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

1. Legal basis for the preparation of the review

The legal basis for this review is a letter (ref. no. RN-D-0002.2.2026) from the Secretary of the Scientific Council of the Institute of Fundamental Technological Research of the Polish Academy of Sciences, signed by Prof. Dr Habil. Eng. Zbigniew Ranachowski, and the attached doctoral dissertation by Hojjat Mousavisogolitappeh entitled "Atomistic Simulation of Crack Propagation in Irradiated Materials". The supervisor of the dissertation is Dr Habil. Aneta Ustrzycka.

2. Overview of the doctoral dissertation

This thesis focuses on investigating the mechanisms underlying irradiation-induced degradation in Fe-Ni-Cr alloy, a representative of 310S steel widely utilized in nuclear reactor environments. By employing molecular dynamics simulations, the study explores the interplay between radiation-induced defects, crack propagation, and deformation mechanisms to assess fracture resistance using energy-based criteria. The research highlights the significant impact of crystallographic orientation and defect accumulation on the ductile-to-brittle transition, providing a novel atomistic framework for understanding post-irradiation fracture behavior in austenitic alloys. The research is motivated by the necessity to ensure the reliability of nuclear energy systems under harsh conditions, especially in terms of radiation-induced embrittlement. At the nanoscale, defects resulting from radiation significantly impact how materials respond to mechanical stress.

The study aims to uncover how radiation-induced defects influence crack propagation and to establish a systematic approach for analyzing defect evolution near crack tips. The primary goal is to create an atomistic framework that integrates defect evolution, orientation-dependent deformation, and crack propagation mechanisms to understand the ductile-to-brittle transition and evaluate radiation-induced embrittlement.

The research aims to address the following questions:

- How do voids (vacancy-type defects) contribute to crack acceleration by causing stress concentrations and local lattice weakening?
- How does the growth and merging of voids compete with mechanisms that may impede crack propagation, induced by clusters of interstitial defects?

The subject of this thesis, "Atomistic Simulation of Crack Propagation in Irradiated Materials," is up-to-date and important due to its direct relevance to the safety and longevity of nuclear

energy systems. The thesis specifically addresses a critical gap in understanding how radiation-induced microstructures compromise fracture behavior and material performance at the atomistic level. While experimental studies available in the literature provide valuable insights, they are inherently limited in capturing the full atomistic mechanisms governing defect formation, interactions, and crack propagation. Molecular dynamics simulations, the core methodology of this thesis, are a powerful and widely used atomistic simulation method for investigating irradiation effects in structural materials, particularly those in nuclear energy systems. MD enables researchers to capture dynamic processes like defect generation, microstructural evolution, and property degradation at temporal and spatial resolutions inaccessible to experimental methods. This capability is crucial for understanding defect dynamics, radiation-induced damage, and fracture processes in crystalline materials. The work establishes a unified framework that integrates qualitative insights into defect-controlled fracture processes with quantitative mechanical characterization, explicitly accounting for crystallographic orientation. This provides a physically and mechanically consistent interpretation of radiation-induced embrittlement and the associated ductile-to-brittle transition.

In my opinion, the thesis tackles a contemporary and vital problem in nuclear materials science, using advanced computational techniques to provide fundamental insights into radiation-induced embrittlement that are crucial for enhancing the safety, longevity, and design of current and future nuclear energy systems.

The dissertation is written in English and comprises a total of 148 pages of A4 typescript. It includes an abstract in both English and Polish, a table of contents, six chapters, seven appendices, and bibliography comprising 187 items. The titles of the individual chapters are as follows:

1. Introduction
2. Background and state of the art
3. Methodology
4. Radiation-induced embrittlement
5. Anisotropic effects in radiation embrittlement
6. Summary, conclusions, and future research

Chapter 1: Introduction introduces the critical problem of radiation-induced embrittlement in nuclear materials, highlighting the limitations of current understanding and the necessity of atomistic simulations to bridge experimental observations with fundamental mechanisms. It sets the stage for the subsequent chapters, which delve into the methodology, specific investigations, and findings regarding crack propagation and fracture resistance in irradiated alloys.

Chapter 2: Background and state of the art lays the groundwork by detailing the harsh nuclear environments, the nature and detection of radiation-induced defects, and the atomistic simulation techniques used to study their impact on material fracture. It emphasizes the critical role of defects and crystallographic orientation in influencing plastic deformation and crack propagation, setting the stage for the detailed investigations in subsequent chapters.

Chapter 3: Methodology provides the foundational methodological details for the atomistic simulations, covering the theoretical underpinnings of MD, the choice of simulation parameters

and ensembles, and the computational tools and techniques used to ensure accurate and reliable analysis of crack propagation in irradiated materials.

