Available online at www.sciencedirect.com

ScienceDirect

Procedia Structural Integrity 23 (2019) 203–208

Structural Integrity
Procedia

www.elsevier.com/locate/procedia

9th International Conference on Materials Structure and Micromechanics of Fracture

On crack propagation in homogeneous and composite materials under mixed mode loading conditions

Martin Lederer[a,*], Agnieszka Betwar Kotas[a], Golta Khatibi[a] and Herbert Danninger[b]

[a]Christian Doppler Laboratory for Lifetime and Reliability of Interfaces in Complex Multi-Material Electronics, TU Wien, Institute CTA, Getreidemarkt 9, 1060 Wien, Austria
[b]Institute of Chemical Technologies and Analytics, TU Wien, Getreidemarkt 9, 1060 Wien, Austria

---

Abstract

The direction of crack propagation under mixed mode loading conditions is investigated by FEM simulation in comparison with delamination experiments performed in the 4 point bending mode. Composites consisting of aluminum nitride attached to copper by active metal brazing were delaminated with use of a central notch for crack initiation. The main crack line propagated along the interface direction. However, SEM micrographs revealed that the crack line propagating along the interface is subjected to bifurcation. Small cracks digress from the main delamination line under kinking angles of 90° until they are stopped at the copper substrate. The observed behavior of crack propagation is studied by Linear Elastic Fracture Mechanics and by nonlinear Finite Element Analysis. In fact, the bifurcation angle of 90° can be considered as an indication for dominant influence of geometrical nonlinearities at the crack tip. Finite Element Analysis is performed in two stages starting from macroscopic level and then the analysis of crack tip behavior is continued on a microscopic level. On the macroscopic level, the whole experimental setup is simulated in order to derive an approximation of the stress distribution around the crack tip. Thereafter, the analysis is further extended on microscopic level, whereby local mesh refinement is continued until the element size approaches the dimension of the lattice constant. Thus, high stress values at the crack tip lead to considerable amounts of material rotation. Consequently, the observed direction of crack extension may be derived from the maximum hoop stress criterion.

Keywords: hoop stress criterion, mixed mode loading, delamination, bifurcation of cracks, finite strain elasticity

---

* Corresponding author. Tel.: +43-1-58801-164393.
E-mail address: martin.lederer@tuwien.ac.at

10.1016/j.prostr.2020.01.087

1. Introduction

Composites of copper layers attached to aluminum oxide or aluminum nitride are commonly used in power electronics. According to Wei et al. (2018) aluminum nitride is often favored as insulator, because of its excellent thermal conductivity aside from its expedient mechanical properties. During processing and operation of the devices, the substrates are subjected to thermo-mechanical fatigue with a predominant cyclic bending loading mode. In spite of existing failure mechanisms, packages used for power electronics are often required to reach lifetimes of up to 30 years under operation conditions. Therefore, testing the adhesive properties of interfaces is indispensable. Ben Kabaar et al. (2017) employed the four point bending method for testing the adhesive strength of copper - ceramic interfaces through delamination. Thereby, crack initiation was induced by a central notch.

The present investigation of adhesive behavior is mainly focused on the direction of crack propagation. Usually, a delaminating crack is constrained along the interface under test. Nevertheless, bifurcation of the main crack line is here reported. Short cracks were branching from the main line until they arrived at a material layer of higher fracture toughness, where they were stopped ultimately. Therefore, it is the purpose of this study to improve our understanding of the underlying mechanisms leading to bifurcation of cracks.

Crack branching is often considered as dynamic process. Cox et al. (2005) stated that at some scale every fracture is dynamic. In accordance, Bobaru and Zhang (2015) argued that even if a fracture advances in quasi-static manner on macroscopic level, the dynamic of rupture of atomic bonds still plays an important role. An interesting theory of dynamic crack branching in brittle materials was proposed by Katzav et al. (2007). Following common standards, this approach was developed in the frame of Linear Elastic Fracture Mechanics.

On the other hand, it has been stated that the linear theory is incapable of capturing all aspects of fracture mechanics. Buehler et al. (2003) have suggested that hyperelasticity may play a governing role in the dynamics of fracture. They concluded that the material response may be subjected to a change of stiffness when approaching the limit to failure.

