Structural Integrity 5

Series Editors: José A. F. O. Correia · Abílio M. P. De Jesus

Emmanuel E. Gdoutos

Editor

Proceedings of the First International Conference on Theoretical, Applied and Experimental Mechanics

Springer

Structural Integrity

Volume 5

The *Structural Integrity* book series is a high level academic and professional series publishing research on all areas of Structural Integrity. It promotes and expedites the dissemination of new research results and tutorial views in the structural integrity field.

The Series publishes research monographs, professional books, handbooks, edited volumes and textbooks with worldwide distribution to engineers, researchers, educators, professionals and libraries.

Topics of interested include but are not limited to:

- Structural integrity
- Structural durability
- Degradation and conservation of materials and structures
- Dynamic and seismic structural analysis
- Fatigue and fracture of materials and structures
- Risk analysis and safety of materials and structural mechanics
- Fracture Mechanics
- Damage mechanics
- Analytical and numerical simulation of materials and structures
- Computational mechanics
- Structural design methodology
- Experimental methods applied to structural integrity
- Multiaxial fatigue and complex loading effects of materials and structures
- Fatigue corrosion analysis
- Scale effects in the fatigue analysis of materials and structures
- Fatigue structural integrity
- Structural integrity in railway and highway systems
- Sustainable structural design
- Structural loads characterization
- Structural health monitoring
- Adhesives connections integrity
- Rock and soil structural integrity

More information about this series at http://www.springer.com/series/15775

Emmanuel E. Gdoutos
Editor

Proceedings of the First International Conference on Theoretical, Applied and Experimental Mechanics

Springer

Editor
Emmanuel E. Gdoutos
Office of Theoretical and Applied Mechanics
Academy of Athens
Athens
Greece

ISSN 2522-560X ISSN 2522-5618 (electronic)
Structural Integrity
ISBN 978-3-319-91988-1 ISBN 978-3-319-91989-8 (eBook)
https://doi.org/10.1007/978-3-319-91989-8

Library of Congress Control Number: 2018944306

Printed on acid-free paper

This Springer imprint is published by the registered company Springer International Publishing AG part of Springer Nature
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

This volume contains 42 six-page papers and 59 two-page abstracts presented at the "First International Conference on Theoretical, Applied and Experimental Mechanics," (ICTAEM_1) held in Paphos, Cyprus, June 17–20, 2018. The papers/abstracts are arranged in four topics and two special symposia with 69 and 32 papers/abstracts, respectively. The papers of the tracks have been contributed from open call, while the papers of the symposia have been solicited by the respective organizers.

ICTAEM_1 will focus in all aspects of theoretical, applied, and experimental mechanics including biomechanics, composite materials, computational mechanics, constitutive modeling of materials, dynamics, elasticity, experimental mechanics, fracture, mechanical properties of materials, micromechanics, nanomechanics, plasticity, stress analysis, structures, wave propagation. During the conference, special symposia covering major areas of research activity organized by members of the Scientific Advisory Board will take place.

The attendees of ICTAEM_1 will have the opportunity to interact with the most outstanding world leaders and get acquainted with the latest developments in the area of mechanics. ICTAEM_1 will be a forum of university, industry, and government interaction and exchange of ideas in an area of utmost scientific and technological importance.

I am sure that besides the superb technical program, you will enjoy the majestic town of Paphos with its unique beaches and scenic beauty, many areas of historical interest and archeological importance, the delicious local cuisine, and the traditional Cypriot hospitality.

More than a hundred participants attended ICTAEM_1. The participants of ICTAEM_1 came from 25 countries. Roughly speaking, 36% came from Europe, 25% from the Far East, 7% from the Americas, and 32% from other countries. I am happy and proud to have welcomed in Paphos well-known experts who came to discuss problems related to the analysis and prevention of failure in structures. The tranquility and peacefulness of this small town provided an ideal environment for a group of scientists and engineers to gather and interact on a personal basis. Presentation of technical papers alone is not enough for effective scientific communication. It is the healthy exchange of ideas and scientific knowledge, formal and informal discussions, together with the plenary and contributed papers that make a fruitful and successful meeting. Informal discussions, personal acquaintance, and friendship play an important role.