Chapter 4: Radiation-induced embrittlement presents a comprehensive atomistic investigation into how radiation-induced defects modify crack propagation and plastic deformation in Fe-Ni-Cr alloys, leading to radiation-induced embrittlement. It highlights the competing roles of different defect types and quantifies the reduction in fracture resistance using energy-based metrics, establishing a clear link between microstructural damage and macroscopic embrittlement.
This chapter is extracted from the paper:
A. Ustrzycka, H. Mousavi, F. J. Dominguez-Gutierrez, and S. Stupkiewicz: Atomistic study of radiation-induced ductile-to-brittle transition in austenitic steel. *International Journal of Mechanical Sciences*, 303 (2025) 110567. The statement of author contributions placed at the end of the chapter describes in details the contribution of the PhD Candidate.

Chapter 5: Anisotropic effects in radiation embrittlement elaborates on how crystallographic orientation significantly influences radiation-induced embrittlement in Fe-Ni-Cr alloys. It highlights that while defect populations may be similar across orientations, the material's response to crack propagation and plastic deformation varies considerably due to the interplay between defect-induced mechanisms and the availability of slip systems, ultimately modulating the ductile-to-brittle transition.
The chapter is extracted from the following publication:
H. Mousavi, S. Stupkiewicz, and A. Ustrzycka: Molecular Dynamics Study of the Role of Anisotropy in Radiation-Driven Embrittlement. *International Journal of Plasticity* 201 (2026) 104686, with the detailed description of the PhD Candidate contribution.

Finally, Chapter 6: Summary, conclusions, and future research contains the thesis overview, underlines core contributions, and indicates future research directions.

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3. Summary of the achievements of the doctoral dissertation

The research presented in the dissertation addresses an important challenge of irradiation-induced degradation in structural materials used in nuclear energy systems, focusing on the complex interplay between microstructural damage and mechanical response. It establishes an atomistic framework to clarify how radiation-induced defects govern crack propagation, fracture resistance, and the ductile-to-brittle transition (DBT) in austenitic $Fe_{55}Ni_{19}Cr_{26}$ alloy. The work emphasizes the necessity of linking defect-level mechanisms with quantitative mechanical responses, providing a physically and mechanically consistent interpretation of radiation-induced embrittlement, explicitly accounting for crystallographic orientation. The main achievements consist in the explanation of the following issues:

1. Competing mechanisms. The study demonstrates that fracture behavior in irradiated $Fe_{55}Ni_{19}Cr_{26}$ alloy is governed by competing interactions between radiation-induced

defect populations and crack-tip plastic deformation mechanisms. It shows that irradiation does not introduce a single dominant embrittlement mechanism; instead, fracture resistance and crack propagation behavior arise from a balance between defect-assisted crack acceleration and defect-induced crack shielding. The dominance of either acceleration or shielding is controlled by defect evolution and crystallographic constraints on plastic accommodation at the crack tip.

2. Role of defects. Vacancy-type defects (voids) play a central role by acting as weak zones that reduce lattice cohesion and promote crack advance through absorption and linkage mechanisms. As irradiation progresses, their accumulation and spatial connectivity increasingly facilitate crack propagation, driving a gradual transition toward more brittle fracture. Interstitial-type defect clusters impede dislocation motion and restrict plastic flow, limiting crack-tip stress relaxation. Their influence transitions from crack-shielding to plasticity-suppressing behavior as void populations become dominant contributors to crack acceleration.
3. Plasticity-controlled DBT. A key outcome is the identification of plastic energy dissipation as the controlling factor for fracture resistance under irradiation. Embrittlement is directly associated with a progressive loss of plastic work at the crack tip, while the energy for crack surface formation remains largely unaffected. This confirms that irradiation-induced DBT is fundamentally a plasticity-controlled phenomenon. The thesis defines DBT as a progressive shift in the balance between defect-assisted crack acceleration and defect-induced crack shielding, mediated by the orientation-dependent capacity for plastic deformation and energy dissipation at the crack tip. This provides a mechanistic definition of radiation-induced DBT in terms of evolving defect populations and diminishing plastic energy dissipation.
4. Influence of crystallographic orientation. The thesis extends mechanistic understanding by explicitly accounting for crystallographic orientation, revealing that the fracture response of an irradiated material cannot be described solely by defect density or type. Instead, it is strongly governed by the lattice's orientation-dependent capacity to accommodate plastic deformation. The same radiation-induced defect populations can lead to markedly different fracture behaviors depending on available slip systems and crack-tip deformation pathways. Orientation (001) exhibits inherently limited plasticity, with stress localization intensifying under irradiation, promoting an early shift toward brittle-like crack advance. Irradiation primarily reinforces an already brittle response. Orientation (011) shows pronounced sensitivity to irradiation. Defect-induced obstruction of stacking fault propagation and immobile dislocation junctions sharply suppress plastic dissipation, leading to rapid degradation of fracture resistance and an accelerated transition to brittle fracture. Orientation (111) retains a greater capacity to incorporate radiation-induced defects into extended deformation structures due to its multiple slip systems. This enables sustained crack-tip plasticity and elevated energy dissipation, allowing it to resist embrittlement even in irradiated conditions. The ductile-to-brittle transition is defined as a progressive shift in the balance between defect-assisted crack acceleration and defect-induced crack shielding, mediated by the orientation-dependent capacity for plastic deformation and energy dissipation at the crack tip.