A different aspect of hyperelasticity is emphasized in the present approach. The linear theory can lead to violation of material objectivity when applied to large deformations. In fact, the linearized strain tensor is not an objective tensor, because the related material response is not frame indifferent, when a deformation is super imposed by rigid body rotation. This problem increases in the vicinity of crack tips. Therefore, nonlinear FEM simulations are here performed in order to determine the amount of material rotations.

2. Experiments

Interfaces of aluminum nitride and copper were tested in four point bending using a central notch for crack initiation. A similar setup was first suggested by Charalambides et al. (1989). Here, samples consisting of 5 layers were produced by soldering a copper sheet of 1 mm thickness onto a copper - aluminum nitride - copper sandwich structure. The interface under test connecting aluminum nitride and copper was fabricated by active metal brazing (AMB). The AMB interface layer had a thickness of 20 µm and consisted of an alloy containing Ag, Al and Ti.

During bending the load increased linearly, until a sudden drop was observed at a critical load of about 150 N, which indicated fracture of the notch in the ceramic. At this stage, a small delamination crack was generated right after cracking of the substrate in the vicinity of the notch. Thus, the delamination crack propagated along the Cu - ceramic interface. In fact, the crack split up into branches at both sides of an AlN wedge, which remained in the midsection of the sample. A detailed description of the experimental setup may be found in Lederer et al. (2018).

The direction of crack propagation can be seen in SEM micrographs depicted in Figure 1. Due to brittleness the fracture toughness of the AMB layer is by far lower than that of copper, but it is nearly equivalent to that of aluminum nitride. The horizontal main line of the delaminating crack followed the interface between copper and AlN. In addition, short vertical cracks digressing from the main line were seen in SEM micrographs. These short cracks were ultimately stopped at the copper layer. The angle between the main crack line and the short cracks was typically 90°.

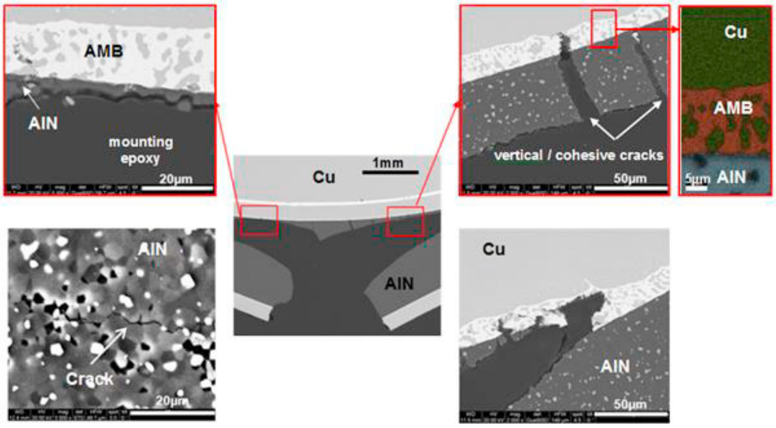

Fig.1. SEM micrograph of AlN-Cu interface fracture surface after testing in 4 point bending. The main delamination crack has developed in horizontal direction, while bifurcating short cracks are digressing in vertical direction.

3. Finite Element simulations including geometrical nonlinearities

A simulation of the complete experimental setup is depicted in Figure 2. The composite sample from top to bottom consisted of 1000 µm copper / 100 µm solder / 300 µm copper / 1000 µm aluminum nitride and 250 µm copper layers. The copper was modelled according to kinematic hardening on the basis of elasto-plastic material data obtained from tensile test and nano-indentation. Thereby, two types of copper were distinguished: The copper sheet soldered onto the top showed enhanced hardening due to fine grain size, whereas the coarse grained copper attached to aluminum nitride exhibited lower flow stress. The bolts made of steel were simulated with use of contact elements.