I am proud to have hosted ICTAEM_1 in the beautiful town of Paphos, and I am pleased to have welcomed colleagues, friends, old and new acquaintances.

I very sincerely thank the authors who have contributed to this volume, the symposia/sessions organizers for their hard work and dedication, and the referees who reviewed the quality of the submitted contributions. The tireless effort of the members of the Organizing Committee as well as of other numerous individuals and people behind the scenes is appreciated. I am deeply indebted to Dr. Stavros Shiaeles for his hard work and dedication in the organization of the conference. Finally, a special word of thanks goes to Dr. Maria Shiaele for her continuous collaboration and support.

March 2018 Emmanuel E. Gdoutos

Contents

Miscellaneous (Biomechanics, Compu-tational mechanics, Dynamics, Nano-mechanics, Plasticity, Structures, Wave propagation)

Investigation into the Breakdown of Continuum Fracture Mechanics at the Nanoscale: Synthesis of Recent Results on Silicon

Pasquale Gallo(✉), Takashi Sumigawa, Takahiro Shimada, Yabin Yan, and Takayuki Kitamura

Department of Mechanical Engineering and Science, Kyoto University, Kyoto-daigaku-Katsura, Nishikyo-Ku, Kyoto-Shi 615-8540, Japan
pasquale.gallo@aalto.fi

Abstract. The present contribution reviews some recent results on the experimental characterisation of the nanoscale fracture toughness of silicon by using pre-cracked specimens and alternatively the theory of critical distances (TCD). Later, the results are discussed to provide the ultimate dimensional limit of the continuum fracture mechanics at the nanoscale in the light of sophisticated discrete atomic simulations at the onset of brittle fracture. The results show that the fracture toughness of Si is independent of the scale, crystal orientation and the singular stress field length. This confirms the atomistic nature of the brittle fracture. Moreover, the continuum fracture mechanics fails below a singular stress field approaching 2 nm.

Keywords: Fracture nanomechanics · Nanoscale · Silicon
Quantum mechanics

1 Introduction

Conventional fracture mechanics [1] has been primarily investigated starting from the II World War, leading to the well-known linear elastic fracture mechanics (LEFM). In the last decade, the miniaturisation of electronic devices driven by the increasing demand for high-density integrations have brought problems of material behaviour at very small scales into the domain of fracture mechanics. At micro and nanoscale, indeed, the material still fails by nucleation and propagation of cracks, but the continuum assumption basing the LEFM has to face the discrete nature of atoms [2]. The so-called *fracture nanomechanics* poses entirely new challenges, both from the experimental and theoretical point of view. However, the nanoscale investigation of fracture has sparked the interest of the scientific community [3–5].

In the above background, the experimental characterisation of fracture behaviour at the nanoscale and the investigation of the low limit of the continuum theory are at the present relevant and challenging aspects. Therefore, the present work presents recent experimental tests on the evaluation of single crystal Si fracture toughness at the nanoscale [6, 7]. Results obtained from pre-cracked samples and by using the theory of

E. E. Gdoutos (Ed.): ICTAEM 2018, SI 5, pp. 205–210, 2019.
https://doi.org/10.1007/978-3-319-91989-8_45

critical distances (TCD) [8] are compared to highlight pros and cons of each procedure. Later, in Sect. 3, the experimental results are discussed in the light of complex discrete atomic simulations at the onset of brittle fracture [9] to provide the ultimate dimensional limit of the continuum fracture mechanics.

2 Experimental Characterization of Si Fracture Toughness at the Nanoscale

2.1 Procedure Based on Pre-cracked Samples

Recently, the K_{IC} of Si has been investigated accurately by Sumigawa et al. [6]. Those authors employed pre-cracked specimens accurately realised to avoid large curvature at the crack tip. First, a V-notch was realised by focused ion beam (FIB) processing system along the cleavage plane Si(011), and later a pre-crack was generated by gradually opening the notch. The opening displacement was controlled and applied through a wedge-shaped diamond indenter. Image of a sample is reported in Fig. 1. Four samples with several pre-crack lengths were generated by cutting the upper part of the notch. Details are reported in [6].

