{1,1}+K_{I I}^{2} M_{2,1}^{2,1} \\
\mathbf{U}_{1}= & 2 K_{T}\left(K_{I} M_{1,1}^{1,2}+K_{I I} M_{2,1}^{1,2}\right) \\
\mathbf{U}_{2}= & K_{I}^{2}\left(m_{1,1}^{1,1}\left(M_{1,1}^{1,1}\right)^{2}+2 m_{2,1}^{1,1} M_{1,1}^{1,1} M_{2,1}^{1,1}+m_{2,1}^{2,1}\left(M_{2,1}^{1,1}\right)^{2}\right) \\
& +K_{I I}^{2}\left(m_{1,1}^{1,1}\left(M_{2,1}^{1,1}\right)^{2}+2 m_{2,1}^{1,1} M_{2,1}^{1,1} M_{2,1}^{2,1}+m_{2,1}^{2,1}\left(M_{2,1}^{2,1}\right)^{2}\right) \\
& +2 K_{I}\left(k_{1,3} M_{1,3}^{1,1}+k_{2,3} M_{2,3}^{1,1}\right)+2 K_{I I}\left(k_{1,3} M_{1,3}^{2,1}+k_{2,3} M_{2,3}^{2,1}\right) \\
& +2 K_{I} K_{I I}\left(m_{1,1}^{1,1} M_{1,1}^{1,1} M_{1,2}^{1,1}+m_{2,1}^{1,1}\left(\left(M_{2,1}^{1,1}\right)^{2}+M_{1,1}^{1,1} M_{2,1}^{2,1}\right)+m_{2,1}^{2,1} M_{1,1}^{2,1} M_{2,1}^{2,1}\right)
\end{aligned}
$$

The first summand $\mathbf{U}_{0}$ is equal to $-2 \mathscr{G}_{0}$. The formal derivation of formula (28) was given in [AN02]. But from a mathematical point of view, it has to be shown, in what sense an approximation as constructed here is "good". Problems of this kind have to be treated in weighted Sobolev spaces. Special techniques from asymptotic analysis are needed to calculate the order of $h$ this construction approximates the solution $u^{h}$ in weighted Sobolev norms. A rigorous mathematical justification of formula (28) was given in [Ste09].

For a straight crack elongation, the first coefficients $M_{i, l}^{j, k}(0)$ can be found from the relation

$$
-\partial_{x_{1}} U^{j, 1}(x)=M_{j, 1} V^{1,1}(x)+M_{j, 2} V^{2,1}(x), \quad j=1,2
$$

there holds [Naz05]

$$
\begin{array}{ll}
M_{1,1}^{1,1}(0)=M_{1,1}, & M_{2,1}^{1,1}(0)=M_{1,2} \\
M_{1,1}^{2,1}(0)=M_{2,1}, & M_{2,1}^{2,1}(0)=M_{2,2}
\end{array}
$$

In the case of isotropic materials, direct calculations show

$$
\begin{equation*}
M_{1,1}=M_{2,2}=\frac{\lambda+2 \mu}{2 \mu(\lambda+\mu)}, \quad \quad M_{1,2}=M_{2,1}=0 \tag{29}
\end{equation*}
$$

where $\lambda$ and $\mu$ are the Lamé constants. In isotropic materials, a crack propagates along a straight crack shoot, if $K_{I I}=0$. In this case, formula (28) reads

$$
\Delta \mathbf{U}=-\frac{1}{2}\left(\frac{(\lambda+2 \mu)}{2 \mu(\lambda+\mu)} K_{I}^{2}\right) h+\ldots
$$

and this is the classical GRIFFITH formula [Gri21] (see also [SPI65], [NP96]). For anisotropic materials the following result was proven in [Ste09]:

If the crack lies on an axis of elastic symmetry, this means $a_{31}=a_{32}=0$, and $K_{I}>0$, the crack can only kink, if $K_{I I} \neq 0$.

The connection to the IRWIN fracture criterion. Besides the energy principle, there are various fracture criteria in the literature for predicting crack propagation. We only want to show the connection between the energy principle and the stress criterion introduced by Irwin [Irw57]. For a more detailed discussion on fracture criteria see e.g. [NP96] or [Erd00]. Similar to the model described in the previous sections, the IRWIN stress criterion is based on the idea that the behavior near the crack tip can be expressed in terms of asymptotic expansions. But for the behavior at the crack tip stress intensity factors are supposed to be the deciding quantities and a fracture criterion can be formulated as follows (for Mode-I cracks): A crack propagates, if the stress intensity factor reaches some critical value:

$$
K_{I}^{\sigma}:=\lim _{x_{1} \rightarrow 0+}(2 \pi r)^{1 / 2} \sigma_{22}\left(u ; x_{1}, 0\right) \geq K_{I C}
$$

A similar criterion can be formulated for general crack scenarios [RS09]. As long as $K_{I}^{\sigma}$ does not reach a critical value, the crack is stationary. If the critical value is reached, crack propagation is locally only stable, if the change of $K_{I}^{\sigma}(h)$ with growing crack length $h$ is negative. Otherwise we have $K_{I}^{\sigma}(h)>K_{I}^{\sigma}(0)>K_{I C}$ and the crack is locally instable.

We show, how the stress criterion is related to the energy principle discussed before and assume, that $K_{I I}^{\varepsilon}=0$ and the crack propagates along a straight crack shoot. Taking into account that the power-law are normalized to strains, the change of $K_{I}^{\varepsilon}$ in terms of the crack elongation is [Ste09]

$$
\begin{equation*}
\left.\frac{\mathrm{d}}{\mathrm{~d} h} K_{I}^{\varepsilon}(h)\right|_{h=0+}=\frac{3}{2} k_{1,3}^{\varepsilon}+K_{I}^{\varepsilon}\left(m_{1,1}^{1,1} M_{1,1}^{1,1}+m_{2,1}^{1,1} M_{2,1}^{1,1}\right) \tag{30}
\end{equation*}
$$

Using the coefficients $M_{i, j}$ from the relation

$$
-\partial_{x_{1}} U^{j, 1}(x)=M_{j, 1} V^{1,1}(x)+M_{j, 2} V^{2,1}(x), \quad j=1,2
$$

depending on the normalization of the power-law solutions, the change of total energy in the case of a straight crack elongation can be written as

$$
\begin{align*}
& \Delta \Pi(h)= h(2 \gamma(0)- \\
&-\left.\frac{1}{2}\left(K_{I}^{\varepsilon}\right)^{2} M_{1,1}\right)  \tag{31}\\
&-h^{2} \frac{K_{I}^{\varepsilon}}{2}\left(M_{1,1}\left(\frac{3}{2} k_{1,3}^{\varepsilon}+K_{I}^{\varepsilon}\left(m_{1,1} M_{1,1}+m_{1,2} M_{2,1}\right)\right)\right. \\
&\left.+M_{1,2}\left(\frac{3}{2} k_{2,3}^{\varepsilon}+K_{I}^{\varepsilon}\left(m_{1,2} M_{1,1}+m_{2,2} M_{1,2}\right)\right)\right)+\ldots
\end{align*}
$$

A short calculation shows the following relations between the strain and the stress intensity factors in the case $K_{I I}^{\varepsilon}=0$ :

$$
K_{I}^{\varepsilon}=\frac{1}{2\left(A^{-1}\right)_{11}} \frac{\operatorname{det}\left(M^{\sigma}\right)}{M_{2,2}^{\sigma}} K_{I}^{\sigma}, \quad K_{I I}^{\sigma}=-\frac{M_{1,2}^{\sigma}}{M_{2,2}^{\sigma}} K_{I}^{\sigma}
$$

Especially, $K_{I I}^{\varepsilon}=0$ is not equivalent to $K_{I I}^{\sigma}=0$. Defining

$$
K_{I C}^{\varepsilon}:=2\left(\left(M_{1,1}^{\varepsilon}\right)^{-1} \gamma(0)\right)^{1 / 2}
$$

according to the energy principle the crack can only propagate, if $K_{I}^{\varepsilon}>K_{I C}^{\varepsilon}$. With the relations above, this is the case if and only if

$$
K_{I}^{\sigma}>4\left(A^{-1}\right)_{11} \frac{M_{2,2}^{\sigma}}{\operatorname{det}\left(M^{\sigma}\right)}\left(\left(M_{1,1}^{\varepsilon}\right)^{-1} \gamma(0)\right)^{1 / 2}=: K_{I C}^{\sigma}
$$

This means, that beginning of crack propagation is characterized similar by the energy principle and the IRWIN stress criterion. For isotropic materials, this is a classical result in fracture mechanics [Ric72], [NP96].
The IrWin stress criterion characterizes locally instable crack propagation by

$$
\left.\frac{\mathrm{d}}{\mathrm{~d} h} K_{I}^{\sigma}(h)\right|_{h=0+}>0
$$

Using the relations (30) and (31) locally instable crack propagation based on the energy principle can occur, if

$$
-\frac{K_{I}^{\varepsilon}}{2}\left(\left.M_{1,1}^{\varepsilon} \frac{\mathrm{d}}{\mathrm{~d} h}\right|_{h=0+}+M_{1,2}^{\varepsilon}\left(\frac{3}{2} k_{2,3}^{\varepsilon}+K_{I}^{\varepsilon}\left(m_{1,2}^{\varepsilon} M_{1,1}^{\varepsilon}+m_{2,2}^{\varepsilon} M_{1,2}^{\varepsilon}\right)\right)\right)>0
$$

Because of $K_{I}^{\varepsilon} \geq 0$ as well as $M_{1,1}^{\varepsilon}>0$, this is equivalent to IRWIN's characterization if and only if $M_{1,2}^{\varepsilon}=0$ and this depends on the material properties, see [Ste09] for more details. In the case of isotropic materials, the equivalence of both criteria is well-known (see e.g. [Ric72], [NP96], [GS01]). This can be seen directly. Due to the relations (29) and $K_{I}^{\varepsilon}=K_{I}^{\sigma}, K_{I I}^{\varepsilon}=K_{I I}^{\sigma}$ the change of stress intensity factors in (30) simplifies to

$$
\left.\frac{\mathrm{d}}{\mathrm{~d} h} K_{I}(h)\right|_{h=0+}=\frac{3}{2} k_{1,3}+\frac{\lambda+2 \mu}{2 \mu(\lambda+\mu)} K_{I} m_{1,1}
$$

This is also a well-known classical result [Ric72].

