MICROMECHANICS AND CRACK SPECTRA

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Micromechanics can describe defects and their mechanical interactions by means of analytical and computer methods as well. Some results are reported concerning simulation of defect interaction connected with cracks. Two experimental methods are discussed which allow to measure microdeformations within crack-tip regions by means of lasers (holographic J measurement etc.) and scanning electron microscopy ("micro-moiré method). A hypothesis is established concerning crack electron spectra due to the microdeformation effects. The latter is explained in terms of the deformation potential approach.

INTRODUCTION

Modern fracture mechanics is assumed to be based upon two main pillars: phenomenological (macroscopic) fracture modeling and structural (microscopic, micromechanical) fracture mechanics. However, most fracture problems can only be solved taking into account both macroscopic and microscopic aspects. The concept of the crack tip immediate surroundings ("process region" etc) is a characteristic example, how the microscopic approach and the phenomenological concept "meet" each other within a "transition region" of modeling. Within the nearest crack tip region defect mechanisms play the dominant part in the fields of crack initiation and crack propagation as well. Mechanical interaction between different kinds of defects (such as point defects, voids, dislocations, microcracks etc., see e.g. (1)-(3))

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can be studied by means of simulation models (see e.g. (6),(2)) and experiments which provide a more precise information on the micromechanical deformation behaviour in the defected regions (see (2),(1o),(11),(9), (17)). Besides analytical and semi-analytical defect models ((14)-(16),(18)) the development and application of powerful computer simulation programmes have become a new branch of research in "MICROMECHANICS OF DEFECTS": Finite Element Method (FEM) and Boundary Element Method (BEM) both have been successfully applied to the micromechanical level too (1o),(18). The systematic study of mechanical defect interaction phenomena using the above-mentioned methods, however, is only possible by means of more "physically" refined models in micromechanics of defects. The authors have been working in this field for some years now (see e.g. (1),(2),(4), (13)-(16)).It is one of their experiences that so-called "hybrid models"(already well-known from solid mechanics) should also provide a good basis for systematic investigation of defects on the microscopic level (1). One of the greatest advantages of these kinds of models is that they could "combine" different aspects (even to a certain extent "inconsistent" views) of physical modeling, e.g. the continuum point of view on the one hand and the discrete nature of lattice structure on the other. Inside the "process region", where the pure phenomenological approach to fracture mechanics does not work, "continuum Micromechanics" and "lattice Micromechanics" meet at a point of so-called "mesoscopic modeling". The void-void interaction problem, for example, which is of great importance for ductile fracture (crack initiation etc.) can be described in terms of continuum mechanics to a certain extent, after some additional aspects of thermodynamical field coupling effects (connected with the concept of "internal" pressure, local temperature field around the voids etc.) have been taken into account. Then we immediately arrive at the field interaction problems in general, such as mechanical- thermal field coupling etc. (1),(2),(13).

We do not want to go more into details here, as we dealt with these kinds of effects in recent papers (13),(4). Crack tip temperature fields, however, also react on the mechanisms of defect interaction because of the dependence of defect activation on the "local" temperature field. Other kinds of field interactions have been shown to influence the crack behaviour too, e.g. the electromagnetic-mechanical field coupling effects (19). On a pure phenomenological level of modeling there is no real chance neither to find out the reason nor to arrive at a suitable "practical" picture about the defect behaviour in the near crack tip region. But we also know that even the mostly advanced microscopic theory of micromechanics (let's say microphysics or lattice physics) today in no case of practical importance has been able to solve the very complicated problems of lattice distortion within the defected regions around a real crack tip. This conflict in the framework of continuum fracture mechanics can be "weakened" in three ways:

i) To enlarge the degree of freedom in the phenomenological models taking into account field coupling effects such as mechanical-thermal field interaction (temperature-dependent fracture mechanics as field theory etc.).

ii) To improve the experimental diagnostics of local deformation and temperature fields in the near crack tip region (see below)

iii) To establish certain kinds of "hybride models" on the mesoscopic level of "continuum -micromechanics".

All the three steps mentioned above are equally important and will contribute to progress in this field. The third approach is arranged at the "micro-macro-border" of fracture modeling. However, this can only be successfully achieved using the main results - but not all sides- of i and ii, as the "simplification" of the model (one important aim of most hybrid models) requires the incorporation of essential outlines of the more comprehensive "large models" and of the experiments as well.