The dissertation is well-structured and clearly written, facilitating a comprehensive understanding of its complex subject matter.

4. Critical and discussion remarks

(1) Editorial remarks

(a) List of symbols. Against the backdrop of an otherwise carefully prepared dissertation, a significant shortcoming is the absence of a list of symbols, abbreviations, and mathematical notation.

(b) Inconsistent notation. The doctoral dissertation exhibits inconsistencies in the notation used for vectors and tensors, which could potentially affect clarity. Vectors and tensors are not uniformly represented throughout the text. For instance, in Figure 3.6, they are depicted using italic bold fonts. However, in other parts of the text, such as in equations and general discussions, straight bold fonts are used, and in many instances, italic fonts with an upper arrow are employed to denote vectors. This variation in typographical representation can be confusing for the reader. To enhance readability and maintain academic rigor, it is important to adopt a consistent typographical style for all mathematical symbols, particularly for vectors and tensors, throughout the entire document. Symbol "N" is written either in straight font (usually in equations) or in italic font (usually in the text). Does it denote the same quantity? See for ex. Equation (3.20). The potential energy is denoted either with "U" (for ex. Eq. 3.42) or with "E" (for ex. Eq. 3.44). Letter "E" is also used for the total energy (page 33).

(c) Other editorial shortcomings. The dissertation contains instances of imprecise wording, for example: (page 10) "N is the total number of atoms in the material" – in what amount? A mole? Some reference volume?; (page 32) "The numerator represents the weighted average" – it represents the weighted integral.
In formula (3.17) the symbol of scalar product is missing (in the third part of the formula).
Formula (3.19) is not explained.
Eq. (3.20) is unclear. What is the meaning of the integral $\int d^{\mathrm{dN}}p$ (or $\int d^{\mathrm{dN}}r$)?
Figure 4.3 lacks the (a) (b) and (c) designators
There is a discrepancy between Figure 2.9 and its description in the caption and in the text (the angles are swapped with each other).
Why the thermostat variable is not multiplied by the number of degrees of freedom in Eq. (3.31), as it is in Eq. (3.24)?
The definition of the volume-averaged virial stress tensor, Π_{ij}, as presented in Equation (3.35), exhibits a confusing mix of absolute and index notation, which can lead to ambiguity in interpretation (the same problem appears in Equation 3.36). Indices i and j are used as *atom indices* in the descriptive text for r_{ij} and f_{ij}, directly after the term Π_{ij} where i and j are *Cartesian component indices*. This mixed notation requires careful interpretation to distinguish between atom identifiers and vector components, which can be confusing for readers trying to fully grasp the definition of the virial stress tensor.

The above errors are *minor shortcomings*, and do not diminish the overall quality of the dissertation, which is, in general, carefully prepared.

(2) Discussion-type remarks

(a) Simplifying assumptions

While atomistic simulations offer greater accuracy than continuum-scale approaches, they still simplify the physical state of matter. Molecular dynamics (MD) models atomic motion using classical mechanics - atoms are treated as point masses governed by Newton's second law, with forces derived from interatomic potential energy functions. This inherently simplifies the quantum mechanical nature of atomic interactions.

Common potentials include the Lennard-Jones (LJ) potential, which captures pairwise short-range repulsion and long-range attraction, and the Embedded Atom Method (EAM), which incorporates local electron density to model many-body metallic bonding. Despite this added complexity, both remain classical approximations. The LJ potential is inadequate for metals and complex alloys due to its inability to account for many-body effects and electron-density dependence, while EAM, though more sophisticated, still relies on effective rather than explicit quantum mechanical interactions.

MD simulations provide high spatial and temporal resolution into phenomena such as atomic rearrangements, defect nucleation, dislocation motion, and crack propagation. However, quantum effects - such as electron delocalization and bond breaking/formation - are only implicitly captured through potential functions, not explicitly calculated.

