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REVIEW

of the doctoral dissertation **by Hojjat Mousavisogolitappeh MSc.**
entitled "*Atomistic Simulation of Crack Propagation in Irradiated Materials*"

Identification description: computer printout with the rights of a manuscript, 148 pages, 181 references.

Doctoral thesis supervisor: dr hab. Aneta Ustrzycka

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GENERAL ASSESSMENT OF THE DISSERTATION: TOPIC, PURPOSE, AND SCOPE OF WORK

The doctoral candidate Hojjat Mousavisogolitappeh set out to develop an atomistic description of the influence of radiation defects on crack propagation and fracture resistance in Fe–Ni–Cr alloys, with particular emphasis on the role of voids, dislocation loops, crystallographic orientation and the loss of the ability to dissipate energy plastically at the crack tip. The subject of this thesis can be considered innovative in the sense that the author attempts to integrate three key issues into a single atomistic model: the evolution of radiation defects, crack propagation, and orientation-dependent mechanisms of plastic deformation. Particularly valuable is the treatment of fracture in irradiated material as the result of competition between defects that promote fracture propagation, especially voids, and defects capable of locally shielding the fracture tip, such as selected interstitial clusters and dislocation loops.

A valuable contribution (generally in doctoral dissertations) would be to formulate a research hypothesis that would allow the author's scientific arguments to be organized logically. From a formal point of view, it would be preferable to clearly distinguish the research hypothesis within the thesis, as it is currently scattered amongst the description of the motivation, the aim of the work and the research questions. This is not a criticism, but a suggestion for the future. Nevertheless, given the generally formulated objective of the dissertation, I consider the selection of research methods and tools described in the subsequent chapters of the dissertation to be appropriate. In my opinion, this dissertation tackles a difficult and complex topic and is a valuable reference work for other researchers. The structure of the dissertation is correct and typical for this type of study.

The thesis is divided into six main chapters and seven technical appendices. Its structure is logical and guides the reader from the general scientific context, through a description of the methodology, to a presentation of the results concerning the fracture behaviour of irradiated materials.

Chapter 1 provides an introduction to the subject matter of the thesis. The author outlines the importance of the durability of structural materials used in nuclear environments, discusses the effects of irradiation on microstructure and mechanical properties, and sets out the main motivation for the research. This chapter also defines the aim of the thesis, the scope of the analyses, and the main research questions concerning the influence of radiation defects on crack propagation and the transition from ductile to brittle behaviour.

Chapter 2 contains a literature review and the theoretical background of the thesis. It discusses radiation environments, the properties of materials used under irradiation conditions, the mechanisms of radiation defect formation, and their experimental identification. The author also presents the fundamentals of collision cascade simulations, plasticity mechanisms in FCC-structured metals, and issues in atomistic fracture mechanics. This chapter provides the reader with a solid introduction to the subject of radiation defects, dislocation loops, voids, SFT, and their influence on material behaviour at the crack tip.

Chapter 3 is devoted to the research methodology. The author discusses the fundamentals of molecular dynamics, the statistical ensembles used, the method for determining virial stresses and thermodynamic quantities, interatomic potentials, system relaxation procedures, and boundary conditions. The chapter also presents a general scheme for simulation and data processing, which forms the basis for the analyses carried out in the remainder of the thesis.

Chapter 4 concerns radiation-induced brittleness in Fe–Ni–Cr alloy. The author analyses the influence of radiation defects on crack propagation, plastic deformation mechanisms and changes in fracture resistance. Particular attention is paid to the interaction of the crack with voids, dislocation loops and defect clusters. In this chapter, an energy-based approach has also been applied to assess fracture resistance, distinguishing between the contributions associated with the formation of new surfaces and plastic dissipation.

Chapter 5 extends the analysis to include the influence of crystallographic orientation on the behaviour of irradiated material. The author compares crack propagation in selected orientations, namely (001), (011) and (111), analysing differences in the activation of slip, twinning, dislocation emission and local plasticity mechanisms. This chapter also contains a quantitative assessment of the stress–strain relationship, crack length evolution, traction–separation analysis and fracture energy. This chapter is a key part of the work, as it demonstrates that the effect of irradiation depends not only on the defect population but also on the crystallographic geometry of the material.