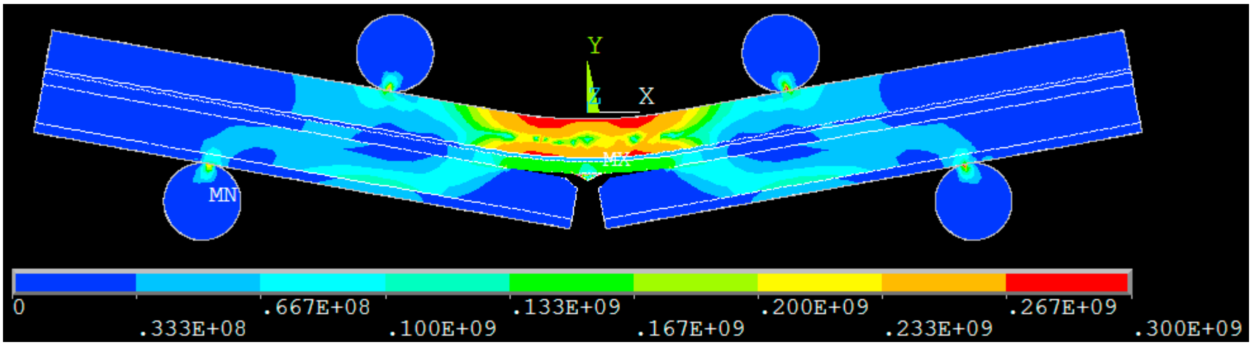

Fig. 2. Plot of the von Mises stress [Pa] for the complete experimental setup including the bolts.

The four point bending setup generates a crack tip stress field of mixed mode 1 and mode 2 behavior. The angle of mode mixity can well be determined from the macroscopic simulation of the entire model. However, further mesh refinement in the region around the crack tip leads to unrealistically high values of plastic equivalent strain in the adjacent copper layer, because strain gradient effects are not considered in conventional plasticity theory.

On the other hand, a thorough analysis of geometrical nonlinearities in the 20 µm thin AMB layer requires a finer mesh. In order to enable mesh refinement to element sizes of atomic scale, the analysis of crack propagation was complemented by simulation of a microscopic crack tip model. In the microscopic simulation, the direction of crack propagation is derived from the maximum hoop stress criterion in combination with an elliptic crack. For the example depicted in Fig. 3, the aspect ratio of the ellipse relating the major axis *a* to the minor axis *b* was chosen as 1500. Further, the strategy of mesh refinement is also illustrated in Fig. 3:

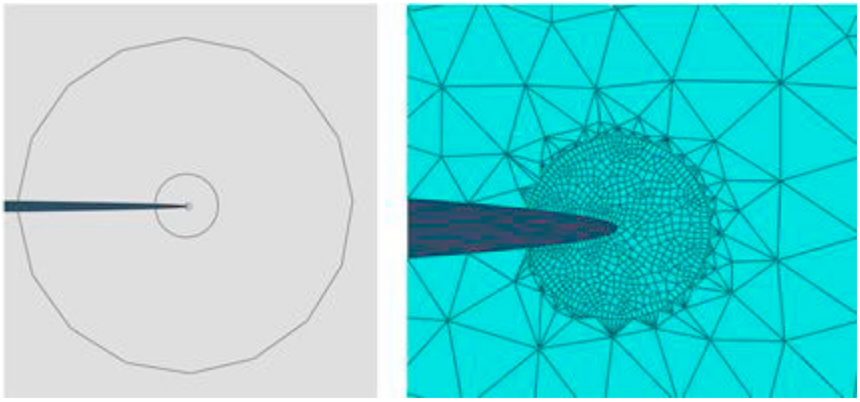

Fig. 3. Partitions with radius of 100 nm, 20 nm and 2 nm were defined for the purpose of mesh refinement. The element sizes corresponding to the mesh of the innermost partition are in the range of crystallographic lattice constants.

Actually, Figure 3 shows only a detail of the nonlinear elastic microscopic model. The crack of the microscopic model was embedded in an AMB interface layer, which was sandwiched in between two adjacent layers of copper and aluminum nitride. However, the adjacent materials were represented by reduced material volume compared to the entire model depicted in Figure 2.