### 3.2 The Change of Potential Energy in Inhomogeneous Materials

As shown in the previous section, the asymptotic decomposition of the displacement field near the crack tip in an inhomogeneous material slightly changes. Especially the first terms are the same as in the case of homogeneous materials, but related to elastic properties frozen at the crack tip. Inspired by this fact, we transfer the method of matched asymptotic expansion described above to inhomogeneous materials in order to construct an asymptotic approximation of the displacement field $u^{h}$ for the calculation of the change of potential energy. In particular, it turns out that the inner expansion can be constructed from solutions of the elasticity problem in stretched coordinates, but with constant material properties. In contrast to the case of homogeneous materials, we are not be able to construct an arbitrary number of asymptotic terms. Because only the first terms of the asymptotic decomposition are known explicitly, also only the first two terms of the expansion of the change of the potential energy can be constructed as well.

As in the previous paragraph, we always exclude the pair of indices $(2,2)$ in the following. We define three weight functions related to the material properties at the crack tip $x_{0}$ :

$$
\zeta^{j, k}(x):=V_{0}^{j, k}+\widetilde{\zeta}^{j, k}(x)
$$

The functions $V_{0}^{j, k}$ are singular power-law solutions related to material properties at the crack tip as introduced in (23) and $\zeta^{j, k}$ are solutions to the homogeneous problem

$$
\mathscr{L}(x, \nabla) \zeta^{j, k}(x)=0, \quad x \in \Omega_{0}, \quad \mathscr{N}(x, \nabla) \zeta^{j, k}(x)=0, \quad x \in \partial \Omega_{0}
$$

With the same arguments as in the proof of (13) it can be shown, that for SIFs the following integral representation hold:

$$
K_{j, k}=\int_{\Omega_{0}} f(x) \cdot \zeta^{j, k}(x) d x+\int_{\Gamma} p(x) \cdot \zeta^{j, k}(x) d x, \quad j=1,2, \quad k=1,2
$$

The functions $\widetilde{\zeta}^{j, k}$ are solutions of the problem

$$
\begin{array}{ll}
\mathscr{L}(x, \nabla) \widetilde{\zeta}^{j, k}(x)=-\mathscr{L}(x, \nabla) V_{0}^{j, k}(x), & x \in \Omega_{0} \\
\mathscr{N}(x, \nabla) \widetilde{\zeta}^{j, k}(x)=-\mathscr{N}(x, \nabla) V_{0}^{j, k}(x), & x \in \partial \Omega_{0}
\end{array}
$$

Using the TAYLOR expansion of the elasticity operator,

$$
\mathscr{L}=\mathscr{L}^{(0)}+\mathscr{L}^{(1)}+\ldots, \quad \mathscr{N}=\mathscr{N}^{(0)}+\mathscr{N}^{(1)}+\ldots
$$

and the following properties of the power-law solutions,

$$
\mathscr{L}^{(0)}(\nabla) V_{0}^{j, k}(x)=0, \quad \mathbb{R}^{2} \backslash \Xi_{\infty}^{ \pm}, \quad \mathscr{N}^{(0)}(\nabla) V_{0}^{j, k}(x)=0, \quad x \in \Xi_{\infty}^{ \pm}
$$

it can be seen directly, that the solutions $\widetilde{\zeta}^{j, k}$ have finite energy. Moreover, they admit an asymptotic decomposition

$$
\widetilde{\zeta}^{j, k}(x)=m_{1,1}^{j, k}\left(U_{0}^{1,1}(x)+U_{1}^{1,1}(x)+\ldots\right)+m_{2,1}^{j, k}\left(U_{0}^{2,1}(x)+U_{1}^{2,1}(x)+\ldots\right)+\ldots, \quad|x| \rightarrow 0
$$

Based on the same arguments as in the previous paragraph, we approximate the displacement field $u^{h}$ in some distance to the crack tip by an expansion

$$
u^{h} \sim v(h ; x)=u^{0}(x)+a_{1,1}(h) \zeta^{1,1}(x)+a_{2,1}(h) \zeta^{2,1}(x)+a_{1,2}(h) \zeta^{1,2}(x)
$$

where $a_{j, k}(h)$ are some coefficients to be found. The asymptotic decomposition of this approximation near the crack tip reads

$$
\begin{aligned}
v(h ; x)= & K_{I} U_{0}^{1,1}(x)+K_{I I} U_{0}^{2,1}(x)+K_{T} U_{0}^{1,2}(x) \\
& +a_{1,1}(h)\left(V_{0}^{1,1}(x)+m_{1,1}^{1,1} U_{0}^{1,1}(x)+m_{2,1}^{1,1} U_{0}^{2,1}(x)+m_{1,2}^{1,1} U_{0}^{1,2}(x)\right) \\
& +a_{2,1}(h)\left(V_{0}^{2,1}(x)+m_{1,1}^{2,1} U_{0}^{1,1}(x)+m_{2,1}^{2,1} U_{0}^{2,1}(x)+m_{1,2}^{2,1} U_{0}^{1,2}(x)\right) \\
+ & a_{1,2}(h)\left(V_{0}^{1,2}(x)+m_{1,1}^{1,2} U_{0}^{1,1}(x)+m_{2,1}^{1,2} U_{0}^{2,1}(x)+m_{1,2}^{1,2} U_{0}^{1,2}(x)\right)+\mathcal{O}\left(|x|^{3 / 2}\right), \quad|x| \rightarrow 0
\end{aligned}
$$

Because this expansion contains singular power-law solutions $V_{0}^{j, k}$ only related to material properties frozen at the crack tip, we construct the inner expansion from singular solutions of the second limit problem with constant material properties:

$$
w(h ; \xi)=b_{1,1} h^{1 / 2} \eta_{0}^{1,1}(\xi)+b_{2,1} h^{1 / 2} \eta_{0}^{2,1}(\xi)+b_{1,2} h \eta_{0}^{1,2}(\xi)
$$

The functions

$$
\eta_{0}^{j, k}:=U_{0}^{j, k}+\widetilde{\eta}_{0}^{j, k}, \quad j=1,2, \quad k=1,2
$$

are singular solutions of the elasticity problem in the whole plane with a semi-infinite kinked crack and constant elastic properties frozen at the initial crack tip $x_{0}$ :

$$
\mathscr{L}^{(0)}\left(\nabla_{\xi}\right) \eta_{0}^{j, k}(\xi)=0, \quad \xi \in \Omega_{\infty}, \quad \mathscr{N}^{(0)}\left(\nabla_{\xi}\right) \eta_{0}^{j, k}(\xi)=0, \quad \xi \in \partial \Omega_{\infty}
$$

They also admit an asymptotic decomposition at infinity,

$$
\widetilde{\eta}_{0}^{j, k}(\xi)=M_{1,1}^{j, k}\left(\theta ; x_{0}\right) V_{0}^{1,1}(\xi)+M_{2,1}^{j, k}\left(\theta ; x_{0}\right) V_{0}^{2,1}(\xi)+M_{1,2}^{j, k}\left(\theta ; x_{0}\right) V_{0}^{1,2}(\xi)+\ldots, \quad|\xi| \rightarrow \infty
$$

where the coefficients $M_{i, j}\left(\theta ; x_{0}\right)$ now depend on the kink angle and the material properties frozen at the crack tip $x_{0}$. With the same argumentation as in the case of homogeneous materials we see, that both expansions only coincide in some region, where $|x|$ is small and $|\xi|$ is large, if and only if

$$
\mathbf{K}+\mathbf{m} \cdot \mathbf{a}(h)=\mathbf{b}, \quad \mathbf{a}(h)=\mathbf{M}\left(h ; \theta ; x_{0}\right) \cdot \mathbf{b}
$$

This is the case, if

$$
\mathbf{a}(h)=\mathbf{M}\left(h ; \theta ; x_{0}\right) \cdot\left(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}\left(h ; \theta ; x_{0}\right)\right)^{-1} \cdot \mathbf{K}, \quad \mathbf{b}=\left(\mathbb{I}-\mathbf{m} \cdot \mathbf{M}\left(h ; \theta ; x_{0}\right)\right)^{-1} \cdot \mathbf{K}
$$

with the $3 \times 3$ matrices $\mathbf{m}$ and $\mathbf{M}\left(h ; \theta ; x_{0}\right)$ composed of the coefficients $m_{i, l}^{j, k}$ and $M_{i, l}^{j, k}\left(h ; \theta ; x_{0}\right)$. We calculate the change of potential energy. Substituting the displacement field $u^{h}$ by the outer expansion $w(h ; \cdot)$ we find

$$
\mathbf{U}\left(\Omega_{h}, u^{h}, F\right) \approx \mathbf{U}\left(\Omega_{h}, w(h ; \cdot), F\right)=-\frac{1}{2}\left(\int_{\Omega_{h}} f(x) \cdot w(h ; x) d x+\int_{\Gamma} p(x) \cdot w(h ; x) \cdot d s\right)
$$

The integrals on the right can be simplified using the relations for the coefficients $a_{j, k}$ :

$$
\begin{aligned}
(f, w)_{\Omega_{h}}+ & (p, w)_{\Gamma}=\left(\left(f, u^{0}\right)_{\Omega_{0}}+\left(p, u^{0}\right)_{\Gamma}+a_{1,1} h\left(\left(f, \zeta^{1,1}\right)_{\Omega_{0}}+\left(p, \zeta^{1,1}\right)_{\Gamma}\right)\right. \\
& \left.+a_{2,1} h\left(\left(f, \zeta^{2,1}\right)_{\Omega_{0}}+\left(p, \zeta^{2,1}\right)_{\Gamma}\right)+a_{1,2} h^{3 / 2}\left(\left(f, \zeta^{1,2}\right)_{\Omega_{0}}+\left(p, \zeta^{1,2}\right)_{\Gamma}\right)\right)+\mathcal{O}\left(h^{2}\right) \\
= & -2 \mathbf{U}\left(\Omega_{0}, u^{0}, F\right)-\frac{1}{2}\left(K_{I}^{2} M_{1,1}^{1,1}\left(\theta ; x_{0}\right)+2 K_{I} K_{I I} M_{2,1}^{1,1}\left(\theta ; x_{0}\right)+K_{I I}^{2} M_{2,1}^{2,1}\left(\theta ; x_{0}\right)\right) h \\
& +2 K_{T}\left(K_{I} M_{1,1}^{1,2}\left(\theta ; x_{0}\right)+K_{I I} M_{2,1}^{1,2}\left(\theta ; x_{0}\right)\right) h^{3 / 2}+\mathcal{O}\left(h^{2}\right)
\end{aligned}
$$

We remark that the volume force $f$ is assumed to be zero near the crack tip $x_{0}$. With the relations for the coefficients $a_{j, k}(h)$, we finally get

$$
\begin{align*}
& \Delta \mathbf{U}=-\frac{1}{2}\left(\left(K_{I}^{2} M_{1,1}^{1,1}\left(\theta ; x_{0}\right)+2 K_{I} K_{I I} M_{2,1}^{1,1}\left(\theta ; x_{0}\right)+K_{I I}^{2} M_{2,1}^{2,1}\left(\theta ; x_{0}\right)\right) h\right.  \tag{32}\\
&\left.+2 K_{T}\left(K_{I} M_{1,1}^{1,2}\left(\theta ; x_{0}\right)+K_{I I} M_{2,1}^{1,2}\left(\theta ; x_{0}\right)\right) h^{3 / 2}\right)+\mathcal{O}\left(h^{2}\right)
\end{align*}
$$

This is the formula (28) for the change of potential energy generalized to the case of inhomogeneous materials. A mathematical justification can be derived with a similar argumentation as for homogeneous materials given in [Ste09].