Chapter 6 contains a summary of the results, final conclusions and proposals for further research directions. The author briefly outlines the main mechanisms responsible for the change in the fracture behaviour of irradiated material, emphasising the role of radiation defects, plasticity limitations and crystallographic orientation. This chapter also presents possible avenues for future research, including the need to further integrate atomistic simulations with higher-scale models.

Appendices A–G supplement the thesis with technical details and supporting analyses. These include, amongst other things, elastic properties and material moduli, analysis of boundary conditions, the selection of a statistical ensemble for fracture simulations, the influence of strain rate, the evaluation of stress distributions at the crack tip, the fundamentals of the cohesion zone model and the laws of traction and separation, as well as implementation details of the crack propagation simulation. The appendices supplement the methodological section of the work and document selected numerical decisions.

In the reviewer's opinion, the issues raised in thesis are important and scientifically relevant. The dissertation is written in correct language using appropriate research methods. However, reading the work raises a number of ambiguities and questions of a scientific nature that should be clarified. These issues will be discussed in detail in the next section of this review.

COMMENTS ON THE DISSERTATION, CRITICAL QUESTIONS, AND DISCUSSION ISSUES

The dissertation is written in correct, understandable language and demonstrates a decent level of editing, no major flaws were found, and some of them are presented later in this review. The rich graphic documentation deserves special mention.

The doctoral student deserves praise for the selection of literature – it includes not only the latest publications, but also earlier publications that are important for this area of research.

The dissertation presents an original and comprehensive approach to the subject, which is undoubtedly a scientific achievement of the doctoral student. Reading the doctoral dissertation also raises a number of questions and issues for discussion, which are presented below:

1. What are the limitations of analysing such similarities between materials like Fe55Ni19Cr26 and 310S steel i.e. representativeness? Which elements of the actual microstructure of 310S steel alloying elements, impurities, grain boundaries, segregation, precipitates, residual stresses, can significantly influence the observed fracture mechanisms? Please comment it.
2. Should the term "ductile to brittle transition" used in the dissertation be understood as a classical ductile to brittle transition, or rather as an atomistic change in the dominant fracture mechanism?
3. How does the author justify the use of this term (DBT) in relation to MD results, without classical experimental data such as impact strength, K_{IC}, J_{IC}, R-curves or the transition temperature? Could the Author comment on available experimental fracture properties of the analysed or related alloys?
4. Continuing on this topic, to what extent can the energy measures used be compared with the classical parameters of fracture mechanics? Can the separation energy from traction-separation analysis and the critical release energy determined in MD be regarded as equivalents of the macroscopic values G_c, J_{IC} or K_{IC}, or rather as local comparative indicators?
5. To what extent are the results sensitive to the limitations of the MD method, particularly cell size, simulation time and very high strain rates? Does the author expect that, with a larger model scale and longer relaxation times, the mechanisms obtained would remain qualitatively the same?
6. How does the author distinguish between the effects of different types of radiation defects on crack propagation?
7. Do you think that, in the case of irradiated materials, the traditional concept of "fracture toughness" needs to be redefined or expanded? Are macroscopic parameters sufficient, or is it necessary to take into account defect populations and local energy dissipation mechanisms?
8. What are the main sources of uncertainty in traction–separation analysis?
9. If we were to attempt to develop such a comprehensive numerical and experimental research procedure for engineering practice, what would the experimental validation of the proposed approach look like? What kind of tests and studies do you think are necessary for validation?
10. In your opinion, how can atomic-scale results be combined with "higher-scale" models?

Maybe, would it be more natural to move towards crystalline plasticity, cohesive zone models, continuous damage models, or perhaps multi-scale methods? Please comment on this issue.

