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外国人特別研究員作成／By Fellow

2019 / 1 / 11
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JSPS Fellow's
Signature (Handwritten only) : Pasquale Gallo

Research Report (by Fellow)
(Cover Page)

I hereby submit the research report of my fellowship.

1. Name (Print) : Pasquale GALLO
2. Nationality : Italy
3. Host Institution : Kyoto University
4. Host Researcher : Prof. Takayuki KITAMURA
5. Title of Research in Japan : Unified fracture mechanics in micro- and mano-materials Based on Strain Energy Density Criterion
6. Fellowship Tenure : From 2016 / 11 / 26 (YYYY) (MM) (DD) To 2018 / 11 / 25 (YYYY) (MM) (DD)

***Notes for writing the Research Report**
***Type this form except the date and the signature.**
Please prepare your Research Report in English or Japanese within three to ten pages including this page. The contents should include:

7. Background of Research

With the continuous miniaturization of electronic devices driven by the ever-increasing demand for high-density integration, the size of elements has been approaching several nanometers. Examples of such devices are micro- and nano-electromechanical systems (MEMS and NEMS) employed as sensors and actuators. These new advances have brought problems of material behavior at the micro/nanometer scale into the domain of fracture mechanics. While for the characterization of fracture and fatigue at the macroscale numerous reliable approaches and theories are available, the small dimensions of MEMS and NEMS pose a tremendous challenge for experimental studies, which in turn prevents theoretical advancements. Especially, basic mechanical properties governing the fracture, such as the fracture toughness, have shown a strong dependence from the local geometries and their reliability is affected by the accurate realization of proper specimens. From the theoretical point of view, when approaching such small scales, it is natural to wonder if continuum theory is valid, if the linear elastic fracture mechanics is a reliable tool and if the limitation (if any) of continuum theories can be quantified.
Some few preliminary results available in the literature, have shown that this topic is currently very challenging and that it deserves special attention from the scientific community. Some examples available for the single crystal silicon showed that a singular stress field of just a few nanometers still governs the fracture. Moreover, the fracture toughness obtained had good agreement with the bulk counterpart, confirming that some mechanical properties seem to be independent of the size. These preliminary results suggest that there is certainly room for an extension of some well-known continuum fracture theories to very small scales, but the definition of the correct parameters governing the fracture and their lower limit of applicability was still unclear. Additionally, it does beg the question of how to approach lower scales, where the discrete nature of atoms can't be neglected. Indeed, when approaching atomic scale and in general beyond the breakdown of continuum theory, the validity and definitions of usual macromechanics parameters (e.g., stress, strain, elastic constant) should be reconsidered. Approaches based on energy seem to be very versatile, and their concepts showed to be easily extensible and valid from

the macroscale until the atomic level. If one considers the brittle fracture of silicon, the Griffith criterion, Energy Release Rate (ERR) have been reformulated successfully to consider the atomic structure and validated by using atomic simulations.
In the above background, the present research had the primary target to conduct a systematic investigation of classic continuum fracture mechanics concepts based on energy at the micro- and nano-scale. The focus is primarily on silicon, that represents the most fundamental and straightforward research target in the field of fracture nanomechanics and represents the starting point before consideration of plastic phenomena (e.g., emission of dislocation). This research tries to answer to questions like: can classic continuum theory be extended at small scale? How to quantify the breakdown of continuum theory? How to characterize the fracture at very small scales? Ultimately, can we provide a unified fracture mechanics theory based on energy parameters?
The investigation of fracture nanomechanics might bring great advancements not only in several academic fields (e.g., multi-physics) but also in industrial miniaturization of future electronic devices. The present research is the first step towards a unified and general formulation of fracture mechanics theory, from macro to the atomic scale, and provides invaluable insight into the micro-mechanisms of fracture and, to some extent, to fatigue.

8. Research methodology

The research has made extensive use of the advanced equipment provided by the host supervisor/institution. Specifically, the work has been conducted by alternating the following work packages:

- Experimental activities: the focus has been on experimental characterization at the micro and nanoscale of fracture of single crystal silicon. In detail, the research has explored geometries rarely considered in the field, such as notched nano-cantilever beams, and common geometry as well (e.g., pre-cracked specimens). The specimens have been realized by Focused Ion Beam processing system (see Fig. 1 as a qualitative example of final sample) starting from a silicon plate. The considered geometries have all similar fabrication process with differences in the final steps.