The first term in formula (32) is widely used for calculating the change of potential energy in inhomogeneous isotropic and some orthotropic materials (see e.g. [KP04b], [KP07] and the literature cited there).

Higher order terms of $\Delta \mathbf{U}$ can not be calculated this way. For the calculation of higher order terms one has to know the structure of the shadow terms in the expansion (21) in more detail. Looking at the construction procedure of the asymptotic approximation sketched here, the shadow terms have to be taken into account in the outer expansion for the calculation of the next asymptotic term of $\Delta \mathbf{U}$. Therefore, they have to be compensated in the inner expansion using additional singular solutions of the second limit problem. This solutions depend especially on higher order derivatives of the Hooke matrix and their asymptotic behavior at infinity depends on the structure of the shadow terms.

## 4. Numerical Simulation of Quasi-Static Crack Propagation

The intention of this chapter is to show ideas, how the theoretical results previously discussed can be used to simulate crack propagation in "real world" problems. The first observation from "real world" problems is, that crack propagation is not a static process. A solid with a crack under simple loading will collapse or not. The final breaking of a solid is really fast and from this moment no simulations or models are needed anymore.

As indicated at the beginning of the foregoing section, quasi-static crack propagation describes another type of very slow crack growth. Let us consider a specimen with a crack under a cyclic loading on parts of the outer boundary and volume forces, for simplicity assumed to be constant in time. If the load is not high enough to break the specimen immediately, the material will fatigue with an increasing number of load cycles and the crack can start to propagate (slowly). Fatigue itself is a very complex process depending on the micro structure of the material and many other factors and can not be described sufficiently with the macroscopic view of linear elasticity theory. At each load cycle a new crack front is being formed and as long as this new crack front is of small length compared to the whole crack length and the dimensions of the specimen, crack propagation is called stable. With a continuing number of load cycles there will be a moment in time, where the crack will become instable and the specimen breaks down.

Even if crack propagation is only slow, how can we apply static results to simulate crack propagation? First, we only consider the case, that deformations are small and linear elasticity theory can be applied to describe the behavior of the specimen under loading. Dynamical aspects as the influence of elastic waves on crack growth can not be modeled with this theory.

A model for quasi-static scenarios. We consider a specimen $\Omega_{0}$ with initial crack $\Xi_{0}$ under cyclic loading. Any load cycle $T$ needs some "real" time which we denote by $\tau(T)$, usually a fractional amount of a second. We approximate the propagated crack per cycle by a linear crack shoot $\Upsilon_{T}\left(\theta_{T}\right)$ to direction $\theta_{T}$ of length $h_{T}$. After $T$ load cycles, we get a piece-wise linear approximation of the crack path:

$$
\Xi_{T}=\Xi_{0} \cup \Upsilon_{1} \cup \Upsilon_{2} \cup \ldots \cup \Upsilon_{T}
$$

with crack tip

$$
x^{T}=\sum_{k=1}^{T}\binom{h_{k} \cos \left(\theta_{k}\right)}{h_{k} \sin \left(\theta_{k}\right)} .
$$

Depending on the load, $h_{k}=0$ is of course possible. To model the time dependency more precisely, we introduce a smooth and bounded vector function $G$ with

$$
G_{i}(T)=G_{i}(T+\tau(T)), \quad 0 \leq G_{i}(t) \leq 1, \quad i=1,2, \quad t \in \mathbb{R}^{+}
$$

for all $T=0,1,2, \ldots$ In order to use the results previously discussed, we define for any cycle $T$ the static load vector

$$
g^{T}(x):=\max _{t \in[T, T+\tau(T)]}\left(G_{1}(t) p_{1}(x), G_{2}(t) p_{2}(x)\right)^{\top}, \quad x \in \partial \Omega_{T}
$$

For example, a periodic cyclic loading with cycle length $\tau=1$ applied at the outer boundary can be modeled to

$$
\widetilde{G}(t, x):=F\left(\frac{1}{2}-\frac{1}{2} \cos (2 \pi t)\right) n(x) \chi(x)
$$

where $F$ is some force, $n$ is the normal vector and $\chi$ is a cut-off function, equal to one on some part of the boundary and zero otherwise. We remark that this is a very basic model for describing the time dependency of the loading, it can be easily adapted to more complicated situations. Also the volume force can be change in time, this is no technical problem but we omit further explanations.

Based on this definition of time dependency we formulate a model for quasi-static crack propagation based on the energy principle: For each cycle $T=0,1,2, \ldots$
(1) calculate SIFs of the displacement field $u^{T}$ as solution of the elasticity problem

$$
\mathscr{L}(x, \nabla) u^{T}(x)=f(x), \quad x \in \Omega_{T}, \quad \mathscr{N}(x, \nabla) u^{T}(x)=g^{T}(x), \quad x \in \partial \Omega_{T}
$$

(2) calculate the global integral characteristics $M_{i, l}^{j, k}\left(\theta ; x^{T}\right)$ related to material properties frozen at the crack tip $x^{T}$ and with the help of all this quantities the change of total energy for different angles $\theta \in[-\pi, \pi]$,
(3) determine the next kink angle $\theta_{T+1}$ as the direction, the total energy has a minimum,
(4) if crack propagation becomes instable, stop the simulation, otherwise elongate the crack about $\Upsilon_{T+1}$.

Crack speed. At last, the length $h$ of the next crack shoot has to be calculated. Implicitly, this is the question of crack speed and this is a more complicated aspect. In the context of quasi-static crack propagation we can interpret crack speed only as "change of crack length per cycle" and in the literature this length is typically denoted by $d a / d N$. Based on the energy principle, the crack can only grow, if energy is released and finally can become instable. But this depends highly on the material. Especially for inhomogeneous materials, it is nearly impossible to find energy release rates from experiments. In the literature, predictions of crack speed are based on other quantities, mostly on stress intensity factors. For some isotropic homogeneous materials there are theoretical approaches, as the Paris law or Formen-Mettu equation given in (33), but in general, experiments are needed to detect so-called $d a / d N$-curves [SR06]:

$$
\begin{equation*}
\frac{d a}{d N}=C\left[\left(\frac{1-\gamma}{1-R}\right) \Delta K\right]^{n} \frac{\left(1-\Delta K_{t h} / \Delta K\right)^{p}}{\left(1-\Delta K_{\max } / K_{C}\right)^{q}} \tag{33}
\end{equation*}
$$

With

$$
\Delta K:=\max _{\tau} K_{I}^{T}(\tau)-\min _{\tau} K_{I}^{T}(\tau)
$$

a cyclic stress intensity factor depending on the load cycle is denoted, $\Delta K_{t h}$ is a threshold value and $K_{C}$ a critical value. With $R$ the ratio $K_{\min } / K_{\max }$ is denoted and $\gamma$ is NewmAn's crack closure function. The constants $C, n, p$ and $q$ depend on the material. Relation (33) is the so-called NASGRO equation [FM90], see also [SR06] and [RS09] for a more detailed discussion.

With experimental data for the change of crack length per cycle at hand, for example $d a / d N$-curves based on SIFs, quasi-static crack propagation can be simulated per load cycle. But crack growth per cycle is very small and the crack shoots $\Upsilon_{T}$ would be to small in comparison to the dimensions of the specimen. Such a simulation needs thousands of simulation steps and very fine and accurate discretizations in every step to detect the change of the crack geometry. We suggest a slightly different approach. We fix a small crack length $h$, usually $h=0.5 \mathrm{~mm}$ is accurate, calculate SIFs and the kink angle based on the energy principle as discussed, but calculate a posteriori, using a model like the Forman-Mettu equation or experimental results, how many cycles the crack would have needed for a crack shoot of this length $h$.

Finite element formulation. For the practical application of the ideas previously shown, solutions of the elasticity problem

$$
\begin{equation*}
\mathscr{L}(x, \nabla) u(x)=f(x), \quad x \in \Omega_{0}, \quad \mathscr{N}(x, \nabla) u(x)=g(x), \quad x \in \partial \Omega_{0} \tag{34}
\end{equation*}
$$

with self-balanced load vectors $\{f, g\} \in L^{2}\left(\Omega_{0}\right) \times L^{2}\left(\partial \Omega_{0}\right)$ are needed. We only want to show basic ideas and consider a configuration $\Omega_{0}$ with an initial crack $\Xi_{0}$, composed of an inhomogeneous material. Solutions in configurations with a piece-wise linear kinked crack can be calculated similar with obvious changes.

The variational formulation of (34) seeks a (weak) solution $u \in V:=H^{1}\left(\Omega_{0}\right)$, such that

$$
a\left(u, v ; \Omega_{0}\right)=(f, v)_{\Omega_{0}}+(g, v)_{\partial \Omega_{0}} \quad \text { for all } \quad v \in V
$$

The finite element approximation uses subspaces

$$
V_{h}:=\left\{v \in H^{1}\left(\Omega_{0}\right):\left.v\right|_{K} \in Q_{1}(K), K \in \mathcal{T}_{h}\right\}
$$

where $\mathcal{T}_{h}$ is a decomposition of $\Omega_{0}$ into quadrilaterals $K($ cells $)$ of width $h_{K}:=\operatorname{diam}(K)$ and $h:=$ $\max _{K \in \mathcal{T}_{h}} h_{T}$ denotes the global mesh width. In this paragraph, we only consider the domain $\Omega_{0}$ without a growing crack and we denote the discretization parameter by $h$ as it is common in the context of finite elements. The space $Q_{1}(K)$ consists of polynomial-like shape functions defined on the cell $K \in \mathcal{T}_{h}$, which are obtained as usual from the space of bilinear functions $Q_{1}(\widehat{K}):=\operatorname{span}\left\{1, x_{1}, x_{2}, x_{1} x_{2}\right\}$ on the reference cell $\widehat{K}=[0,1] \times[0,1]$ (isoparametric bilinears).