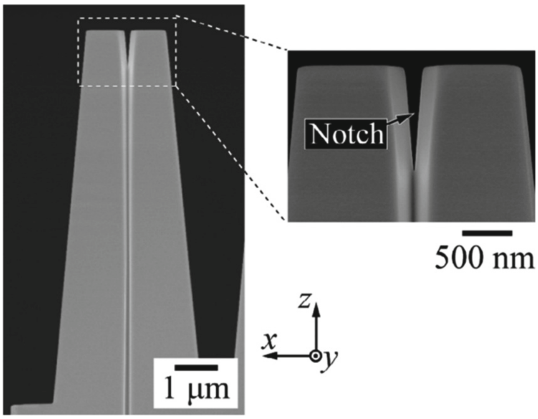

Fig. 1. Example of pre-cracked specimen

The four specimens were tested in a transmission electron microscope (TEM) provided by *in situ* observation camera. Experimental results were later re-analysed by finite element method (FEM) to determine the stress state accurately at the crack tip and the final average K_{IC} of about 1 $MPa^{0.5}$. This value is in agreement with the bulk silicon K_{IC} that is 0.75–1.08 $MPa^{0.5}$. The FEM simulations showed, besides, that all the geometries presented a singular field of $r^{0.5}$, while its length varied from 23 nm to 60 nm. The K_{IC} seems therefore independent of the scale and the singular field length, while the local fracture mechanisms take place at least at those or smaller sizes.

2.2 Procedure Based on Theory of Critical Distances

The fabrication of pre-cracks in nanoscale specimens, even if feasible it is clearly difficult. To avoid strict control on the fabrication process, an alternative strategy using the TCD and notched specimens has been employed by Gallo et al. [7]. TCD in the form of the point method states indeed that failure occurs when the linear elastic maximum principal stress σ_1 at a given distance $L/2$ from the notch root equals the inherent material strength σ_0 [8]. L is called material characteristic length, it is a material property and is defined as follows:

$$L = \frac{1}{\pi}\left(\frac{K_{IC}}{\sigma_0}\right)^2 \tag{1}$$

As stated by Susmel and Taylor [10], the intersection of at least two linear elastic stress field in incipient failure of specimens with *different sharpnesses* gives a correct estimation of both σ_0 and L. Once these two parameters are defined, (1) can be used to the determine $K_{IC} = \sigma_0\sqrt{\pi L}$. This strategy simplifies the experimental procedure since it is based on notches instead of cracks, and a strict control on the final notch geometry is not needed [10].

According to the procedure briefly explained above, notches of different sharpness have been introduced in two nano cantilever beams by FIB processing system. The sharp notch had a radius ρ of about 6.3 nm and an opening angle 2α of 68°; the blunt notch had ρ = 20.2 nm and 2α = 59°. The sharp specimen had a notch depth a of 144 nm while the blunt sample had a notch depth a of 179 nm. The geometry is depicted in Fig. 2(a) while additional details can be found in [7].

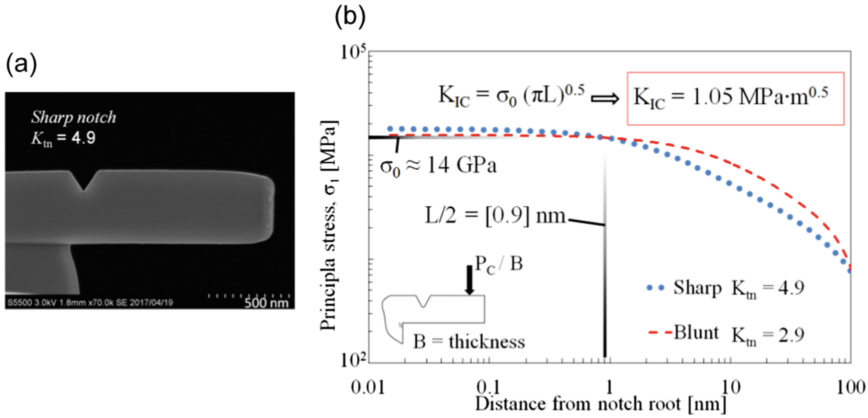

Fig. 2. Example of nanoscale notched specimen (a), and stress fields under the critical load P_C at failure (b)