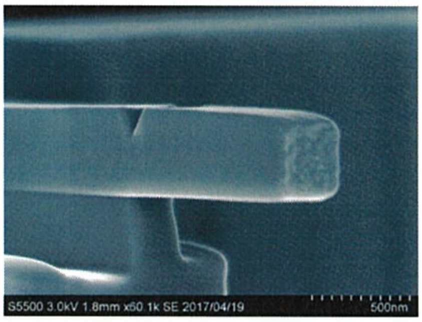

Fig. 1. Example of notched nano-cantilever beam sample.

Once the specimens are realized, they are deposited on the flat tip of a gold wire. The experiments are then conducted in TEM (transmission electron microscope) provided with in-situ observation camera. The load and opening displacement were applied by using a wedge-shaped indenter while a sensor beneath the indenter detected the applied load. Figure 2 gives a qualitative example of the experiment devices and loading procedure.

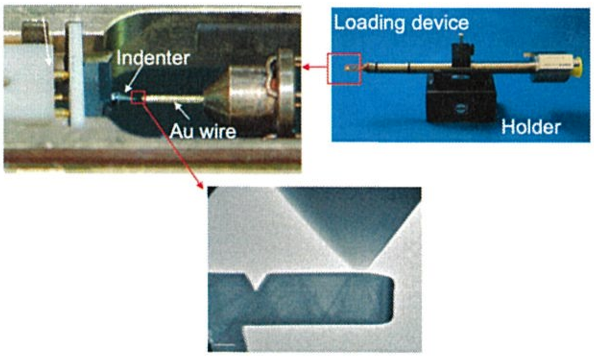

Fig. 2. Example of loading devices and experiments in TEM.

- Theoretical developments: based on the obtained results, several classic fracture mechanics concepts have been considered and applied/developed for the first time at such small scales. The focus has been primarily on energy methods, e.g., averaged strain energy density criterion (aSED) and theory of critical distances (TCD). In particular, by evaluating the parameters of the TCD, it has been possible to evaluate accurately the most

important variables of the aSED criterion, such as the control volume over which the strain energy density is averaged. This has permitted to overcome some practical challenges when characterizing mechanical properties at small scales, e.g., size dependency of mechanical properties. The re-analysis of the results has also underlined limitations of continuum theory, and a new formulation of the aSED criterion has been proposed based on atomic potentials. Based on these results, insight into the breakdown of continuum theory has been provided.
  Finite Fracture Mechanics theory, who has several similarities with the TCD, has been considered late and left as future work.
- Numerical simulations: the re-analysis of the experimental results has made extensive use of numerical tools. Until the breakdown of continuum theory, finite element method has been mainly used to re-analyze stresses and strains at notch root or crack tip. 2D and 3D linear elastic simulations have been realized by considering the anisotropy of single crystal silicon. Beyond the breakdown of continuum theory, where the discrete nature of atoms can't be neglected, atomic simulations have been realized by using LAMMPS molecular dynamics code (Large-scale Atomic/Molecular Massively Parallel Simulator). The simulations have considered specimens of different sizes of crack plates made of silicon. A large number of samples have been tested, varying from a few hundreds of atoms (small specimens) until hundreds of thousands (for larger samples). A bond order potential of modified Stillinger–Weber (SW) form was adopted to characterize the brittle nature of fracture from the crack tip. In the tensile experiments, the thickness dimension was fixed with a periodical boundary to realize a plane strain condition. A stepwise increment of strain was applied to the top and bottom layers of atoms. After each loading increment, the atomic structure was fully relaxed by using Fast Inertial Relaxation Engine (FIRE). The atomistic simulation permitted to obtain for each specimen the critical deformation/load at fracture.

As a future collaboration with the host institution and following the excellent results obtained during the fellowship, the focus has been moved later to the copper and fatigue process by using resonant vibration technique. However, this activity is limited to preliminary experiments and will bring to excellent publications in the near future.

9. Results/impacts

The research plan had mainly three targets: high quality scientific output with the aim to proposed a unified fracture mechanics tool based on aSED criterion that would characterize the fracture from the macro to the nanoscale; dissemination of the obtained results; establishment of a stable international collaboration within all the partners involved in order to promote an active exchange of knowledge and resources that would bring enormous benefit to both Japanese society (and young scholars) and foreign institutions. Currently, excellent results have been obtained in all these three entries:

