XVIII International Conference on Computational Plasticity, COMPLAS 2025
September 2-5, 2025, Barcelona, Spain

ATOMISTIC MODELING OF DEFORMATION AND DAMAGE BEHAVIOR OF METAL MATRIX COMPOSITES

Marcin Maździarz and Szymon Nosewicz

Institute of Fundamental Technological Research Polish Academy of Sciences,
Pawińskiego 5B, 02-106 Warsaw, Poland, E-mail: mmazdz@ippt.pan.pl, snosew@ippt.pan.pl

ABSTRACT

Nickel aluminide (NiAl) is a promising material for high temperature applications, especially as thermal barrier coatings (TBCs). Furthermore, alumina (Al_2O_3) reinforced NiAl matrix composites exhibit excellent mechanical and thermal properties as well as high frictional wear resistance. Deformation and damage behavior is one of the most important issues related to the durability and long-term performance of Al_2O_3 composites with respect to their potential industrial application. Depending on their microstructure and interfacial properties, different damage modes have been identified: matrix/reinforcement interface debonding, reinforcement fracture and matrix cracking. In addition to the atomistic properties of each composite component, the density of material defects, grain orientations, and the nature of grain boundaries significantly affect the macroscopic mechanical properties [1].

The present work aims to determine the deformation and damage behavior of individual NiAl-Al_2O_3 composite components as well as their mechanical parameters using molecular dynamics simulations [2]. The elastic and strength parameters determined by molecular dynamics are the main input data for the micromechanical model.

A series of simulations have been conducted to assess the mechanical properties of single NiAl and Al_2O_3 mono- and polycrystals, as well as NiAl-Al_2O_3 bonding. The simulations encompass uniaxial tensile, uniaxial compressive, and shear tests. The impact of crystallographic orientations in the samples has also been thoroughly investigated.

Acknowledgments
This work was supported by the National Science Centre (NCN – Poland) Research Project: 2020/37/B/ST8/03907.

REFERENCES

[1] M. Maździarz, S. Nosewicz, Atomistic investigation of deformation and fracture of individual structural components of metal matrix composites, Engineering Fracture Mechanics 298 (2024) 109953. doi:10.1016/j.engfracmech.2024.109953.

[2] K. Choudhary, T. Liang, A. Chernatynskiy, S. R. Phillpot, S. B. Sinnott, Charge optimized many-body (COMB) potential for Al_2O_3 materials, interfaces, and nanostructures, Journal of Physics: Condensed Matter 27 (30) (2015) 305004. doi:10.1088/0953-8984/27/30/305004.