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Recencja Rozprawy Doktorskiej:

Atomistic Simulation of Crack Propagation in Irradiated Materials

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Niniejsza ocena została sporządzona na podstawie powołania przez Radę Naukową Instytutu Podstawowych Problemów Techniki PAN w Warszawie z dnia 19 marca 2026 r. Przedłożona praca została przygotowana w języku angielskim, dlatego niniejsza recenzja również sporządzona jest w tym języku, aby umożliwić kandydatowi do stopnia doktora wnikliwe zapoznanie się z jej treścią oraz prowadzenie dyskusji na wymaganym poziomie naukowym, bez ryzyka niejednoznaczności wynikających z nieautoryzowanego tłumaczenia. Konkluzja recenzji i rekomendacja dla Rady Naukowej przedstawione są natomiast w j. polskim.

Dissertation Review:

Atomistic Simulation of Crack Propagation in Irradiated Materials

Author: mgr inż. Hojjata Mousavisogolitappeh

This report has been prepared based on an appointment by the Scientific Council of the Institute of Fundamental Technological Research of the Polish Academy of Sciences in Warsaw, dated March 19, 2026, to evaluate the fulfilment of the requirements for the degree of Doctor with specialisation in Mechanical Engineering.

General information

The doctoral dissertation presents a molecular dynamics (MD) model to assess how radiation-induced defects affect crack propagation and plastic deformation mechanisms under loading conditions compared with those of the unaffected material. The defined framework is focused on the fracture evaluation under mode-I tensile loading conditions in the Fe–Ni–Cr austenite model alloy. The work has primarily a qualitative character, but includes also some quantitative attempts to evaluate fracture resistance using energy-based criteria. The role of crystallographic orientation in the ductile-to-brittle transition is also addressed under specific assumptions.

The scope of the thesis is timely and relevant, as understanding the behaviour of structural materials in nuclear reactors under harsh in-service environments, particularly under neutron irradiation, is critical for the further development of safe, large-scale industrial applications. Investigations on these topics, both from experimental and numerical points of view, are carried out by research teams across the world, to support the country's energy policies. Based on the literature review, the Author appropriately identifies research gaps and defines six key scientific questions that he attempts to answer within the thesis.

The manuscript itself is composed of an introduction with five regular chapters followed by conclusions and perspectives. A literature section contains 187 papers, including many publications of a fundamental nature for this topic, as well as 56 new ones published in the last five years, i.e. in the years 2021-2026. Additionally, at the end of the thesis, seven very useful appendices are provided. The focus on computational materials science and mechanical engineering is clear from the presented content.

Evaluation of the thesis

The title of the thesis is, in general, adequate, as it reflects the content of the dissertation in a broad sense. However, it could have been more focused on the investigated material system, as the replicability of the findings to other irradiated material systems is neither direct nor obvious.

The first chapter of the thesis is an introduction to the topic that presents the motivation for the work undertaken in the area of irradiated stainless steel behaviour under operational conditions. The Author also identifies the six research questions that will be the topic of the dissertation. The overall structure of the dissertation and the content of each of the four main chapters are also summarised, which makes a very good guideline for the reader.

Chapter 2 provides the background and literature review of research on the fracture phenomenon in structural materials under radiation exposure. The characteristics of irradiation environments are introduced, in particular, the challenges associated with exposure to high-energy particles in, e.g., tokamak fusion reactors and large-scale particle accelerators. The role of radiation-induced defects in changes of mechanical material responses is clearly highlighted. The Author also introduces stainless steel 310S as a very good model alloy for studying radiation-induced embrittlement. Radiation defects such as voids, bubbles, dense populations of dislocation loops, vacancy clusters, or stacking fault tetrahedras and associated damage measures are also well characterised at the atomic level. However, some of the experimental capabilities for imaging at this length scale could be further elaborated. In this chapter, the unique experimental capabilities of the MARIA reactor at the National Centre for Nuclear Research (NCBJ) that could be used in such investigations of irradiated materials are also mentioned; unfortunately, such research was beyond the scope of this work.