The authors below are going to give a brief survey about their research activities in the field of "mesoscopic" continuum micromechanical modeling of defect interaction related with crack problems.

THEORETICAL BACKGROUND OF MICROMECHANICS OF DEFECTS

Quite a lot of publications have appeared since the classical papers written by NABARRO, ESHELBY, COTTRELL, KRÖNER etc. which deal with various kinds of models of defects in solids on the basis of continuum micromechanics. Review papers, monographs and conference proceedings report on the powerful development in this field (see e.g. (1),(22)-(26)). Linear and non-linear models of defects and their interaction processes have been published all over the world. Besides the purely elastic approach more general constitutive behaviour - above all inside the "core" regions of the defects- also in the microscopic regions has been taken into consideration. Nonlocal aspects have been reported upon too(22). We do not go into detail here but mention one main aspect of the development in this area of defect modeling which seems us to be a trend in recent fracture micromechanics: This is the full-scale application of computer simulation by means of FEM, BEM and other powerful numerical discretization methods for problems in micromechanics. Hence, it is not essential any longer, whether a model is a linear one or not, as the discetization (by FEM) in principal is also possible for advanced geometrically and physically nonlinear concepts. In case of practical application, however, this situation is somewhat different because good computers and high costs are necessary to solve more complicated nonlocal or nonlinear problems. Besides this we also have to recognize that there are some difficulties with regard of the uniqueness of solutions in the nonlinear models (e.g. branching,inverse and improperly posed problems which are difficult to solve, etc.). But this is not the point of discussion here. The main point, however, is the model itself, i.e. the physical interpretation. In this conference the authors discuss the following examples, where interesting results have been obtained applying computer mechanics on the micromechanics level of defect modeling.

- Simulation of different classes of void problems (three-dimensional) in various materials (isotropic and anisotropic).
- Surface and interface interaction of voids, inclusions and other defects.
- Interaction between voids and microcracks.
- Near crack dislocation behaviour (e.g. crack-flank "COTTRELL atmosphere" etc.).
- BEM simulation of cracks, microcracks, material inhomogeneities (2d and 3d models) by means of deterministic as well as stochastic models.

The results are discussed with regard of the physical relevance of the simulation (e.g. attraction or repulsion effects between the defects and conclusions derived from the outlines of the models).
Various routines of spezialized software have been written. A programme bank system "FAMSAR"- FRACTURE AND MICROMECHANICS, STOCHASTICS AND RELIABILITY- which is to contain a collection of specialized software packages both in the theoretical field and in the field of practical application is under construction. The latter also includes software for experiments (e.g. CAT- COMPUTER AIDED TESTING by means of various experimental techniques, such as x-ray diffraction,

laser beam technique, photoelastic method, acoustic testing, electron microscopic deformation measurement and conventional methods of materials testing and fracture mechanics tests).

As the local deformation field around the cracks shows an important influence on fracture behaviour in the next two chapters a brief survey will be given about two specialized experimental methods which have been developed in the Institute of Mechanics of our Academy of Sciences for the study of near crack tip deformation behaviour:

i) The evaluation of stresses, strains and generalized three-dimensional J-integral by means of laser experiments (holographic interferometric J test) HI-J-TEST.

ii) The "MICRO-MOIRE-METHOD" which has been developed to get information upon displacements, stresses, strains and local fracture parameters in the immediate crack tip surroundings through in-situ experiments within a scanning electron microscope.

GENERALIZED THREE-DIMENSIONAL J BY MEANS OF LASER EXPERIMENTS- THE HOLOGRAPHIC INTERFEROMETRIC J-TEST

Presented here is a combination method of holographic interferometry with a smoothing numerical method bearing in mind mechanical equilibrium to evaluate strain, stress and 3d-J integrals, respectively.(see (11),(17)). One possible way for the extension of classical J to the three-dimensional elastic crack problem was carried out by MIYAMOTO and KIKUCHI in 1980 (see e.g. (27) and (28)).

The J_k -vector is

$$J_k = \int_{\Gamma} (W n_k - u_{i,k} t_{ij} n_j) \, d\Gamma + \int_{A} (W \delta_{k3} - u_{i,k} t_{i3})_{,3} \, dA.$$

Suffices followed by a comma denote differentiation. W is the known strain energy density function. u_i and t_{ij} are the local displacement and stress tensor, respectively.