A series of simulations was performed with the microscopic model considering different conditions of mixed mode loading. The influence of geometric nonlinearities on the results can be deduced from a comparison with analytic results for equivalent loading modes evaluated for the linearized theory. Under mode 1 loading condition, the crack extension is always in straight forward direction regardless whether linear or nonlinear theory is applied. In the case of mode 2 loading, the crack shows a tendency of digressing from the main line leading either to crack curving or to bifurcation. Thereby, the nonlinear theory predicts a larger angle of digression from the main line compared to the linear theory. Figures 4 and 5 show the results of linear and nonlinear approach under pure mode 2 loading conditions:

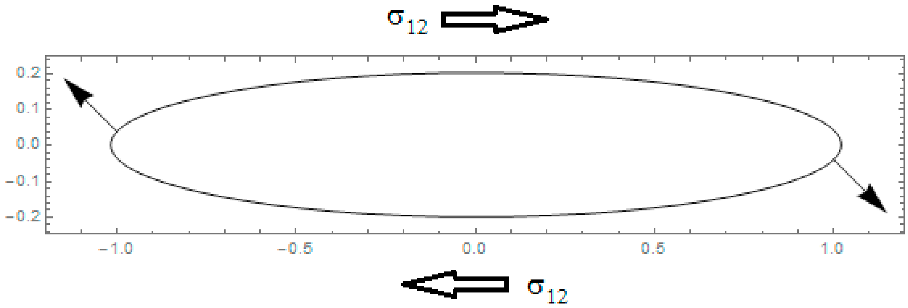

Fig. 4. Linear elastic solution for the direction of crack propagation under mode 2 loading evaluated for an elliptic crack by McClintock (1963). Crack extension is expected under angles of 45°.

Figure 4 illustrates a result first obtained by McClintock (1963) for the case of an elliptic cavity under mode 2 loading evaluated within linear elasticity. In this model based on the maximum hoop stress criterion the crack extension occurs under angle of 45° relative to the horizontal axis. For comparison, Figure 5 shows the result of the geometrically nonlinear model derived with the mesh of Figure 3 for a load level in agreement with crack propagation.

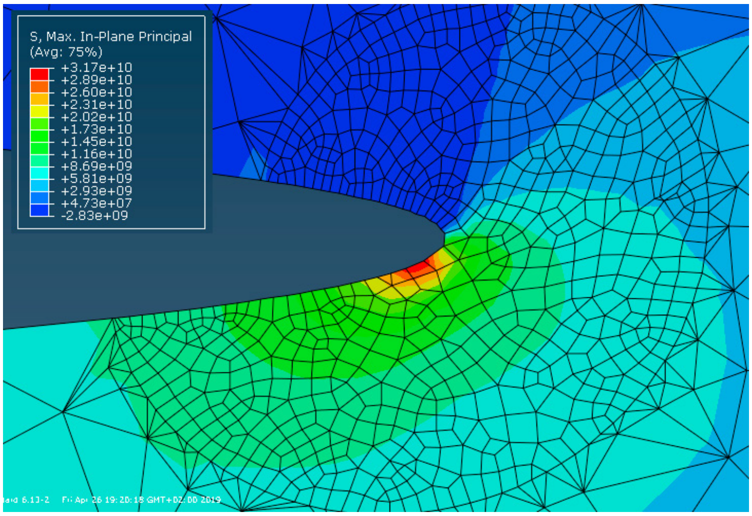

Fig. 5. Plot of the first principal stress for an elliptic crack under mode II loading, shown in true deformation scale. Geometrical nonlinearities were included in this simulation. At the position of maximum stress the angle between normal to the ellipse and horizontal axis is 67.5°.

In the geometrical nonlinear simulation depicted in Fig. 5, the location of maximum hoop stress appears at a position, where the tangent to the deformed ellipse is 67.5° relative to the horizontal axis. It should be recognized that the amount of material rotation depends on the maximum value of strain. Since the stress concentration at the vertex of the ellipse increases with its sharpness, there are larger material rotations for sharper cracks. At this point, it must be said that convergence of the simulation becomes increasingly difficult, when the geometry of the ellipse approaches the shape of a sharp crack. Nevertheless, an extrapolation of the simulation results suggests that for sharp cracks under mode II loading the tangent to the deformed ellipse at the location of maximum hoop stress gets parallel to the crack line. Insofar, a sharp crack under mode 2 loading may be expected to propagate under an angle of 90°.

Mode 1 and mixed mode loading of the microscopic model were also simulated. In general, material rotations are larger in geometrical nonlinear analysis compared to the analytic solution of the linear model.

4. Discussion

The static FEM analysis performed here cannot fully capture the dynamic aspects generated by cracking of atomic bonds. Nevertheless, the simulation of geometrical nonlinearities performed here shows significant influence on the direction of crack propagation. Thereby, the nonlinear aspects of elasticity evaluated here are just a consequence of material frame indifferent treatment of a linear elastic material model. In conclusion, the material rotations found here are certainly of relevance for the theory of crack branching.