We look for solutions $u_{h} \in V_{h}$ to the discrete problem

$$
a\left(u_{h}, v_{h} ; \Omega_{0}\right)=\left(f, v_{h}\right)_{\Omega_{0}}+\left(g, v_{h}\right)_{\partial \Omega_{0}}, \quad v_{h} \in V_{h}
$$

The error $e:=u-u_{h}$ of this approximation scheme fulfills the so-called GalERKIN orthogonality

$$
a\left(e, v_{h} ; \Omega_{0}\right)=0, \quad v_{h} \in V_{h}
$$

Using a nodal basis $\left\{\phi_{h}^{i}, i=1, \ldots, \operatorname{dim}\left(V_{h}\right)\right\}$ of the finite element space $V_{h}$ the discrete problem can be converted to a system of linear algebraic equations for the coefficients $u_{i}$ in the decomposition $u_{h}=\sum_{i=1}^{n} u_{i} \phi_{h}^{i}:$

$$
\mathbf{A} \mathbf{u}=\mathbf{f}
$$

The entries of the "stiffness matrix" A and the "load vector" $\mathbf{f}$ are given by $a_{i j}=a\left(\phi_{h}^{j}, \phi_{h}^{i} ; \Omega_{0}\right)$ and $\left(f, \phi_{h}^{i}\right)_{\Omega_{0}}+\left(g, \phi_{h}^{i}\right)_{\partial \Omega_{0}}$, respectively. For more details we refer to [Cia02], [BS02].

As already mentioned at the beginning of this chapter, a weak solution is unique up to a rigid motion only. Because we consider the pure Neumann problem, the kernel of the stiffness matrix A also has dimension three. A solution $\mathbf{u}$ exists only, if the load vector $\mathbf{f}$ is orthogonal to the kernel of $\mathbf{A}$. If the (continuous) load vectors $\{f, g\}$ are self-balanced, the discrete orthogonality conditions are fulfilled up to numerical errors, resulting from the discretization of the domain and numerical integration. Even if the stiffness matrix $\mathbf{A}$ is not positive definite, a numerical solution can be found using the MinResmethod [PS75] or a modified conjugated gradient method [BL05]. For more details see also [SF07].

### 4.1 Computation of Global Integral Characteristics

With the focus on the simulation of crack propagation, we are not interested in a numerical solution of the elasticity problem itself, but in values of certain functionals of such a solution. For example, SIFs can be found from the integral representation in (24),

$$
K_{j, k}=K_{j, k}(u)=\int_{G_{0}}\left(\mathscr{N} u \cdot V_{0}^{j, k}-u \cdot \mathscr{N} V_{0}^{j, k}\right) d s+\int_{\partial G_{0}}\left(f \cdot V_{0}^{j, k}-u \cdot \mathscr{L} V_{0}^{j, k}\right) d x
$$

or in terms of integrals using weight functions:

$$
K_{j, k}=K\left(\zeta^{j, k}\right)=\int_{\Omega_{0}} f \cdot \zeta^{j, k} d x+\int_{\partial \Omega_{0}} g \cdot \zeta^{j, k} d s .
$$

Both representations are functionals of solutions of the elasticity problem, the first of the displacement field $u$, the second of weight functions $\zeta^{j, k}$, respectively. As we have seen in (26) and (27), similar integral representations hold for the coefficients $m_{i, l}^{j, k}$ and $M_{i, l}^{j, k}(\theta)$.

While calculating such functionals from a numerical solution, one is always left with the question of the accuracy of the obtained values and how this accuracy can be improved. Using a finite element formulation and standard convergence results [Cia02], one can obtain (more or less sharp) error bounds depending on the global mesh size and improving accuracy is always associated with refining the discretization. The simplest strategy is global mesh refinement, in every approximation step each cell of the mesh is being refined. But this needs a lot of computing time and memory. Problems from practical applications we finally want to deal with can reach millions of cells easily and the question is, if this is needed for a numerical functional value of acceptable accuracy. A more efficient strategy for adapting the mesh in such a way that the accuracy of a functional value is being improved, is the "Dual-Weighted-Residual" method ("DWR" method), see [BR96], [RS02] and the literature cited there for more details.

The basic idea is the following: Let $J(\cdot)$ be a linear error functional defined on $V$ we are interested in and $z$ the solution of the so-called corresponding dual problem:

$$
a\left(v, z ; \Omega_{0}\right)=J(v) \quad \text { for all } \quad v \in V
$$

Taking $v=e$ and using the Galerkin orthogonality, cell-wise integration by parts leads to

$$
\begin{align*}
J(e)= & a\left(e, z ; \Omega_{0}\right)=a\left(e, z-I_{h} z ; \Omega_{0}\right) \\
= & \sum_{K \in \mathcal{T}_{h}}\left(\mathscr{L} u-\mathscr{L} u_{h}, z-I_{h} z\right)_{K}+\left(\mathscr{N} u-\mathscr{N} u_{h}, z-I_{h} z\right)_{\partial K} \\
= & \sum_{K \in \mathcal{T}_{h}}\left\{\left(f-\mathscr{L} u_{h}, z-I_{h} z\right)_{K}-\frac{1}{2}\left(\left[\mathscr{N} u_{h}\right], z-I_{h} z\right)_{\partial K \backslash \partial \Omega_{0}}\right.  \tag{35}\\
& \left.+\left(g-\mathscr{N} u_{h}, z-I_{h} z\right)_{\partial K \cup \partial \Omega_{0}}\right\}
\end{align*}
$$

where $\left[\mathscr{N} u_{h}\right]$ is the jump of normal stress over the inter-element boundaries. With $I_{h} z$ we denote the nodal interpolant of $z \in C\left(\overline{\Omega_{0}}\right)$ satisfying $I_{h} z\left(x_{i}\right)=z\left(x_{i}\right)$ for all nodal points $x_{i}$. The relations (35) can be used to estimate the error to

$$
|J(e)| \leq \sum_{K \in \mathcal{T}_{h}}\left\{\left\|\varrho\left(u_{h}\right) ; L^{2}(K)\right\|\left\|\omega(z) ; L^{2}(K)\right\|+\left\|\varrho\left(u_{h}\right) ; L^{2}(\partial K)\right\|\left\|\omega(z) ; L^{2}(\partial K)\right\|\right\}
$$

with the cell- and edge-residuals

$$
\left.\varrho\left(u_{h}\right)\right|_{K}=f-\mathscr{L} u_{h},\left.\quad \varrho\left(u_{h}\right)\right|_{\Gamma \subset \partial K}= \begin{cases}\frac{1}{2}\left[\mathscr{N} u_{h}\right], & \Gamma \subset \partial K \backslash \partial \Omega_{0} \\ g-\mathscr{N} u_{h}, & \Gamma \subset \partial \Omega_{0}\end{cases}
$$

and the weights

$$
\omega(z):=z-I_{h} z
$$

An interpretation of this relations is given in [RS02]. The weights $\omega_{K}$ describe the dependency of $J(e)$ on variations of the cell residuals $\varrho_{K}$ :

$$
\frac{\partial J(e)}{\partial \varrho_{K}} \approx \omega_{K}(z) \approx \max _{K}\left|\nabla^{2} z\right|
$$

see [RS02] and [BS02]. Local regularity properties of the dual solution $z$ are related directly to the error of the functional. Besides the possibility of error estimation, there is another advantage of (35), it can be used for mesh refinement. Knowing the dual solution, the residuals and the weights on the right-hand side of (35) can be computed a posteriori per cell. Such a cell-wise error indicator can be used for an efficient mesh refinement strategy. For example, one can refine a fixed fractional part of the cells with the largest error indicators and coarse the cells with the lowest indicators. This way, only the cells are being refined, which really contributes to the error of the numerical functional value.

In general, the dual solution is not known explicitly and has to be computed numerically. But the dual solution $z$ can not be replaced by an approximation on the current mesh with the same finite element formulation scheme as $u_{h}$, because the error bound would be zero. The dual solution has to be approximated with higher accuracy. This can be done by various techniques [RS02] for example using biquadratic finite elements. This is much more computational work as only computing the solution $u_{h}$, but as we have mentioned at the beginning of this paragraph, we are not interested in the displacement field itself. We are interested in accurate numerical values of functionals and an error bound, this is the price for this.

### 4.2 Computation of Local Integral Characteristics

Besides SIFs also the integral characteristics $M_{i, l}^{j, k}(\theta)$ are needed for the calculation of the change of potential energy. As we have seen in the previous sections, for homogeneous and inhomogeneous materials, the numbers $M_{i, l}^{j, k}(\theta)$ arise as coefficients in the asymptotic expansion at infinity of singular solutions

$$
\eta^{j, k}(\xi)=U^{j, k}(\xi)+\widetilde{\eta}^{j, k}(\xi), \quad j=1,2, \quad n=1,2, \ldots,
$$

of the elasticity problem with constant material properties in the whole elastic plane with a semi-infinite kinked crack:

$$
\begin{array}{ll}
\mathscr{L}\left(\nabla_{\xi}\right) \widetilde{\eta}^{j, k}(\xi)=0, & \xi \in \Omega_{\infty}=\mathbb{R}^{2} \backslash\left(\Xi_{\infty} \cup \Upsilon(\theta)\right), \\
\mathscr{N}\left(\nabla_{\xi}\right) \widetilde{\eta}^{j, k}(\xi)=-\mathscr{N}\left(\nabla_{\xi}\right) U^{j, k}(\xi), & \xi \in \partial \Omega_{\infty} .
\end{array}
$$

We froze material properties at the crack tip and assume in the following, that power-law solutions are always related to this material properties.