The path Γ has been introduced as one surrounding the area A at the crack tip. Note that this local J vector is associated here with fixed planes x_3 = const. of the specimen (see e.g. (11)). Using the property of J as a path-independent quantity of state KAWAHARA and BRANDON (46), KING and HERRMANN (47), FREDIANI (48) and many others already presented suitable methods for experimental evaluation for the original RICE-integral. By WILL et al. a combination of holographic interferometry with special smoothing numerical method has been

introduced to determine three-dimensional J.
This hybrid numerical and experimental technique leads to very accurate results. The method is valuable as it is a non-destructive testing methods with small experimental errors. The accuracy was shown in many experiments for different kinds of materials (from steels to ceramics), e.g. for the three-point loaded bending specimen with an edge crack. Details are given in (11).
The experiments which could be carried out by means of usual continuous laser technique lead to very good results for all components of $\underline{J}$. This could also be proved comparing the values with those obtained by synthetic interferogramms which follow from FEM and BEM simulation tests. It is expected that further development of this new hybrid optical method will lead to a powerful tool in experimental fracture research under suitable conditions.

THE MICRO-MOIRÉ-METHOD

Like all the other experimental field measuring techniques known until now in the area of deformation and fracture evaluation (x-ray analysis, acoustic waves, photoelasticity etc.) also investigations by means of electron microscopes should help to study the near crack tip deformation mechanisms.
Thus, on the one hand we used conventional scanning and transmission electron microscopy and other related techniques to investigate real structure and composition of crack tip region of fracture specimens.
On the other hand we combined this with the idea of the moiré- method known from experimental solid mechanics. A special procedure for generating displacement-induced moire-patterns by means of SEM has been developed (see (9),(3)). It permits to find out the componentsof displacement vector $\underline{u}$ of in-situ deformed bending or tension specimens in microscopic dimensions of surface regions of the specimens.
The micro moire-patterns arise by superposition of similar periodic or quasi-periodic structures. The superposition of two such structures can be written as follows:

$$S(\underline{r}) = \sum_m \sum_n \exp\left\{-2\pi i(m+n)\hat{\underline{b}}\cdot\underline{r}\right\} B_m P_n \exp\left\{-2\pi i n(\hat{\underline{p}}\cdot(\underline{r}-\underline{u}) - \hat{\underline{b}}\cdot\underline{r})\right\}.$$

Here $\underline{r}$ is the position vector, B_m, P_n are Fourier coefficients of the two structures.
$\hat{\underline{b}}$, $\hat{\underline{p}}$ are the spatial frequency vectors of the structures. The formula supposes a sufficiently faint po-

sition dependence of the Fourier coefficients and of the quantities $\hat{\underline{b}}$ and $\hat{\underline{p}}$. This is equivalent to the modulation of the first factor of the superposition structure by an unimportant position-dependent exponential term. The modulation is responsible for the build up of moire interference patterns of both structures. If a specimen grid is superimposed by a so-called analyser grid, then the produced moire fringes are generated by all those geometrical points suffering the same relative displacement perpendicular to the analyser grid. This enables us for an experimental determination of the plane components of the displacement field of in-situ deformed regions by generating moire interference patterns (9). From the micrographs before and after deformation the order of fringes can be identified, so that the displacements can be determined, if the density is known. As it is the case for other kinds of field measuring techniques an automative image processing method can be applied which leads to quantitative results for all field quantities very quickly, e.g. displacements, strains etc. For strains etc. we applied a special smoothing method which gives sufficiently accurate results for further differentiation of the displacements. In a similar way - as it was already shown above for the HI-J-Test- we arrive at the deformation field etc. One result of this scanning micro-moiré-method obtained in the electron microscope is the J-vector. This was carried out for some materials. The method can also be used for a systematic study of the microdeformations within the process zone. This is only dependent upon the kind of microscope available for the experiments. The border of the transition region where the J concept fails, i.e. J looses the property of path-independence, can be defined as "process region". This "experimentally verified process region" has been the aim of current research work in this field within the group of the authors (3o). The procedure is not necessarily restricted to the J concept. Other fracture concepts could be studied too by this experimental method. Integral concepts have been used because of some numerical advantages due to the "smoothing" effect connected with integration of physical quantities. Generalized conservation laws concerned with other integral concepts have been under consideration (a survey of those concepts is given in (12)).

HYPOTHESIS: CHARACTERISTIC "CRACK SPECTRA"

Electron states of cracks – do they exist?