- Scientific outputs: the new findings, obtained through an excellent combination of experimental activity, numerical tools, and sophisticated theoretical developments, have been numerous and of high quality. The results have been published or are currently to be submitted in relevant international scientific journals, such as Theoretical and Applied Fracture Mechanics, Advanced Theory and Simulations. These works successfully combined theoretical formulations of the theory of critical distances (TCD) and strain energy density (SED) to highlight mechanisms of fracture at micro and nanoscale and to quantify the breakdown of continuum fracture mechanics. Results showed that the fracture toughness of silicon is independent of size and crystal orientation — moreover, the studies put forth a new and more simple methodology for the characterization of fracture properties at the micro- and nanoscales. Indeed, the TCD can be applied to a large variety of materials, such as composites materials, polymers, ceramics, and even bio-materials (e.g., bones). It provides a tool for the evaluation of the fracture mechanics properties by characterizing, at the same time, the breakdown of continuum theory. By re-analyzing the results in terms of "energy," it has been found that the averaged SED is still characterizing the fracture at very small scales.
  In conclusion, it is shown that within the limit of continuum fracture mechanics, classic approaches can be easily scaled down to the nanoscale, provided that the main parameters (that become variables) are calibrated to consider the unavoidable scale effect. By contrast, once the low limit of continuum mechanics is reached, one must deal with atomic structure and theories reformulated accordingly. In this case, energy criterions seem more flexible than others in adapting to discrete models. This hypothesis has been confirmed by the results from Molecular Dynamics (MD) experiments on cracked samples. Indeed, based on these last analyses, a unified method for the characterization of fracture from macro-scale to beyond the breakdown of continuum theory has been formulated. The proposed model defines the strain energy density concept as a function of atomic potential, and it is the first step towards a universal formulation of fracture mechanics concept.
- Dissemination of the results: all the obtained results, besides publication in relevant

international scientific journals, have been presented in several international conferences and strongly appreciated. The results have sparked significant interest in the scientific community that has brought to numerous relevant collaborations. The main channel of dissemination of the results has been participating in international conferences related to the field of mechanics of materials and fracture mechanics. These include, for example, "International Conference on Crack Path," "International Conference on the Theoretical, Applied, Experimental Mechanics." The target has been, therefore, primarily researchers and/or academic partners. However, as better explained below, impact on the industry may be relevant as well.

- International Collaboration: the establishment of international network was one of the primary targets of the fellowship. The research has successfully brought and established relevant international connections with several famous universities and countries, such as NTNU (Norway) and China, as demonstrated by international co-authorship. Potentially, collaboration with Italian Universities has also been considered for future papers (see the end of this section for more details on on-going works). The research has strengthened the connection with Aalto University (Finland) as well, and it is currently considered as a primary partner for international grant applications. Specifically, the fellow and Aalto University have recently applied for financial support from Academy of Finland funding body, and the JSPS host supervisor's research team have been included in the research project as principal collaborators. Host researcher is now permanently considered as the overseas partner and therefore involved in any future applications. Moreover, both fellow and host researcher are committed to supporting and promoting the active exchange of young scholars at any level.

The results summarized above had a great impact in academia in the short term, and also in the industry in the long term.
The obtained results are indeed an important step towards a deeper understanding of fracture nanomechanics and a universal formulation of fracture mechanics concept. The effort has been devoted to a completely new and cutting-edge field of science, and the obtained results will support future researchers and young minds. Contribution to the field has been relevant, and the results will surely be considered as pioneers in the future. Concepts like continuum theory and fracture mechanics have been re-interpreted by promoting multidisciplinary approach, e.g., bringing together material science and classic mechanical engineering concepts. A deeper understanding of fracture mechanisms at small scales and transition from macro to nanoscale have been achieved. Future researchers may find the current results useful when also studying the macroscale. Indeed, multiscale modeling may benefit from the proposed findings. To some extent, theoretical bases proposed here may be crucial for the next great challenge that is the investigation of fatigue phenomena.
On the long-term, all the outcomes may provide relevant impact in the industrial field if adequately disseminated. All the proposed developments, indeed, have been provided with the aim to support practical challenges (in addition to the academic advancements). Electronic industries involved in the design of Microelectromechanical systems (MEMS) and Nanoelectromechanical system (NEMS) may surely benefit from the new solutions proposed when characterizing mechanical properties and static assessment of those components. Both the TCD and aSED, indeed, heavily simplified the experimental characterization and numerical analysis. The aSED criterion, for example, presents important mesh independence when using FE methods and therefore models with very low computational cost may be used in the design phase. The TCD, on the other hand, provides a new simpler way to determine fundamental quantities such as fracture toughness and ideal material strength by using notched components. These geometries, indeed, are considerably simpler to be realized and tested than classic experiments based on pre-crack specimens. A further added value is that with reasonable effort extension to fatigue process would be certainly possible.
Concluding, in addition to the publications already available, the research plan has produced excellent results, in collaboration with international partners, that are currently under finalization. In particular, it should be mentioned:
-a final paper based on molecular dynamics simulations is currently under finalization and will be submitted to a relevant international journal at the beginning of 2019. This final work will propose a more general formulation based on the atomic potential of the strain energy density to assess the fracture behavior of the brittle material. The work will also discuss and quantify breakdown of continuum theory. A critical discussion of the results will be carried out by comparing the data with relevant scientific papers available in the literature.
-review/progress report in the field of fracture nanomechanics and energy methods. Upon the invitation of the prestigious international journal "Advanced Theory and Simulations," a review on the recent advancements in the field is scheduled for the summer of 2019, in collaboration with international partners (e.g., NTNU-Norway).
-application of finite fracture mechanics at small scales. In collaboration with Italian researchers, the experimental data obtained during the JSPS fellowship is being re-analyzed by using the finite fracture mechanics theory. Paper will be submitted to international journal later in 2019.

