Crack Development In Al2O3: A DFT Study

Mostafa Fathalian [1], Eligiusz Postek [1] and Tomasz Sadowski [2]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawińskiego 5B,02-106 Warsaw, Poland.

[2] Department of Solid Mechanics, Lublin University of Technology, 20-618 Lublin, Poland.

Keywords: Crack; Al2O3; Fracture toughness; DFT

Correspondence: mfath@ippt.pan.pl.

Abstract: This study employs Density Functional Theory (DFT) simulations to explore the fracture toughness (K_{IC}), surface energy (γ), and Young's modulus (E) of α-Al2O3 (aluminum oxide) while investigating the impact of vacancies on these mechanical properties. Young's modulus and fracture toughness are determined for models with and without vacancies. Fracture toughness and Young's modulus are fundamental indicators of a material's ability to withstand crack propagation and its stiffness, respectively. DFT, a computational approach, facilitates the analysis of atomic-level interactions within materials. Al2O3, a versatile ceramic with exceptional mechanical characteristics, serves as the subject of investigation.

Through DFT simulations, this research delves into the fracture mechanisms and crack propagation behavior of Al2O3, providing insights into its intrinsic fracture toughness. DFT can predict the formation and behavior of defects and dislocations in the material, which can affect its mechanical properties, including fracture toughness. By integrating DFT results with experimental data, a comprehensive understanding of both fracture toughness and Young's modulus is achieved. The research results provide useful information on the behavior of α-Al2O3 in the presence of vacancies. This study advances insights into Al2O3's crack behavior and mechanical attributes, informing its application across aerospace, electronics, and manufacturing. Demonstrating DFT's efficacy in uncovering complex mechanical phenomena, the research guides materials design strategies while forecasting employment opportunities in cutting-edge materials science.

Acknowledgments

This research was funded by the National Science Center, Poland, grant No. UMO 345 2019/33/B/ST8/0126. The calculations were performed at PLGrid national facilities—Academic Computer Centre Cyfronet in Krakow, Academic Computer Centre in Gdansk, and Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland

References

[1] G. Pilania et al., Revisiting the Al/Al2O3 Interface: Coherent Interfaces and Misfit Accommodation, Scientific Reports, (2014) DOI: 10.1038.

[2] Y. Chen et al., Density functional theory study of Ir atom deposited on γ-Al2O3 (001) surface, Physics Letters A, Volume 373, Issue 2, (2009), Pages 277-281.

[3] Y. Chena et al., Interface intrinsic strengthening mechanism on the tensile properties of Al2O3/Al composites, Computational Materials Science,169 (2019) 109131.

[4] K. Chen, M. Bielawski, Interfacial fracture toughness of transition metal nitrides. Surface & Coatings Technology, 203 (2008) 598–601.