Setting up numerical calculations, we are confronted with another problem here: The domain is unbounded. The coefficients $M_{i, l}^{j, k}(\theta)$ can be calculated by an integral over the crack shoot $\Upsilon(\theta)$ as given in (27), but nevertheless we have to compute a numerical solution in an unbounded domain. One possibility is to cut off the domain, for example at radius $R$, and approximate the solution of (36) by a finite element approximation on the bounded domain. By this cutting procedure, a new artificial boundary $\Gamma_{R}$ appears and boundary conditions have to be prescribed here. This artificial boundary conditions (ABCs) have to be constructed in such a way, that the approximation error $\left\|\eta-\eta^{R}\right\|$ gets small for $R \rightarrow \infty$ in suitable Sobolev norms. For some $R \gg 1$ we define

$$
\Omega_{R}:=\left\{\xi \in \Omega_{\infty}:|\xi|<R\right\}, \quad \Gamma_{R}:=\left\{\xi \in \Omega_{\infty}:|\xi|=R\right\}, \quad \Xi_{R}:=\partial \Omega_{R} \backslash \Gamma_{R},
$$

and look for solutions of the elasticity problem in the bounded domain $\Omega_{R}$ with artificial boundary $\Gamma_{R}:$

$$
\begin{align*}
\mathscr{L}\left(\nabla_{\xi}\right) u^{R}(\xi) & =0, & & \xi \in \Omega_{R}, \\
\mathscr{N}\left(\nabla_{\xi}\right) u^{R}(\xi) & =g(\xi), & & \xi \in \Xi_{R}^{+} \cup \Xi_{R}^{-},  \tag{37}\\
\mathscr{N}^{R}\left(\nabla_{\xi}\right) u^{R}(\xi) & =0, & & \xi \in \Gamma_{R} .
\end{align*}
$$

In general there are different possibilities for the choice of the boundary operator $\mathscr{N}^{R}$. In particular for solutions of elliptic problems with an asymptotic decomposition in terms of power-law solutions at infinity, artificial boundary conditions in variational form are given in [NSN04] as follows: With the symmetric bilinear form

$$
\begin{equation*}
b\left(u, v ; \Gamma_{R}\right)_{\Lambda=\lambda}:=R\left(\int_{\Gamma_{R}} A \mathscr{D}_{R}(\lambda) u(\xi) \cdot \mathscr{D}_{R}(\lambda) v(\xi) d s\right) \tag{38}
\end{equation*}
$$

the variational formulation of (37) reads:

$$
\begin{equation*}
u^{R} \in H^{1}\left(\Omega_{R}\right): \quad a\left(u^{R}, v ; \Omega_{R}\right)+b\left(u^{R}, v ; \Gamma_{R}\right)_{\Lambda=-1 / 2}=(g, v)_{\Xi_{R}}, \quad v \in H^{1}\left(\Omega_{R}\right) . \tag{39}
\end{equation*}
$$

The operator $\mathscr{D}_{R}(\Lambda)$ is the strain tensor rewritten in polar coordinates on the boundary $\Gamma_{R}$ with partial derivatives with respect to $\rho$ substituted by $\Lambda$ :

$$
\mathscr{D}\left(\nabla_{\xi}\right)=\rho^{-1} \mathcal{D}\left(\varphi, \partial_{\varphi}, \rho \partial_{\rho}\right), \quad \mathscr{D}_{R}(\Lambda)=R^{-1} \mathcal{D}\left(\varphi, \partial_{\varphi}, \Lambda\right), \quad \xi=(\rho \cos (\varphi), \rho \sin (\varphi)) .
$$

The form (38) is inspired by the following observation, proofed in [NSN04]:

Any power-law solution $U(\xi)=|\xi|^{\lambda} \Phi(\varphi)$ with $\lambda=k / 2, k \in \mathbb{Z}$, fulfills the relation

$$
\begin{equation*}
\left(\mathscr{N}_{R}(\lambda) U, v\right)_{\Gamma_{R}}=-b\left(U, v ; \Gamma_{R}\right)_{\Lambda=\lambda} \tag{40}
\end{equation*}
$$

where $v$ is an arbitrary smooth function.

A solution of (39) is unique and exists, if the right-hand side is self-balanced. Moreover, for the approximation error the following estimation is valid [NSN04]:

$$
\begin{aligned}
\left\|\nabla\left(u-u^{R}\right) ; L^{2}\left(\Omega_{R}\right)\right\|+\left\|(1+|x|)^{-1}\left(u-u^{R}\right) ; L^{2}\left(\Omega_{R}\right)\right\| & \\
& \leq c R^{-1 / 2} \log (R)\left\|g ; L^{2}\left(\Xi_{R}\right)\right\|, \quad c>0
\end{aligned}
$$

For a more detailed discussion on artificial boundary conditions we refer to [NSN04] and the literature cited there.

Similar to the computation of global integral characteristics, we are interested in a cell-based error estimator for the numerical computation of the coefficients $M_{i, l}^{j, k}(\theta)$. In order to apply the dual-weighted-residual approach, we use the integral representation (27) and define the functionals

$$
J^{i, l}\left(\eta^{j, k}\right):=M_{i, l}^{j, k}(\theta)=\sum_{ \pm}\left(\int_{\Upsilon \pm(\theta)} \widetilde{\eta}^{i, l}(\xi) \cdot \mathscr{N}\left(\nabla_{\xi}\right) \widetilde{\eta}^{j, k}(\xi) d s\right)
$$

The finite element approximation of the solutions $\widetilde{\eta}^{j, k}$ reads

$$
\widetilde{\eta}_{h}^{j, k} \in V_{h}: \quad a\left(\widetilde{\eta}_{h}^{j, k}, v_{h} ; \Omega_{R}\right)+b\left(\widetilde{\eta}_{h}^{j, k}, v_{h} ; \Gamma_{R}\right)_{\Lambda=-1 / 2}=-\sum_{ \pm}\left(v_{h}, \mathscr{N} U^{j, k}\right)_{\Upsilon \pm(\theta)}, \quad v_{h} \in V_{h}
$$

but we omit an additional index " $R$ " for finite element solutions of the artificial approximation problem (37). This approximation scheme also features the "GALERKIN orthogonality" for the error $e^{j, k}:=$ $\widetilde{\eta}^{j, k}-\widetilde{\eta}_{h}^{j, k}:$

$$
a\left(e^{j, k}, v_{h} ; \Omega_{R}\right)+b\left(e^{j, k}, v_{h} ; \Gamma_{R}\right)_{\Lambda=-1 / 2}=0, \quad v_{h} \in V_{h}
$$

With a solution $z^{i, l}$ of the dual problem

$$
z^{i, l} \in V: \quad a\left(v, z^{i, l} ; \Omega_{R}\right)+b\left(v, z^{i, l} ; \Gamma_{R}\right)_{\Lambda=-1 / 2}=J^{i, l}(v), \quad v \in H^{1}\left(\Omega_{R}\right)
$$

at hand, the Galerkin orthogonality and integration by parts lead to the following error representa-
tion:

$$
\begin{aligned}
J^{i, l}\left(e^{j, k}\right)= & a\left(e^{j, k}, z^{i, l} ; \Omega_{R}\right)+b\left(e^{j, k}, z^{i, l} ; \Gamma_{R}\right)_{\Lambda=-1 / 2} \\
= & a\left(e^{j, k}, z^{i, l}-I_{h} z^{i, l} ; \Omega_{R}\right)+b\left(e^{j, k}, z^{i, l}-I_{h} z^{i, l} ; \Gamma_{R}\right)_{\Lambda=-1 / 2} \\
= & \sum_{K \in \mathcal{T}_{h}}\left\{\left(\mathscr{L} \widetilde{\eta}^{j, k}-\mathscr{L} \widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{K}+\left(\mathscr{N} \widetilde{\eta}^{j, k}-\mathscr{N} \widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{\partial K}\right\} \\
& +b\left(e^{j, k}, z^{i, l}-I_{h} z^{i, l} ; \Gamma_{R}\right)_{\Lambda=-1 / 2} \\
= & \sum_{K \in \mathcal{T}_{h}}\left\{\left(-\mathscr{L} \widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{K}-\frac{1}{2}\left(\left[\mathscr{N} \widetilde{\eta}_{h}^{j, k}\right], z^{i, l}-I_{h} z^{i, l}\right)_{\partial K \backslash \partial \Omega_{R}}\right. \\
& \left.\quad+\left(\mathscr{N} e^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{\partial K \cap \Gamma_{R}}+\left(-\mathscr{N} U^{j, k}-\mathscr{N} \widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{\partial K \cap \Xi_{R}^{ \pm}}\right\} \\
& \quad+b\left(e^{j, k}, z^{i, l}-I_{h} z^{i, l} ; \Gamma_{R}\right)_{\Lambda=-1 / 2}
\end{aligned}
$$

Up to the integrals over the artificial boundary, this is a cell-wise representation of the error in terms of residuals and weights similar to (35). By construction of the artificial boundary condition, the solution $u^{R}$ of the approximation problem (37) on $\Omega_{R}$ fulfills

$$
b\left(u^{R}, v ; \Gamma_{R}\right)_{\Lambda=-1 / 2}+\left(\mathscr{N} u^{R}, v\right)_{\partial K \cap \Gamma_{R}}=0, \quad v \in H^{1}\left(\Omega_{R}\right)
$$

Using this relation, the error can be estimated to

$$
\begin{align*}
\left|J^{i, l}\left(e^{j, k}\right)\right| \leq & \sum_{K \in \mathcal{T}_{h}}\left\{\left\|\mathscr{L} \widetilde{\eta}_{h}^{j, k} ; L^{2}(K)\right\|\left\|z^{i, l}-I_{h} z^{i, l} ; L^{2}(K)\right\|\right. \\
& +\frac{1}{2}\left\|\left[\mathscr{N} \widetilde{\eta}_{h}^{j, k}\right] ; L^{2}\left(\partial K \backslash \partial \Omega_{R}\right)\right\|\left\|z^{i, l}-I_{h} z^{i, l} ; L^{2}\left(\partial K \backslash \partial \Omega_{R}\right)\right\| \\
& +\left|\left(\mathscr{N} \widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l}\right)_{\partial K \cap \Gamma_{R}}+b\left(\widetilde{\eta}_{h}^{j, k}, z^{i, l}-I_{h} z^{i, l} ; \partial K \cap \Gamma_{R}\right)_{\Lambda=-1 / 2}\right| \\
& \left.+\left\|-\mathscr{N} U^{j, k}-\mathscr{N} \widetilde{\eta}_{h}^{j, k} ; L^{2}\left(\partial K \cap \Xi_{R}^{ \pm}\right)\right\|\left\|z^{i, l}-I_{h} z^{i, l} ; L^{2}\left(\partial K \cap \Xi_{R}^{ \pm}\right)\right\|\right\} \tag{41}
\end{align*}
$$

Besides the numerical error depending on the global mesh width $h$, computed values are always left with an approximation error depending on the radius $R$, which can not be overcome. In [Ste09] the following error estimation for the total error was established:

$$
\left|M_{i, l}^{j, k}(\theta)-M_{h}^{R}\right| \leq c\left(R^{-1 / 2} \log (R)+h^{1 / 2}\right)\left\|U^{j, k} ; L^{2}\left(\Xi_{R}\right)\right\|\left\|U^{i, l} ; L^{2}\left(\Xi_{R}\right)\right\|, \quad c>0
$$

The constant $c$ depends on the shape of $\Upsilon(\theta)$, but not on $h$ and $R$. We see, that in order to get a small approximation error, the radius $R$ has to be chosen very large, but in order to get a small numerical error, the global mesh width $h$ has to be chosen very small. For a large radius $R$ a small mesh width $h$ will result in a lot of cells $K$ in the discretization of the domain $\Omega_{R}$. One has to balance this two influences on the global error. A tendency for the choices of $R$ and $h$ can be seen from the following example: Evaluating the quantity $\log (50) / \sqrt{50} \approx 0.55$, a very fine discretization of the domain $\Omega_{R}$ is needed to reach a global mesh width $\sqrt{h} \approx 0.55$. This indicates that the main influence on the accuracy of the numerical values of $M_{i, l}^{j, k}(\theta)$ is the global mesh width and we will see this from numerical examples in the next paragraph.