Simulation accuracy is therefore directly tied to how well these potentials represent real atomic interactions. Despite careful parameterization against experimental and first-principles data, they remain approximations. In essence, treating atoms as classical interacting particles - akin to billiard balls - is a deliberate trade-off: it enables the study of larger systems over longer timescales than quantum mechanical methods allow, but means matter is described through an *effective*, rather than *fundamental*, representation.

In light of the above discussion, the question arises as to what are **the most significant simplifications** adopted in the analysis, referred to:

- idealized material and defect configurations
- simulation conditions and scope
- theoretical framework simplifications?

Is it possible to estimate how these simplifying assumptions affect the accuracy of model predictions?

(b) Mechanisms of radiation-induced embrittlement and their experimental validation

The thesis identifies that radiation-induced defects, such as voids and dislocation loops, play competing roles in crack propagation. Voids facilitate crack advance by reducing local cohesion and forming preferential paths, while dislocation loops impede propagation by obstructing slip and deflecting the crack front. It is important to note that the findings presented are primarily derived from atomistic simulations and are not directly verified by experiments. The work highlights that advanced microscopy methods like Transmission Electron Microscopy and 3D Atom Probe Tomography provide experimental validation of defect types and their spatial distributions, and help link nanoscale defect structures with macroscopic hardening, fracture resistance, and embrittlement. However, these experimental techniques are used to *inform* the

simulations rather than *verify* the specific fracture mechanisms and quantitative trends predicted by the simulations. Validation through controlled irradiation experiments is crucial to strengthen confidence in atomistic predictions and facilitate their incorporation into multiscale modeling frameworks. How might experimental techniques, beyond those currently available, be developed to directly observe and quantify the competing nanoscale interactions in real-time within irradiated materials, especially considering the complex interplay of defect types and their spatial distributions?

(c) Role of crystallographic orientation

The study emphasizes that crystallographic orientation significantly influences crack-tip plasticity, stress redistribution, and defect shielding, leading to orientation-dependent fracture responses. Given that real engineering materials are polycrystalline, how can the insights gained from single-crystal simulations be effectively upscaled and integrated into models for polycrystalline materials, where grain boundaries introduce additional complexities and anisotropic effects?

(d) Energy-based fracture analysis and DBT

- The thesis uses an energy-based approach, decomposing the critical energy release rate (G_c) into surface energy (γ_s) and plastic work (w_p), to quantify irradiation-induced embrittlement. The results show that the reduction in G_c with increasing dpa is primarily due to the suppression of w_p, while γ_s remains relatively stable. What are the implications of this finding for designing new radiation-tolerant alloys, particularly in terms of microstructural engineering to enhance plastic energy dissipation under irradiation?
- The thesis's approach to estimating critical fracture energy by using a near-absolute zero temperature reference to suppress plasticity is a methodological choice aimed at isolating the surface energy contribution. However, many austenitic stainless steels, including 310*S*, are known to retain pronounced ductility and toughness even at cryogenic temperatures, close to absolute zero. Therefore, the assumption that plasticity is effectively suppressed at 10 K to yield a "near-brittle reference" might introduce a source of error when applied to austenitic stainless steels. If these steels retain significant ductility and plastic deformation mechanisms at 10 K, then the plastic work may not be negligible, and the critical fracture energy value might still contain a substantial plastic contribution, rather than purely representing the surface energy. This could lead to an underestimation of the true plastic work at higher temperatures if the cryogenic reference is not truly brittle. In the paper by Xu and Demkowicz (2020), on which the fracture energy derivation is based, experimentally determined values of fracture energy (for pure Ni and Ni-base alloys) were significantly different than the values predicted in that paper. Were the fracture energy estimations presented in the thesis verified in any way with experimental results?
- In general, at temperatures near absolute zero, classical mechanics collapses, and quantum mechanics dictates the state. Was the possibility of near-zero specific phenomena taken into account when estimating the fracture energy? Can they significantly affect the final result?

(e) Future research directions

The thesis suggests extending the analysis to body-centered cubic (bcc) materials and exploring the role of helium-related damage, as well as investigating polycrystalline systems. Among these future directions, which one holds the most immediate practical significance for the nuclear industry, and what specific challenges will have to be overcome to make substantial progress in that area?

5. Final conclusion

I conclude that the doctoral dissertation entitled *"Atomistic Simulation of Crack Propagation in Irradiated Materials"* by Hojjat Mousavisogolitappeh, submitted for my review, presents an original and valuable solution to a scientific problem, and meets the requirements set for doctoral dissertations by the Act *Ustawa z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce.* **I recommend that it be admitted to public defense.**