Within the chapter, the Author also addresses the capabilities of numerical simulations of irradiation defects based on MD and the concept of collision cascades initiated by primary knock-on atoms (PKA). This section presents a series of fundamental works alongside the most recent ones, highlighting the high potential of these approaches in scientific research of fundamental nature. The same observation is relevant to the state-of-the-art description of plastic deformation mechanisms operating at crack tips, as well as to fracture mechanics at the atomic level. Information on stress intensity factor, ductile-to-brittle transitions, traction-separation, crack-tip plasticity, or the role of crystallographic orientation is well discussed. Eventually, based on the presented literarure review, a clear goal of the thesis is defined: „by explicitly modeling the interaction between advancing cracks and radiation-induced defects, this work aims to quantify how microstructural disorder alters dislocation activity, energy dissipation, and the overall fracture response" and „… (this work) establishes a predictive framework for identifying the conditions leading to ductile-to-brittle transition in irradiated materials."

Chapter 3 presents the methodology and computational techniques framework that was used within the research. First, the molecular dynamics framework, including classical mechanics, statistical ensembles, ergodicity, as well as thermodynamic interpretation concepts, is described. The discussion of the Newtonian and Hamiltonian formulations, boundary conditions, along with the simulation ensembles (NVE, NVT and NPT) in MD, is very comprehensive and valuable, especially for readers unfamiliar with atomistic simulations. The Author describes these thermodynamic ensembles used to regulate temperature, pressure, and energy across simulation stages, along with the numerical integration schemes applied to ensure stable atomic trajectories. Additionally, a clear explanation of how the macroscopic mechanical and thermodynamic quantities (stress, pressure, and temperature) can be obtained from MD results is presented. However, a more extensive discussion of available interatomic potentials beyond the Lennard-Jones and EAM (Embedded Atom Method) would be beneficial. At the end of the chapter, the Author also describes the workflow for simulation, data transfer, and results visualisation, which is quite classical for this class of simulations and includes available software: LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), OVITO (Open Visualization Tool) and Atomsk. Therefore, a clear indication of the novelty of the proposed framework should be better highlighted. In general, the chapter is very well written and informative; however, it has a textbook character with a lot of standard information.

Based on the presented information, identified goals, and described simulation workflow, the Author has conducted the main scientific part of his doctoral dissertation.

The core conducted research in Chapters 4 and 5 has already been positively reviewed by editorial boards and independent reviewers in the prestigious scientific journals (International Journal of Mechanical Sciences and International Journal of Plasticity), which confirm that the defined goals were justified, and the research itself was properly planned and implemented. However, in this review, I will still present the general characteristics of these works and provide a summary of the results, along with additional critical comments.

In Chapter 4, an atomistic analysis of the ductile-to-brittle transition (DBT) in irradiated austenitic stainless steel was presented by Mr. Mousavisogolitappeh. The key aspect was to investigate crack–radiation defect interactions in the selected $Fe_{55}Ni_{19}Cr_{26}$ alloy, which was used in the thesis as the model system. At the beginning, the significance of radiation-induced embrittlement was described once more as a motivation for this part of the investigation. Then, the MD model, interatomic potentials, and the procedure for generating and controlling radiation defects were described in detail. Potential data were acquired from the literature. The