Overall, the dissertation is readable and generally well prepared. However, it contains several editorial and proofreading imperfections that slightly reduce its formal quality. Here are some examples:

1. From an editorial perspective, it would be beneficial to include a list of key abbreviations and symbols – particularly as some of these have been used inconsistently throughout the work, as discussed in the following points.
2. Some figure captions are too long and in places contain interpretative elements that could be moved to the main text. This is not a formal error, but it affects the editorial clarity of the dissertation (e.g. page 6-7)
3. The thesis uses various variants of the term for the same phenomenon: **ductile-to-brittle transition, ductile to brittle transition, transition from ductile to brittle behaviour**. This is not a substantive error, but it highlights the need to standardize the terminology.
4. Figure 2.5 contains several images taken from different publications, and the sources are listed collectively in the caption. This is acceptable, but lacks editorial clarity. It would be better to attribute the source to each panel, e.g. (a1) Mansur, 1994; (a2) Klimenkov et al., 2013. The current notation may make it difficult to determine unequivocally which image comes from which source.
5. The bibliography includes entries such as: "*Max Planck Institute for Plasma Physics (n.d.). Wendelstein 7-X Stellarator, https://...*". It is advisable to standardise the citation of online sources and include the date of access, particularly for image and institutional sources.

Once again, it should be emphasized that the above comments are only for discussion and in no way detract from the positive reception of the results of the work and the goals achieved by the doctoral student, and have been presented by me in accordance with the maxim *nemo sine vitiis est.*

SUMMARY

The significant and creative contribution **of Hojjat Mousavisogolitappeh, M.Sc.,** to the development of materials engineering lies in the fact that he presented a solution to the research problem, i.e., ***Atomistic Simulation of Crack Propagation in Irradiated Materials***, on the basis of which the following achievements can be identified:

1. Development and application of a coherent atomistic framework for analysing crack propagation in irradiated material. I consider the integration, within a single computational procedure, of the generation of radiation-induced defects, the simulation of crack propagation, and the quantitative assessment of the material's response using mechanical and energy parameters to be a significant achievement. Particularly valuable here is the transition from the mere visualisation of atomic mechanisms to the analysis of fracture resistance using energy release rate and traction–separation laws.

2. Demonstration that cracking in irradiated material results from the interplay of degradation mechanisms and crack shielding. The author demonstrated that voids may promote crack acceleration through local weakening and stress concentration, whereas interstitial clusters and dislocation loops may, under certain conditions, contribute to crack-tip shielding. This interpretation is one of the most interesting mechanistic outcomes of the work.

3. Identification of the role of crystallographic orientation in the radiation-induced embrittlement of the Fe–Ni–Cr alloy. A particularly valuable aspect of the dissertation is the demonstration that irradiation-assisted fracture is controlled not only by the type and distribution of defects, but also by crystallographic orientation, slip-system activity, and the capacity for plastic energy dissipation at the crack tip. In this context, the analysis of the (001), (011), and (111) orientations represents an important original contribution of the thesis.

FINAL CONCLUSION

for admission to public defense

Taking into account the entirety of the dissertation and the achievements of the author of the thesis, I conclude that **the doctoral dissertation of Hojjat Mousavisogolitappeh, M.Sc., meets** the requirements of article 13 ust 1. – „Ustawa o stopniach naukowych i tytule naukowym oraz o stopniach i tytule w zakresie sztuki z dnia 14 marca 2003 roku (Dz. U. z 2017 r. poz. 1789 z pozn. zm.)" in connection with art. 179 ust. 1." Ustawa z dnia 3 lipca 2018 r. Przepisy wprowadzające ustawę – Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2018 r., poz.1669 z późniejszymi zmianami)". In view of the above, I hereby submit a request for the admission of **Hojjat Mousavisogolitappeh, M.Sc.,** to the public defense of his reviewed thesis as a doctoral dissertation representing the discipline of Mechanical Engineering.

Wrocław, 25th May, 2026

Dr hab. inż. Grzegorz Lesiuk, prof. uczelni