## 5. Examples

Finally, we show some numerical results. We consider a symmetric compact tension (CTS-) specimen (see figure 4) especially developed for simulating mixed-mode situations [Ric85]. Using a special designed loading device, a force $F$ can be applied directed at any angle $0^{\circ} \leq \alpha \leq 90^{\circ}$ to the crack and several scenarios from pure Mode-I to pure Mode-II can be realized at the crack tip. Depending on the angle $\alpha$, the resulting forces at the holes are (see figure 4)

$$
\begin{array}{ll}
F_{1}=F_{8}=F\left(\frac{1}{2} \cos (\alpha)+\sin (\alpha)\right), & F_{2}=F_{7}=F \sin (\alpha) \\
F_{3}=F_{6}= \begin{cases}F_{1}-2 F_{2}, & \alpha<22.56^{\circ}, \\
0, & \text { otherwise },\end{cases} & F_{4}=F_{5}= \begin{cases}2 F_{2}-F_{1}, & \alpha>22.56^{\circ} \\
0, & \text { otherwise }\end{cases}
\end{array}
$$

The force and the length units are selected to $F=10000 \mathrm{~N}$ and $w=90 \mathrm{~mm}$, the specimen is of thickness 10 mm . The initial crack length is $a=45 \mathrm{~mm}$ for calculating stress intensity factors and $a=57 \mathrm{~mm}$ for computing crack paths. CARTESIAN coordinates are centered at the initial crack tip.
The CTS-specimen is well studied for isotropic homogeneous materials and is suitable to test numerical methods. Interpolated and numerical values for SIFs are given e.g. in [Ric85] and experimental results for crack paths in this specimen made of aluminium alloy 7075-T651 under different loading angles are shown in [RS09].


Figure 4: Compact tension (CTS-)specimen.

All numerical computations are done with the software package MCrack2D, developed at the Institute of Analysis and Applied Mathematics at the University of Kassel. MCrack2D is a pure research code with the intention to realize an exact-as-possible transfer of analytical models to numerics in order to test and improve theoretical ideas and make them finally applicable to real-world problems. Today,

MCrack2D can handle anisotropic, homogeneous and especially functional graded materials. Within MCrack2D the library deal.II (see [BHK07] and dealii.org) is used for finite element calculations coupled with the mesh generator Cubit from Sandia National Laboratories (cubit.sandia.gov) and other in-house developed modules for handling crack problems. The library deal.II uses finite elements based on quadrilateral cells only and provides very fast algorithms for assembling matrices, for solving systems of algebraic equations and also mesh refinement using hanging nodes (see the documentation at dealii.org for detailed information). In MCrack2D we use bilinear and biquadratic Lagrange elements. The mesh generator Cubit is controlled with the script language Python and nearly arbitrary geometries can be handled.

In the following we present numerical results for SIFs, the local integral characteristics $M_{i, j}(\theta)$ and results for the initial kink angle of the crack. Finally, we compute crack paths. In order to compare our results with the literature, we start with an isotropic homogeneous material, Aluminium Alloy 7075-T651. To show the influence of an anisotropy and of the surface energy, we show results for an orthotropic material with two axes of elastic symmetry given in $\left[\mathrm{BSHW}^{+} 05\right]$. Finally, we calculate the crack path for a functionally graded material.
All numerical results for SIFs are computed using formulae (24), where the integration domain $G$ is chosen as a circle of diameter 1 mm (see figure 6). All this calculations use the same initial mesh, adaptively refined eight times using the dual-weighted-residual approach and the error estimator from (35). Displacement fields are approximated by bilinear elements, dual solutions by biquadratic elements and computed by solving the elasticity problem (2), algebraic linear systems are solved with a modified conjugated gradient method using projections (see e.g. [SF07]). Numerical values for the local integral characteristics $M_{i, l}^{j, k}(\theta)$ are evaluated using (27). Adaptive mesh refinement is based on the error estimator given in (41) and algebraic linear systems are solved with a conjugated gradient method coupled with a geometrical multigrid preconditioner developed in [JK11]. Kink angles are calculated as the minimum of the difference of the surface energy and the energy release rate (25):

$$
\begin{aligned}
\theta_{0} & =\min _{\theta \in(-\pi, \pi)}\left(2 \gamma(\theta)-\mathscr{G}_{0}(\theta)\right) \\
& =\min _{\theta \in(-\pi, \pi)}\left(2 \gamma(\theta)-\frac{1}{2}\left(K_{I}^{2} M_{1,1}^{1,1}(\theta)+2 K_{I} K_{I I} M_{2,1}^{1,1}(\theta)+K_{I I}^{2} M_{2,1}^{2,1}(\theta)\right)\right)
\end{aligned}
$$

The integral characteristics $M_{i, 1}^{j, 1}(\theta)$ are calculated numerically for a set of discrete values $\theta$ and the minimum is found by cubic spline interpolation. For the simulation of crack paths we always consider a periodic cyclic loading and fix the crack shoot length to 0.5 mm . The circle mesh at the grid tip is always the same, but the specimen is being refined completely in every simulation step.

### 5.1 Numerical Results for Homogeneous Materials

We consider the CTS-specimen as described in figure 4 composed of Aluminium alloy 7075-T651 with LAMÉ constants $\lambda=56023 \mathrm{~N} / \mathrm{mm}^{2}, \mu=26364 \mathrm{~N} / \mathrm{mm}^{2}$, related to elastic moduli by $a_{11}=a_{22}=\lambda+2 \mu$, $a_{21}=\lambda, a_{31}=a_{32}=0, a_{33}=\mu$. Numerical results of SIFs for different loading angles $\alpha$ are given in table 2. In comparison to the numerical and interpolated values given in table 1 from [Ric85], our values are slightly larger and the question appears, which results are more accurate? To answer this question, we look at the error $J(e)$ evaluated during the refinement steps, exemplary shown for $K_{I}$ and an load angle $\alpha=0^{\circ}$ in table 3 together with the number of DoF, the minimal and maximal diameter of cells $K$ and the averaged cell diameter. In every step, about $30 \%$ of the cells with the largest error indicators are being refined, this increases the number of DoF about a factor of two. We see that at the same time the numerical error $J(e)$ is reduced by factor of two and this shows the good performance of the dual-weighted-residual approach. After eight refinement steps we get an numerical
value $J\left(u_{h}\right)=379.7451$ and an error about $|J(e)| \approx 0.0716$. But especially this absolute value of the error $|J(e)|$ should not be overstated. This value is only an estimation and there can be also rounding errors and errors from numerical integration. Nevertheless, $|J(e)|$ should always overestimate the real absolute error of the numerical value.
We remark, that $K_{I}$ becomes negative for a pure Mode-II scenario $\left(\alpha=90^{\circ}\right)$. But this means penetration of crack surfaces and is physically not possible. The negative value indicates the contact of crack surfaces, which also can be seen from experiments and is realistic for this scenario [RS09]. Up to now, we do not use a non-penetration condition in computations and if a calculated value $K_{I}$ becomes negative, we set this quantity to zero for the calculation of kink angles.

Table 1: Stress intensity factors from [Ric85], initial crack length $a=45 \mathrm{~mm}$.

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $K_{I, \text { int }}$ | 371.75 | 359.08 | 321.94 | 262.87 | 185.87 | 96.21 | 0.00 |
| $K_{\text {II,int }}$ | 0.00 | -47.64 | -92.04 | -130.17 | -159.43 | -177.82 | -184.10 |
| $K_{I, \text { num }}$ | 375.19 | 359.34 | 319.70 | 257.61 | 178.35 | 85.87 | 10.56 |

Table 2: Calculated stress intensity factors, MCrack2D.

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $K_{I}$ | 379.74 | 364.79 | 324.95 | 262.84 | 182.81 | 90.33 | -8.29 |
| $K_{I I}$ | 0.0033 | -47.23 | -91.45 | -130.10 | -159.89 | -178.79 | -185.49 |
| $K_{T}$ | $-1.63 \mathrm{E}-05$ | $-2.76 \mathrm{E}-05$ | $-3.85 \mathrm{E}-05$ | $-5.12 \mathrm{E}-05$ | $-6.04 \mathrm{E}-05$ | $-6.55 \mathrm{E}-05$ | $-6.61 \mathrm{E}-05$ |
| $k_{1,3}$ | 2.87 | 2.59 | 2.12 | 1.45 | 0.67 | -0.14 | -0.95 |
| $k_{2,3}$ | 0.01 | 0.37 | 0.72 | 1.07 | 1.34 | 1.52 | 1.59 |

Table 3: Calculated stress intensity factor $K_{I}$ and errors, MCrack2D.

| $n$ | $\#$ DoF | $J\left(u_{h}\right)$ | $\|J(e)\|$ | $h_{\min }$ | $h_{\max }$ | $\sum_{K} h_{K} / \#$ cells |
| :--- | ---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 64442 | 377.5210 | 9.0125 | 0.0439 | 4.43 | 1.66 |
| 1 | 122092 | 378.5908 | 4.5787 | 0.0218 | 4.43 | 1.14 |
| 2 | 243710 | 379.2338 | 2.2640 | 0.0109 | 4.43 | 0.75 |
| 3 | 478668 | 379.4759 | 1.1652 | 0.0055 | 4.43 | 0.51 |
| 4 | 946754 | 379.6424 | 0.5716 | 0.0027 | 3.29 | 0.36 |
| 5 | 1845438 | 379.6923 | 0.2901 | 0.0013 | 2.83 | 0.25 |
| 6 | 3606162 | 379.7333 | 0.1410 | 0.0006 | 2.83 | 0.18 |
| 7 | 6999588 | 379.7451 | 0.0716 | 0.0003 | 2.10 | 0.13 |