The loading experiments are conducted in a TEM, and the load is applied through an indenter after accurate alignment. Displacements and loads are recorded. The stress fields at incipient failure are later re-analysed by FEM and overlapped in a single graph in Fig. 2(b) together with stress concentration factors (net section). The intersection point revealed a σ_0 of about 14 MPa and $L/2$ of about 0.9 nm. By employing (1) the final K_{IC} was 1.05 MPa$^{0.5}$. The results are therefore in agreement with [6] and macro counterpart values (0.75–1.08 MPa$^{0.5}$). Moreover, being the material characteristic length L a representative scale parameter of the mechanisms involved in the fracture process, the procedure provides a more precise information compared to Sect. 2.1 and suggests that those mechanisms take place at least at 2 nm or even smaller size [6].

3 Discussion: Breakdown of Continuum Theory

The results of Sect. 2.1 suggests K_{IC} is independent of the singular stress field length and therefore that the fracture mechanisms take place below 23–60 nm [6]. However, a precise estimation of the size was not provided. The TCD material characteristic length L evaluated in Sect. 2.2 and extended recently in [7] is, instead, a representative length scale parameter that assumes different values as the fracture mechanisms involved change scale [11]. The results briefly reported here suggest that the fracture develops at a scale of about 2 nm. At this small scale, one must deal with atomic structure, and further considerations can be done only with atomic simulations. These have been conducted recently by Shimada et al. [9]. Fracture tests were performed *in situ* using center cracked nanoscale plates of Si. The width of the specimens $2W$ varied from 2.1 to 276 nm while the crack length $2a$ was kept equal to one-third of $2W$. The experiments were first re-analysed from a continuum theory point of view, and it was shown that the singular stress field of $r^{0.5}$ shrinks as the plate width does. However, when the width is very small and the stress intensity factor (SIF) K region approaches 1 nm, the fracture is no longer governed by the merely SIF.

To investigate this statement and to highlight the atomistic nature of fracture, the experiments have been re-analysed by instability mode analyses [12] and density-functional theory (DFT). With these approaches, the deformation mode of atoms at the onset of brittle fracture is accurately determined. Both DFT and instability mode analyses showed that the crack advances along the cleavage plane (110) by atomic *bond breaking*. This phenomenon is observed for all of the specimens, regardless of the size, as Fig. 3 shows.

Moreover, a fracture-process zone Λ_f of about 0.4–0.6 nm is defined as the zone where the discrete motion of atoms is concentrated. When the K-dominant zone Λ_K is geometrically too much small and close to the fracture-process zone (i.e. very small specimens), continuum theory breaks down. Concluding, the ultimate dimensional limit for the single crystal silicon is quantified as the range 3–6Λ_f roughly 2 nm. It should be pointed out that the TCD employed in Sect. 2.2 estimated a material characteristic length of 1.8 nm, and therefore very close to ≈2 nm. This confirms that the material characteristic length is representative of the mechanisms scale involved in the fracture process.

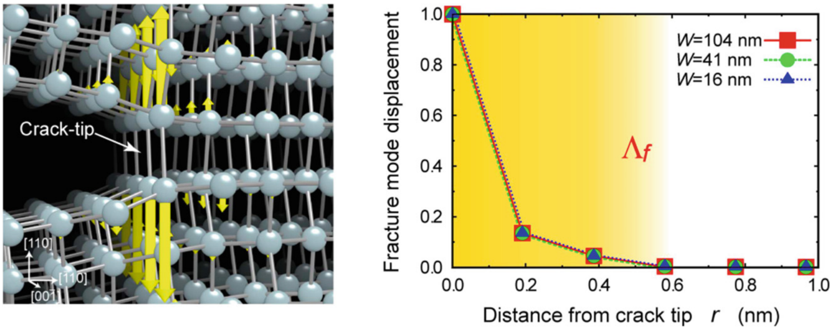

Fig. 3. Fracture mode at the onset of brittle fracture (left), and fracture mode displacement normalized by the maximum displacement at the crack-tip for different size of specimens (right); reproduced from [9] under CC BY 4.0 license permission (https://creativecommons.org/licenses/by/4.0/)

4 Conclusion

The results showed that the fracture toughness of Si is independent of the size and the crystal orientation. Regardless of the methods employed, i.e. using accurate pre-cracked samples or notched components combined with TCD, the K_{IC} has a value of approximately 1 $MPa^{0.5}$. Since the value is in good agreement with the macro counterpart, it can be concluded that from the macroscale to nanoscale the mechanisms involved in the fracture process are the same.

