Investigating the Mechanical Characteristics of Al_2O_3 through Density Functional Theory and Molecular Dynamics

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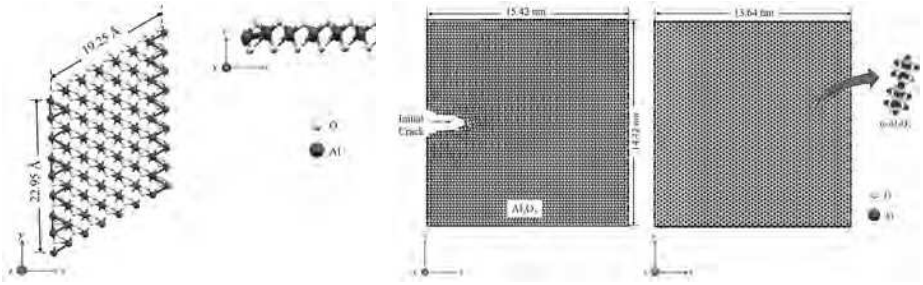
1. Introduction

This exploration highlights the essential role of ceramics, notably aluminum oxide (Al_2O_3), in various technological applications due to its remarkable properties, including high mechanical strength and electrical insulation [1]. It underscores the transformative impact of computational approaches such as density functional theory (DFT) and molecular dynamics (MD) simulations in unraveling Al_2O_3's mechanical characteristics. The focus is on key attributes like surface energy, Young's modulus, and fracture toughness, providing insights into the atomic-scale mechanisms governing these features. Through the application of DFT and MD simulations, a deeper understanding emerges regarding how cracks initiate, propagate, and influence overall fracture behavior, contributing to the advancement of enhanced materials for diverse applications [2,3].

2. Simulation methodology

The simulation process can be segmented into two components: initial DFT simulations and subsequent MD calculations. Both DFT and MD simulations focus on examining Alumina, characterized by a hexagonal crystal structure known as corundum.



(a) (b)

Fig. 1. (a) The defect-free structures of α-Al_2O_3 configuration after relaxation. (b) Schematic representation of the α-Al_2O_3 simulation model, dimensions, and coordinate system.

3. Discussion

The study delves into the effects of asymmetric oxygen (O) and aluminum (Al) vacancies on the surface of α-Al_2O_3, examining their impact on mechanical and electronic properties. Vacancies, crucial in modeling with density functional theory (DFT), alter stress distribution

and local strain fields, influencing mechanical properties such as strength, ductility, and fracture toughness. They also introduce changes in electronic characteristics, affecting electrical conductivity and optical attributes. The investigation encompasses four models with distinct point vacancies and a defect-free supercell, exploring geometric parameters and calculating Young's modulus. The findings reveal varying degrees of structural alterations and disruptions in the crystal lattice associated with O and Al vacancies. A simulated tensile test explores the fracture processes of α-Al_2O_3, providing insights into stress–strain curves and ultimate strength. It is critical for understanding the material's structural limits and irreversible changes in its atomic arrangement. Crack growth in α-Al_2O_3 during z-direction tensile testing with MD provides vital insights into nanoscale material behavior. The observed events include initial crack appearance at zero strain, subsequent elongations triggering crack initiation and propagation, and eventual failure. The stress near the crack tip gradually increases until cracking begins and progresses steadily.

4. Software

In this study, the SIESTA package code was employed for conducting density functional theory (DFT) calculations, while MD simulations were executed using the LAMMPS software [4]. To conduct computations and simulations, high-performance computing (HPC) resources, specifically PLGrid, were utilized.

5. Conclusions

Aluminum vacancies demand higher energy than oxygen vacancies, making their occurrence less likely in natural conditions. Young's modulus significantly decreases with aluminum vacancies, impacting elongation in tensile tests. Fracture toughness diminishes notably with introduced aluminum vacancies. MD simulations yield a fracture toughness of 2.8 MPa·√m for α-Al2O3, aligning well with DFT calculations and experimental data.

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References

1. P. Narottam, J. L. Bansal: Ceramic Matrix Composites: Materials, Modeling and Technology. Wiley, 2014; ISBN 978-1-118-23116-6.
2. M. Fathalian, E. Postek, T. Sadowski: Mechanical and Electronic Properties of Al(111)/6H-SiC Interfaces: A DFT Study. Molecules 2023, 28. doi:10.3390/molecules28114345.
3. S. Blonski, S. H. Garofalini: Molecular Dynamics Simulations of α-Alumina and γ-Alumina Surfaces. Surf. Sci. 1993. 295, 263–274, doi:10.1016/0039-6028(93)90202-U.
4. S. Plimpton: Fast Parallel Algorithms for Short-Range Molecular Dynamics. J. Comput. Phys. 1995.117, 1–19, doi: 10.1006/jcph.1995.1039.