For isotropic materials, the local integral characteristics $M_{i, 1}^{j, 1}(0)=M_{i, j}(0)$ for a straight crack shoot
are known explicitly (29):

$$
M_{1,1}(0)=M_{2,2}(0)=\frac{\lambda+2 \mu}{2 \mu(\lambda+\mu)}=2.5033 E-05, \quad \quad M_{1,2}(0)=M_{2,1}(0)=0
$$

In order to show the influence of the radius $R$ of the artificial circle boundary on the numerical results, we first calculate $M_{1,1}(0)$ for different values $R$ and we refine the mesh adaptively using the error estimator from (41) till the global mesh width $h_{\max }$ is in the same order of magnitude for the different finite element discretizations. The results together with the global mesh width $h_{\max }$, the number of degrees of freedom ( DoF ), the numerically estimated error $|J(e)|$ and the absolute error are given in table 4. An adaptive refined mesh is shown in figure 5 . The results clearly show, that the total error decreases with larger radius $R$ using nearly the same global mesh width $h_{\text {max }}$, but this higher precision can only by obtained with a numerous higher number of DoF. The results for $R=50$ take eight refinement steps, the results for $R=250$ take fourteen refinement steps, always computing a bilinear and a biquadratic finite element solution. Looking to the last row in table 4, we see the results for $R=50$ after fourteen refinement steps. Here, $h_{\max }$ is much smaller and also the number of DoF is lower than for $R=250$, but the precision is nearly the same. All this results clearly indicate the influence of the mesh width. The calculated error $|J(e)|$ is a bit larger for $R=50$ than for $R=250$ and computing more refinement steps will finally result in a higher precision for $R=250$, of course, but this will need a lot more computing time, not needed for the calculation of kink angles. We remark, that the numerically calculated value $|J(e)|$ is smaller than the absolute error. This quantity estimates the error of the functional value calculated with a solution of the approximation problem depending on $R$. Because we are always left with an approximation error depending on $R$, this value can be smaller. We will not reach the exact value and this is reflected here. Using $R=50$ and approximately 5 million DoF, calculated values for $M_{i, j}(\theta)$ for $\theta$ between $-90^{\circ}$ and $+90^{\circ}$ are plotted in figure 12 to 15. Numerical values are calculated for nineteen different kink angles and interpolated by a cubic spline.

Table 4: Calculated values $M_{1,1}(0)$ and errors, MCrack2D.

| R | $\# \mathrm{DoF}$ | $h_{\max }$ | $M_{1,1}^{R, h}$ | $\|J(e)\|$ | $\left\\|M_{1,1}^{R, h}-M_{1,1}\right\\|$ |
| ---: | ---: | ---: | :---: | :---: | :---: |
| 50 | 116118 | 6.25 | $2.4640 \mathrm{E}-05$ | $1.11 \mathrm{E}-07$ | $3.22 \mathrm{E}-07$ |
| 100 | 910386 | 6.33 | $2.4912 \mathrm{E}-05$ | $1.51 \mathrm{E}-08$ | $1.20 \mathrm{E}-07$ |
| 150 | 2019246 | 9.22 | $2.4950 \mathrm{E}-05$ | $7.21 \mathrm{E}-09$ | $8.28 \mathrm{E}-08$ |
| 250 | 7455810 | 7.96 | $2.4993 \mathrm{E}-05$ | $1.94 \mathrm{E}-09$ | $3.97 \mathrm{E}-08$ |
| 50 | 5035998 | 1.59 | $2.4992 \mathrm{E}-05$ | $2.37 \mathrm{E}-09$ | $4.00 \mathrm{E}-08$ |

Using this numerical values the initial kink angle can be calculated for different load scenarios. Here, the surface energy is constant for all directions and does not have an influence on the kink angle. The results for an initial kink length $a=45 \mathrm{~mm}$ are presented in table 5 compared to results from the literature also based on the energy principle. Our numerical values are also in good agreement with the experimental results obtained in [RS09].
Finally we calculate the crack path for an load angle $\alpha=90^{\circ}$ and an initial crack with length $a=57 \mathrm{~mm}$. The result is shown in figure 7 . We stop the simulation after 47 simulation steps when a critical value $K_{V}=0.5 K_{I}+0.5 \sqrt{K_{I}^{2}+5.336 K_{I I}^{2}}=972 N / \mathrm{mm}^{3 / 2}$ is reached (compare with [RS09]). The length of each crack shoot is fixed to 0.5 mm . The crack path is nearly similar to the cracks obtained from experiments results given in [RS09]. Because we only calculate a two-dimensional problem, we can not
expect total agreement with "real-world".


Figure 5: Artificial grid, adaptively refined for $M_{1,1}(0), R=50$.

Table 5: Comparison of kink angles $\theta_{0}$, Aluminium Alloy 7075-T651.

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| MCrack2D | $0 .^{\circ}$ | $14.39^{\circ}$ | $28.44^{\circ}$ | $41.76^{\circ}$ | $54.15^{\circ}$ | $65.65^{\circ}$ | $75.79^{\circ}$ |
| [Nui75] | $0 .^{\circ}$ | $14.3^{\circ}$ | $27.8^{\circ}$ | $40.9^{\circ}$ | $53.2^{\circ}$ | $64.2^{\circ}$ | $70.5^{\circ}$ |
| [HPU74] | $0 .^{\circ}$ | $15.1^{\circ}$ | $29.6^{\circ}$ | $43.1^{\circ}$ | $55.2^{\circ}$ | $65.7^{\circ}$ | $75.1^{\circ}$ |
| [ABDV80] | $0 .^{\circ}$ | $14.4^{\circ}$ | $29.2^{\circ}$ | $42.0^{\circ}$ | $54.4^{\circ}$ | $66.1^{\circ}$ | $79.0^{\circ}$ |

Numerical results for an orthotropic material. We consider the CTS-specimen composed of an anisotropic material with two axes of elastic symmetry given in $\left[\mathrm{BSHW}^{+} 05\right]$. In contrast to isotropic materials, the surface energy depends in the direction of the crack. At an axis of elastic symmetry, surface energy has a minimum and if $a_{31}=a_{32}=0$, surface energy is also symmetric. Because we do not have any other data at hand, we model the surface energy to

$$
\gamma(\theta)=\frac{c_{2}-c_{1}}{2}(1-\cos (4 \theta))+c_{1}, \quad c_{1}=3.5, \quad c_{2}=4.0
$$

In the following, we are not interested in absolute numerical values, we only want to show, that surface energy really has an influence on kink angles and crack paths. Depending on the symmetry axes, one


Figure 6: Meshed CTS-specimen with circle mesh around the tip.


Figure 7: Crack path, Aluminium alloy 7075-T651, $\alpha=90^{\circ}$.
can define CARTESIAN "material" coordinates $z$, related to "crack" coordinates $x$ by an angle $\beta$, see also figure 8:

$$
x=m \cdot z, \quad \quad m=\left(\begin{array}{cc}
\cos (\beta) & \sin (\beta) \\
-\sin (\beta) & \cos (\beta)
\end{array}\right)
$$

We show numerical results for different material angles $\beta$ and calculated crack paths for $\beta=0^{\circ}$ (the crack is on an axis of elastic symmetry) and $\beta=45^{\circ}$. Depending on the angle $\beta$, elastic moduli in crack coordinates are given in table 6. Values for SIFs with initial crack length $a=45 \mathrm{~mm}$ are given in table 7 and 8 , kink angles in table 9 . The influence of the surface energy on the kink angles can be seen from figure 19 and 20. But there is another influence of the surface energy. In table 9 we see, that there is no kink angle for load angles greater then $\alpha=75^{\circ}$. In this case, the minimum of the change of total energy is positive and we do not have crack propagation and no kink angle. With an initial crack length of $a=57 \mathrm{~mm}$ the simulated crack paths depending on the (also plotted) axes of elastic symmetry are presented in figure 9 and figure 10 . The influence of the surface energy can be clearly seen. But we remark again, that we only use a model for the surface energy. The absolute values of kink angles and energy release for this material can not be seen from this calculations.


Figure 8: Material and crack coordinate systems.

Table 6: Elastic moduli for different material angles $\beta$.

|  | $a_{11}$ | $a_{21}$ | $a_{22}$ | $a_{31}$ | $a_{32}$ | $a_{33}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| $\beta=0^{\circ}$ | 10080.60 | 806.45 | 8064.52 | 0.00 | 0.00 | 4000.00 |
| $\beta= \pm 15^{\circ}$ | 9912.32 | 839.72 | 8166.31 | $\mp 309.64$ | $\mp 194.39$ | 4033.27 |
| $\beta= \pm 30^{\circ}$ | 9476.81 | 906.25 | 8468.75 | $\mp 494.12$ | $\mp 378.88$ | 4099.80 |
| $\beta= \pm 45^{\circ}$ | 8939.52 | 939.52 | 8939.52 | $\mp 504.03$ | $\mp 504.03$ | 4133.06 |

### 5.2 Numerical Results for a Functionally Graded Material

Finally we consider the CTS-specimen composed of Aluminium alloy 7075-T651 with a local gradation in one space direction. We choose the Hooke matrix to

$$
A(x)=(1+\delta(x)) A, \quad \delta(x):= \begin{cases}c \sin \left(\frac{\left(x_{1}-16\right)}{4} \pi\right), & 16<x_{1}<20  \tag{42}\\ 0, & \text { otherwise }\end{cases}
$$



Figure 9: Crack path, orthotropic Figure 10: Crack path, orthotropic material, $\beta=0^{\circ}$.
material, $\beta=45^{\circ}$.

The gradation is modeled with the function $\delta$ (see figure 11) and the intensity of the gradation can be controlled by the factor $c$, where $c>0$ increases and $c<0$ decreases the stiffness of the material in the region $16<x_{1}<20$. Because this function is not smooth, we flatten out $A(x)$ at the points $x_{1}=16$ and $x_{1}=20$. This is only technical and we do not go into details. The motivation of this simple example is just: "What can happen, if the material is locally functionally graded?"