0.008, 0.038, 0.152, and 0.266 dpa (displacements per atom) were set, leading to a total of 20, 100, 400, and 700 cascades, which were considered during the investigation. The method for initiating and tracking crack propagation was also explained by the Author. An important component in this chapter is the introduction of an energy-based analysis that separates plastic and surface contributions to the total fracture energy. The model assumptions are well presented, however, the selection of such a dpa range should be better motivated. These levels of dpa seem to correspond to a quite early stage of damage accumulation and may not be representative of the higher doses typical of service conditions. They can be sufficient to capture initial defect formation and their interaction with crack-tip plasticity, but may not be sufficient to account for long-term microstructural evolution (e.g. void coarsening). The Author also notes that the simulation box dimensions were selected based on convergence tests, but these interesting results have not been presented in the thesis. The discussion on the statement „This system size was verified to be sufficient for resolving crack-tip plasticity, dislocation activity, and defect–crack interactions without introducing significant boundary artifacts, while maintaining computational efficiency" should also be more elaborated. On the contrary, it is worth mentioning that a lot of very interesting information and data, from the scientific and replicability of results point of view, like discussion on the role of boundary conditions, is gathered and well described in the appendices.

In this part, the investigation of crack propagation was carried out with the use of unirradiated and irradiated samples with various defects. Additionally, to make the fundamental investigation, a set of analyses was done with models including isolated defects (small/large voids, dislocation loops and rigid inclusions). Such an investigation is practically impossible in any other way than with the use of numerical analysis, highlighting its role in a better understanding of underlying physics. Overall, based on the simulation results, the Author was able to demonstrate that different types of defects influence fracture mechanics in a competing manner and as a function of the applied dose. For example, voids promote strain localisation and favour initiation of brittle propagation. At the same time, dislocation loops can dissipate energy and deflect or, at higher defect density regions, arrest the crack path, increasing the contribution of plastic deformation. The Author also points out that as the irradiation level increases, there is a decrease in plastic work and a transition toward a brittle-dominated regime. The novelty aspects of the findings are well stated in the text. In this chapter, to help data interpretation, an energy-based fracture analysis was also proposed that assumes two factors: surface energy and plastic work. The presented results analysis raised a couple of questions. It is not clear how many times each MD simulation, e.g. from Fig. 4.12, was repeated to take into account stochastic events. Also, it is not clear why only exemplary results for particular initial models after various dpa are presented, e.g., 0.152 dpa. The discrepancies in maximum applied dpa values are also observed, as shown in Figure 4.9, which reports dpa at the level of 0.494, which was not mentioned earlier. Fig. 4.13 requires more extensive explanation, as there is no clear relation in the results with increasing dpa level. Finally, the microstructural–mechanical linkage mentioned on page 78 is not fully clear based on such a limited material volume, including only some minor defect types, neglecting many others, including grain boundaries. Such microstructural simplifications and the restriction to a single loading mode limit the direct applicability of the results to real engineering materials. At the same time, the results are usually dependent on the selected interatomic potential, raising questions about the quantitative robustness of the reported defect vs. crack interaction mechanisms.

Some of the simplifications of the setup investigated in Chapter 4 are addressed in Chapter 5, where the Author considered additional sources of heterogeneities in the material response to loading, in particular, the role of crystalographic orientation.

Therefore, Chapter 5 deals with the influence of crystallographic anisotropy on the slip-system activity, defect–dislocation interactions or crack-tip plasticity, eventually affecting ductile-to-brittle transition. The (001), (011), and (111) fcc orientations were tackled. The same simulation methodology used earlier was applied in this part of the investigation. The approach is systematic and well justified, but again it limits the study to relatively low irradiation doses (0.152 dpa) and neglects interesting effects of, e.g., helium. The representativeness of the results obtained from the models presented in Figure 5.1 should also be elaborated. In general, the thesis examines, in a comprehensive manner, stress–strain response, crack-length evolution and traction–separation analysis, allowing for the estimation of atomic-scale fracture energy. Overall, the results convincingly demonstrate that radiation-induced embrittlement is strongly orientation-dependent, with the (011) orientation showing a pronounced ductile-to-brittle transition due to defect-induced suppression of plasticity, while the (111) orientation retains ductility due to multiple active slip systems.

It is evident that both Chapters 4 and 5 provide an approach for a fundamental investigation of the fracture behaviour under specific loading conditions in a specific material system. The research outcome is undoubtedly valuable and contributes to the state-of-the-art in this area. Despite the mentioned strengths, this research is constrained by typical limitations of MD simulations, like finite model size or dependence on the selected interatomic potential. Furthermore, the absence of experimental validation or multiscale modelling limits the broader applicability of the findings. Addressing these limitations in future research would make a significant impact on the field.