However, it must be admitted that the quantitative evaluation of material rotations in the vicinity of sharp cracks is confronted with numerical difficulties. In the present study, mesh refinement down to element size of atomic scale was necessary to derive the results for the stresses around an elliptic cavity with aspect ratio of 1500. This aspect ratio is still away from a truly sharp crack, but further mesh refinement would be necessary to evaluate sharper cracks.

5. Summary and Conclusions

Interfaces between copper and aluminum nitride fabricated by active metal brazing were delaminated in four point bending using a central notch for crack initiation. Thereby, branching of crack lines was found experimentally. Short cracks digressed under angle of 90° from the main crack line until they were ultimately stopped at a material of higher fracture toughness. From the viewpoint of Linear Elastic Fracture Mechanics, however, smaller bifurcation angles are expected. Therefore, Finite Element simulations were performed in order to include geometrical nonlinearities in the analysis.

The Finite Element Analysis was carried out in two stages starting from a simulation of the complete experimental setup. At this first stage, a reasonable good approximation of the stress field around the crack tip could be derived. However, a precise analysis of geometrical nonlinearities requires advanced mesh refinement down to element sizes of atomic scale. Therefore, a second analysis was carried out on microscopic level. It was the purpose of this analysis to obtain the material rotations in the vicinity of the crack tip with use of a material frame indifferent theory.

The results obtained from the simulations were compared to analytical calculations carried out within the linear theory. Predictions of the kinking angle derived from the linearized theory are typically smaller than the corresponding results of finite elasticity. In the frame of Linear Elastic Fracture Mechanics, the solution of mixed mode loading is simply derived from superposition of the solutions for modes I and II. In the case of the nonlinear theory, it becomes extremely difficult to obtain convergence of the solution for sharp cracks. Nevertheless, reasonable estimates may be derived from extrapolation of simulation results for ellipses representing nearly sharp crack shapes. Finally, model calculations were compared to experiments of crack propagation performed by four point bending of composite structures. In conclusion, bifurcations of the main crack line and kinking angles of up to 90° appear to be plausible.

Acknowledgements

The financial support by the Austrian Federal Ministry for Digital and Economic Affairs and the National Foundation for Research, Technology and Development is gratefully acknowledged.

References

Ben Kabaar A., Buttay C., Dezellus O., Estevez R., Gravouil A., and Gremillard L., Characterization of materials and their interfaces in a direct bonded copper substrate for power electronics applications, Microelectronics Reliability, Vol. 79, pp. 288-296, (2017)

Bobaru F. and Zhang G., Why do cracks branch? A peridynamic investigation of dynamic brittle fracture , International Journal of Fracture, Vol. 196, pp. 59-98, (2015)

Buehler M. J., Abraham F. F. and Gao H., Hyperelasticity governs dynamic fracture at a critical length scale, Nature, Vol. 426, pp. 141-146, (2003)

Charalambides P. G., Lund J., Evans A. and McMeeking R., A test specimen for determining the fracture resistance of bimaterial interfaces. Journal of Applied Mechanics, 56, 77– 82 (1989)

Cox B. N., Gao H., Gross D. and Rittel D., Modern topics and challenges in dynamic fracture. Journal of the Mechanics and Physics of Solids, Vol. 53(3), pp. 565–596, (2005)

Katzav E., Adda-Bedia M. and Arias R., Theory of dynamic crack branching in brittle materials, International Journal of Fracture, Vol. 143, pp. 245-271, (2007)

Lederer M., Betzwar Kotas A., Khatibi G. and Danninger H., Characterization of adhesion properties by delamination of ceramic-metal interfaces in four point bending, Key Engineering Materials, Vol. 774, pp. 66-71, (2018)

McClintock F. A., Journal of Basic Eng. 85, Discussion , pp. 525-527, (1963)

Wei X., Xu H., Zhang J., Zhang H., Cao Y., Cui S., and Tang W., Comparative studies on microstructures, strengths and reliabilities of two types of AlN direct bonding copper substrates, Ceramics International, Vol. 44, pp. 18935-18941, (2018)