Of course, they do. That is not the point. The question is: Are they connected with characteristic physical or mechanical quantities describing the crack configuration?

We are first going to give some further explanation:

From quantum mechanics it is known that dislocations and other lattice defects may give rise to strain fields that effect the electrons (see e.g. (31) – (44)). Thus, it is a known fact that bound electron states in the strain fields of dislocations in germanium occur ((33),(34)). The interest in the electronic properties of dislocations in semiconductors has been considerable since GALLAGHER in 1952 first showed the existence of additional acceptor levels in plastically deformed germanium. Experiments seem to indicate the occurrence of a "dislocation band" in the gap between valence and conducting electrons in semiconductor materials. There are many publications which deal with field coupling effects between the deformation field (i.e. lattice distortions) and electron states in the homogenious unbounded medium. There exist great differences with regard to the theoretical approach for different materials (metals, semiconductors etc.) In some special cases the approximation of so-called "deformation potential" theory can be applied. This rough estimation already leads to correction terms in the Hamiltonian and may lead to essential effects due to lattice distortion around the defects. KLEINMAN and many others dealt with such kinds of problems in general without considering the crack problem (see (40), (38)). CLAESSON presented another formulation of a simplified model (33) which is based on the following decomposition of the Hamiltonian:

$$H = H_o + H_\varepsilon + H_c ,$$

where H_o represents the Hamiltonian of the perfect crystal, H_ε is the term due to strain contribution and H_c denotes the core contribution (due to dislocation core structure). This model disregards the electron-electron interactions and leads to expressions for H_ε containing terms like this:

$$H_\varepsilon = H_\varepsilon^{(1)} + H_\varepsilon^{(2)} + H_\varepsilon^{(3)} , \quad H_\varepsilon^{(1)} \sim \sum_{i,j} A_{ij}\, \varepsilon_{ij} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j}$$

$$H_{\varepsilon}^{(2)} = \Sigma \mathcal{B}_{ij} \beta_{ij} \; ; \; H_{\varepsilon}^{(3)} \sim C \varepsilon_{I} .$$

Here ε_{ij} and β_{ij} are the strain and distortion tensor, respectively. ε_I is the volume dilatation (trace of ε). A_{ii} and β_{ij} and C are related to quantum mechanics. They are of lesser importance with regard to our discussion. This coupling between defect deformation and electron structure of solids (H is responsible for the electron states! From H a modified SCHROEDINGER equation follows which contains the field quantities of defect distortion)due to dislocation can formally be extended to near-surface defects too. The influence of elastic lattice distortion near boundary surfaces (and similar near crack flanks!) is an essential effect which is well-known (see e.g. MICHEL (1),(2) or LOTHE (42)). The surface-influence upon the electron states is , however, a very complicated problem in modern quantum mechanics and probably could also be neglected in a first-order approach. If we only have a look at the lattice influence, we know from continuum micromechanics of defects that the trace ε_I shows a decisive influence on the elastic interaction energy terms between the defects (see (14)-(16),(1),(2)). This means that the defect interaction energy also exerts a non-vanishing influence on H_{ε} and thus on the electron states. From this simple consideration and some quantitative estimations of the terms which enter H we already can draw the conclusion that the crack flank interaction of defects (point defects as well as dislocation) must also lead to a contribution to the electron energy level. This also remains valid for collective behaviour of defects. Taking into account the concept of "process region", we must arrive at the conclusion that "characteristic" crack spectra exist, if the defect arrangement around cracks is a characteristic one which could be related to the crack quantities (geometrical quantities such as crack length inherent material properties and even to fracture concepts like J). This remains an open question for present day fracture theory. It should, however, be possible to answer it, if the micromechanics of defects will be able to answer the question whether there is a definite arrangement of microdefects within the process region or not. We think that the proof for the static case is sufficient. All kinds of dislocation models of cracks rely on this assumption. The two problems (electron states of cracks and characteristic defect arrangements) are stronly related to each other. The authors express their positive opinion about such a characteristic defect structure af a definite crack configuration unless this will not be decided in the near future. A unique arrangement of microdefects will lead to additional states in the "electron gas" around the crack region. This in consequence will lead to crack spectra which should also be excitable by suitable experiments. This, eventually, could lead to improved methods for non-destructive crack diagnostics, if the transition probabilities between these characteristic crack electron states is high enough. This will lead to further questions for research work in the theoretical and experimental fields of micromechanics of cracks.

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