Note: As much as possible, describe the contents and results of your research in a manner that is easily understandable to a non-specialist in your field. Provide a concrete description if (1) papers related to your work have been published in major academic journals, (2) particularly outstanding research results were achieved, or (3) patent applications have been made or other tangible outcomes achieved through the research.

10. Research Presentations during the period of the fellowship (Name of the conference, title, place, date)
International Conference on the Theoretical, Applied, Experimental Mechanics; Investigation into the breakdown of continuum fracture mechanics at the nanoscale: synthesis of recent results on Silicon, Paphos (Cyprus), 17-20 June 2018;
IIW18, Fatigue design of laser stake-welded T-joints made of thin plates under tension and bending loads, Bali (Indonesia), 14-20 July 2018;
6th International Conference on Crack Paths, Experimental characterization at nanoscale of single crystal silicon fracture toughness, Verona (Italy), 19-21 September 2018;
5th Nano Today Conference, Hawaii (USA), 6-10 December 2017.

11. A list of paper published during or after the period of the fellowship, and the names of the journals in which they appeared (Please fill in the format below). Attach a copy of each article if available.

Author(s)	Title	Name of Journal	Volume	Page	Date	Note
P. Gallo; T. Sumigawa; T. Shimada; Y. Yan; T. Kitamura.	Investigation into the breakdown of continuum fracture mechanics at the nanoscale: synthesis of recent results on Silicon.	Proceedings of the First International Conference on Theoretical, Applied and Experimental Mechanics	5	205-210	2019	Published in ***Structural Integrity*** book series, Springer.
P. Gallo; T. Sumigawa; T. Kitamura.	Experimental characterization at nanoscale of single crystal silicon fracture toughness.	Fracture and Structural Integrity	*In Press*	*In Press*	2018	
P. Gallo; T. Sumigawa; T. Kitamura; F. Berto.	Static assessment of nanoscale notched silicon beams using the averaged strain energy density method.	Theoretical and Applied Fracture Mechanics	95	261-269	2018	
P. Gallo; Y. Yan; T. Sumigawa; T. Kitamura.	Fracture behavior of nanoscale notched silicon beams investigated by the Theory of Critical Distances.	Advanced Theory and Simulations	1	1700006	2017	Most cited work (updated at 11-2018)
P. Gallo; M. Guglielmo; J. Romanoff; H. Remes.	Influence of crack tip plasticity on fatigue behavior of laser stake-welded T-joints made of thin plates.	International Journal of Mechanical Sciences	136	112-123	2018	
M. Ayatollahi; F. Berto; A. Campagnolo; P. Gallo et al.	Review of local strain energy density theory for the fracture assessment of V-notches under mixed mode loading.	Engineering Solid Mechanics	5	113-132	2017	
M. Acanfora; P. Gallo; S.J. Razavi et al.	Numerical evaluation of T-stress under mixed mode loading through the use of coarse meshes.	Physical Mesomechanics	21(2)	124-134	2018	
P. Gallo; H. Remes; J. Romanoff.	Influence of crack tip plasticity on the slope of fatigue curves for laser stake-welded T-joints loaded under tension and bending.	International Journal of Fatigue	99	125-136	2017	
P. Gallo; S. Bressan; T. Morishita; et al.	Analysis of multiaxial low cycle fatigue of notched specimens for type 316L stainless steel under non-proportional loading.	Theoretical and Applied Fracture Mechanics	89	79-89	2017	
P. Gallo; T. Sumigawa; T. Kitamura; F. Berto.	Evaluation of Strain Energy Density control volume for a nano-scale singular stress field.	Fatigue and Fracture of Engineering Materials and Structure	39	1557-1564	2016	

12. Awards during the period of the fellowship (Name of the award, Institution, date etc.)
• Top Reviewer Award, Fatigue and Fracture of Engineering Materials and Structures, August 2017;
• Outstanding Reviewer Award, Wear (2018), International Journal of Fatigue (2017);