If pre-cracked samples are employed, even a small curvature at the crack tip can generate large discrepancy on the final fracture toughness.

On the other hand, the TCD has shown several advantages: (i) it simplifies the experimental procedure since the realisation of an effective crack tip is not necessary; (ii) it yields an approximated magnitude of fracture process provided by the material characteristic length $L = 1.8$ nm. This value has been verified by discrete atomic simulations and instability mode analysis that captured the deformation mode of atoms at the onset of a brittle fracture. The analyses showed, for the silicon, a fracture process zone of 0.4–0.6 nm and the low limit of the continuum fracture mechanics of about 2 nm, in agreement with L. For singular stress fields size approaching the lower limit, continuum theory fails and discrete nature of atoms should be considered.

Acknowledgements. This work was supported by the Japan Society for the Promotion of Science (JSPS) International Research Fellow program (Grant No. 16F16366); JSPS KAKENHI (Grant No. JP15H02210, JP26630009, and JP25000012); JSPS Grant-in-Aid for Specially Promoted Research (Grant No. 25000012).

References

1. Liebowitz, H.: Fracture. Academic Press, New York (1968)
2. Kitamura, T., Sumigawa, T., Hirakata, H., Shimada, T.: Fracture Nanomechanics, 2nd edn. Pan Stanford Publishing, Singapore (2016)
3. Gallo, P., Sumigawa, T., Kitamura, T., Berto, F.: Evaluation of the strain energy density control volume for a nanoscale singular stress field. Fatigue Fract. Eng. Mater. Struct. **39**, 1557–1564 (2016). https://doi.org/10.1111/ffe.12468
4. Huang, K., Shimada, T., Ozaki, N., Hagiwara, Y., Sumigawa, T., Guo, L., Kitamura, T.: A unified and universal Griffith-based criterion for brittle fracture. Int. J. Solids Struct. **128**, 67–72 (2017). https://doi.org/10.1016/j.ijsolstr.2017.08.018
5. Sumigawa, T., Shimada, T., Tanaka, S., Unno, H., Ozaki, N., Ashida, S., Kitamura, T.: Griffith criterion for nanoscale stress singularity in brittle silicon. ACS Nano **11**, 6271–6276 (2017). https://doi.org/10.1021/acsnano.7b02493
6. Sumigawa, T., Ashida, S., Tanaka, S., Sanada, K., Kitamura, T.: Fracture toughness of silicon in nanometer-scale singular stress field. Eng. Fract. Mech. **150**, 161–167 (2015). https://doi.org/10.1016/j.engfracmech.2015.05.054
7. Gallo, P., Yan, Y., Sumigawa, T., Kitamura, T.: Fracture behavior of nanoscale notched silicon beams investigated by the theory of critical distances. Adv. Theory Simul., 1700006 (2017). https://doi.org/10.1002/adts.201700006
8. Taylor, D.: The Theory of Critical Distances: A New Perspective in Fracture Mechanics. Elsevier, Oxford (2007)
9. Shimada, T., Ouchi, K., Chihara, Y., Kitamura, T.: Breakdown of continuum fracture mechanics at the nanoscale. Sci. Rep. **5**, 8596 (2015). https://doi.org/10.1038/srep08596
10. Susmel, L., Taylor, D.: The theory of critical distances as an alternative experimental strategy for the determination of K_{Ic} and ΔK_{th}. Eng. Fract. Mech. **77**, 1492–1501 (2010). https://doi.org/10.1016/j.engfracmech.2010.04.016
11. Taylor, D.: The theory of critical distances: a link to micromechanisms. Theor. Appl. Fract. Mech. **90**, 228–233 (2017). https://doi.org/10.1016/j.tafmec.2017.05.018
12. Kitamura, T., Umeno, Y., Fushino, R.: Instability criterion of inhomogeneous atomic system. Mater. Sci. Eng. A **379**, 229233 (2004). https://doi.org/10.1016/j.msea.2004.02.061