The computed stress intensity factors at the initial crack tip ( $a=45 \mathrm{~mm}$ ) for different angles $\alpha$ and several values of the gradation factor $c$ are presented in table 10 and 11 . We can see the influence of the gradation. Increasing the factor $c$ results in a decreasing SIF $K_{I}$ and an (slightly) increasing SIF $K_{I I}$. As one expects, increasing the stiffness of the material, even away from the crack tip, reduces crack opening and effects in a higher sliding of the crack faces and vice versa. But looking to table 12 , the influence of this effects on the initial kink angle $\theta_{0}$ is only small. At last we compute the crack path for a loading angle $\alpha=90^{\circ}$ and a gradation factor $c=5.0$. The result is shown in figure 11 . Increasing the stiffness of the material acts like a local "barrier" on the crack. The crack does not cross the gradation zone. We finally want to remark, that these numerical results have to be interpreted carefully. Especially in functionally graded materials crack propagation depends significantly on the local material properties as the surface energy. Such effects are not be taken into account in this simulation, because we have only considered a theoretical model for a functional graded material with no additional data at hand.

## 6. Conclusion

In this chapter, some ideas for simulating quasi-static crack propagation in functionally graded materials were presented. Based on a mathematical formulation of the Griffith' energy principle, formulae for the change of potential energy in homogeneous and inhomogeneous materials were shown based on asymptotic decompositions of solutions of the linear elasticity problem. These asymptotic decompositions consists of power-law solutions and a normalization of this solutions related to the energy fracture criterion was discussed. Differences between homogeneous and inhomogeneous materials were figured out in detail. In order to make theoretical results applicable for practical problems, a quasi-static framework for crack propagation was shown. Methods for the numerical calculation of certain quantities of interest in this context were presented. Numerical results for homogeneous and inhomogeneous


Figure 11: Crack path in FGM, $c=5.0, \alpha=90^{\circ}$, MCrack2D.
materials were shown and are in good agreement with experiments. Quasi-static crack propagation in functionally graded materials can be predicted for plane problems, but for the application to practical problems and especially to determine the speed of the crack, experimental data such as surface energy are necessarily needed.

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Figure 12: $M_{1,1}(\theta)$, Aluminium alloy Figure 13: $\quad M_{1,2}(\theta)$, Aluminium alloy 7075-T651. 7075-T651.



Figure 14: $M_{2,1}(\theta)$, Aluminium alloy Figure 15: $\quad M_{2,2}(\theta)$, Aluminium alloy 7075-T651. 7075-T651.

Table 7: Calculated SIFs $K_{I}$, orthotropic material, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $\beta=-45^{\circ}$ | 377.56 | 366.57 | 330.58 | 271.99 | 194.86 | 104.45 | 6.93 |
| $\beta=-30^{\circ}$ | 410.87 | 398.29 | 358.53 | 294.22 | 209.86 | 111.19 | 4.95 |
| $\beta=-15^{\circ}$ | 439.68 | 424.69 | 380.70 | 310.61 | 219.35 | 113.14 | -0.76 |
| $\beta=0^{\circ}$ | 451.35 | 433.91 | 386.83 | 313.21 | 218.24 | 108.39 | -8.83 |
| $\beta=+15^{\circ}$ | 439.68 | 420.60 | 372.79 | 299.38 | 205.57 | 97.75 | -16.72 |
| $\beta=+30^{\circ}$ | 410.87 | 391.39 | 345.18 | 275.25 | 186.58 | 85.18 | -22.01 |
| $\beta=+45^{\circ}$ | 377.56 | 358.81 | 315.57 | 250.65 | 168.66 | 75.17 | -23.44 |

Table 8: Calculated SIFs $K_{I I}$, orthotropic material, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $\beta=-45^{\circ}$ | -11.06 | -57.66 | -100.57 | -137.44 | -164.95 | -181.22 | -185.14 |
| $\beta=-30^{\circ}$ | -10.17 | -58.19 | -102.47 | -140.52 | -169.00 | -185.96 | -190.25 |
| $\beta=-15^{\circ}$ | -6.17 | -55.58 | -101.42 | -141.04 | -171.05 | -189.40 | -194.84 |
| $\beta=0^{\circ}$ | $2.66 \mathrm{E}-03$ | -50.09 | -96.96 | -137.86 | -169.36 | -189.32 | -196.38 |
| $\beta=+15^{\circ}$ | 6.17 | -43.48 | -90.35 | -131.64 | -163.96 | -185.11 | -193.65 |
| $\beta=+30^{\circ}$ | 10.18 | -38.22 | -84.19 | -124.96 | -157.21 | -178.75 | -188.11 |
| $\beta=+45^{\circ}$ | 11.06 | -35.94 | -80.65 | -120.41 | -151.95 | -173.14 | -182.53 |

Table 9: Calculated kink angles $\theta_{0}$, orthotropic material, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $\beta=0^{\circ}$ | $0.00^{\circ}$ | $9.9^{\circ}$ | $21.0^{\circ}$ | $37.9^{\circ}$ | $63.9^{\circ}$ | $76.2^{\circ}$ | -- |
| $\beta=+15^{\circ}$ | $-4.6^{\circ}$ | $7.3^{\circ}$ | $26.7^{\circ}$ | $50.3^{\circ}$ | $62.5^{\circ}$ | $70.1^{\circ}$ | -- |
| $\beta=+30^{\circ}$ | $-7.0^{\circ}$ | $13.5^{\circ}$ | $36.3^{\circ}$ | $48.4^{\circ}$ | $56.9^{\circ}$ | $63.6^{\circ}$ | -- |
| $\beta=+45^{\circ}$ | $-0.3^{\circ}$ | $21.6^{\circ}$ | $33.9^{\circ}$ | $43.2^{\circ}$ | $50.7^{\circ}$ | $56.5^{\circ}$ | -- |



Figure 16: $M_{1,1}(\theta ; \beta)$, orthotropic material.


Figure 17: $M_{1,2}(\theta ; \beta)=M_{2,1}(\theta ; \beta)$, orthotropic material.


Figure 18: $M_{2,2}(\theta ; \beta)$, orthotropic material.


Figure 19: $\mathscr{G}_{0}(\theta)$ and $2 \gamma(\theta)$, orthotropic material, $\alpha=90^{\circ}, \beta=0^{\circ}$.


Figure 20: $\mathscr{G}_{0}(\theta)$ and $2 \gamma(\theta)$, orthotropic material, $\alpha=90^{\circ}, \beta=45^{\circ}$.

Table 10: Computed SIFs $K_{I}$, FGM, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $c=-0.75$ | 394.28 | 378.59 | 337.04 | 272.30 | 189.00 | 92.83 | -9.67 |
| $c=-0.25$ | 382.87 | 367.76 | 327.55 | 264.91 | 184.21 | 90.96 | -8.49 |
| $c=+0.00$ | 379.74 | 364.79 | 324.95 | 262.84 | 182.81 | 90.33 | -8.29 |
| $c=+0.25$ | 377.16 | 362.34 | 322.79 | 261.11 | 181.63 | 89.77 | -8.19 |
| $c=+0.75$ | 372.88 | 358.28 | 319.20 | 258.20 | 179.60 | 88.76 | -8.12 |
| $c=+2.00$ | 364.67 | 350.47 | 312.29 | 252.51 | 175.53 | 86.59 | -8.26 |
| $c=+5.00$ | 351.01 | 337.45 | 300.70 | 242.83 | 168.41 | 82.51 | -9.01 |

Table 11: Computed SIFs $K_{I I}$, FGM, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $c=-0.75$ | 0.0034 | -47.99 | -92.96 | -132.33 | -162.70 | -181.97 | -188.85 |
| $c=-0.25$ | 0.0033 | -47.33 | -91.66 | -130.43 | -160.32 | -179.29 | -186.04 |
| $c=+0.00$ | 0.0033 | -47.23 | -91.45 | -130.10 | -159.89 | -178.79 | -185.49 |
| $c=+0.25$ | 0.0033 | -47.17 | -91.33 | -129.90 | -159.61 | -178.46 | -185.13 |
| $c=+0.75$ | 0.0032 | -47.13 | -91.22 | -129.68 | -159.30 | -178.06 | -184.68 |
| $c=+2.00$ | 0.0031 | -47.14 | -91.22 | -129.52 | -159.00 | -177.65 | -184.19 |
| $c=+5.00$ | 0.0030 | -47.29 | -91.43 | -129.61 | -158.95 | -177.46 | -183.87 |

Table 12: Calculated kink angles $\theta_{0}$, FGM, MCrack2D

|  | $\alpha=0^{\circ}$ | $\alpha=15^{\circ}$ | $\alpha=30^{\circ}$ | $\alpha=45^{\circ}$ | $\alpha=60^{\circ}$ | $\alpha=75^{\circ}$ | $\alpha=90^{\circ}$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $c=-0.75$ | $0.0^{\circ}$ | $14.1^{\circ}$ | $27.9^{\circ}$ | $41.3^{\circ}$ | $53.9^{\circ}$ | $65.5^{\circ}$ | $75.8^{\circ}$ |
| $c=-0.25$ | $0.0^{\circ}$ | $14.3^{\circ}$ | $28.3^{\circ}$ | $41.6^{\circ}$ | $54.1^{\circ}$ | $65.6^{\circ}$ | $75.8^{\circ}$ |
| $c=+0.00$ | $0.0^{\circ}$ | $14.4^{\circ}$ | $28.4^{\circ}$ | $41.8^{\circ}$ | $54.2^{\circ}$ | $65.7^{\circ}$ | $75.8^{\circ}$ |
| $c=+0.25$ | $0.0^{\circ}$ | $14.5^{\circ}$ | $28.5^{\circ}$ | $41.9^{\circ}$ | $54.3^{\circ}$ | $65.7^{\circ}$ | $75.8^{\circ}$ |
| $c=+0.75$ | $0.0^{\circ}$ | $14.6^{\circ}$ | $28.7^{\circ}$ | $42.1^{\circ}$ | $54.4^{\circ}$ | $65.8^{\circ}$ | $75.8^{\circ}$ |
| $c=+2.00$ | $0.0^{\circ}$ | $14.9^{\circ}$ | $29.2^{\circ}$ | $42.6^{\circ}$ | $54.8^{\circ}$ | $66.0^{\circ}$ | $75.8^{\circ}$ |
| $c=+5.00$ | $0.0^{\circ}$ | $15.5^{\circ}$ | $30.2^{\circ}$ | $43.5^{\circ}$ | $55.6^{\circ}$ | $66.5^{\circ}$ | $75.8^{\circ}$ |

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