Chapter 6 presents conclusions and plans for future work. The main outcome is a direct representation of the fact that irradiation does not cause just one main embrittlement mechanism. Instead, fracture resistance and crack growth depend on a balance between two effects: defects can either speed up crack growth or help slow it down by shielding the crack tip. Which effect dominates depends on how the defects evolve and on the crystal structure, which controls how the material can deform at the crack tip. At the same time, in this chapter, the Author clearly demonstrates that he is aware of the model limitations and has a well-defined plan for future research. This is very good evidence that he is a mature scientist, with a good understanding of his achievements and future challenges.

Detailed comments

The thesis is well written, adhering to the standards of scientific and technical writing. The quality of the illustrations is at a good level, and their clarity is exemplary. The work contains a negligible number of minor mistakes, e.g., similar information or abbreviation descriptions, like EAM, are repetitively provided in subsequent subchapters.

Open questions

Please provide explanations of the following questions in written form:

1. Explain why an alloy composition closer to EC316LN was not used during the investigation. It seems that it would be more representative of reactor structural steels.
2. What are the differences between EAM and EAM11?.
3. Explain why the EAM-type interatomic potential was used in this investigation.
4. Explain if any in-house code was created to support the defined simulation workflow.
5. Explain why the dpa level in the research was kept at relatively small levels.
6. Provide exemplary results highlighting convergence test results used to define the MD simulation box dimensions.
7. Comment on the computational resources used for the simulations and the computing times.
8. Comment on the repetitiveness of the results for the same initial setup. Explain, for example, how many times each MD simulation was carried out to obtain an average response of the investigated system.
9. Explain what the „species" on page 59 means.
10. Extend the discussion of results from Fig. 4.13 to make them more informative.
11. Comment on the possible influence of microstructural simplifications and a particular loading mode on the direct applicability of the results to real engineering materials.
12. Elaborate on the representativeness of the results obtained from models presented in Fig. 5.1.
13. Explain what are the physical reasons for the sharp increase in void volume in Fig. 5.3.
14. Explain why the results are often limited only to a single dpa value, e.g. in Fig. 5.4.
15. Explain why different numbers of configurations were investigated: four for (011) and three for (001) and (111).
16. Explain the possible experimental setup for the validation of such simulation results.

Conclusion remarks

The PhD candidate, based on the identified research gaps and proposed assumptions, properly conducted the work in his dissertation, demonstrating the required level of scientific maturity. He presented the skills and knowledge necessary to independently formulate and solve a scientific problem. He is also able to identify limitations of the results and define the future direction of research. Therefore, I fully support his candidature for a doctorate in the mechanical engineering discipline.

Przedstawione powyżej uwagi krytyczne są w dużej mierze dyskusyjne i wynikają z zainteresowania recenzenta przedstawioną rozprawą. Praca z tego typu modelami numerycznymi oraz w skali wymiarowej, z którą zmierzył się doktorant, jest niezmiernie skomplikowana, złożona i zawsze będzie zostawiać pole do szerokiej polemiki naukowej. W związku z powyższym, przedstawione uwagi nie obniżają pozytywnej oceny

przedstawionej rozprawy doktorskiej.

Uważam, że opiniowana rozprawa doktorska, jest dziełem dysertabilnym i spełnia warunki określone Ustawą z dnia 20 lipca 2018r. Prawo o szkolnictwie wyższym i nauce. W związku z powyższym wnioskuję o dopuszczenie mgr inż. Hojjata Mousavisogolitappeh do dalszych etapów przewodu doktorskiego.

Signed by / Podpisano przez:

Łukasz Madej
Akademia Górniczo-Hutnicza im. Stanisława Staszica w Krakowie

Date / Data: 2026-04-21 07:32