Multiscale prediction of the elastic response of NiAl-based materials using atomistic and micromechanical calculations

Szymon Nosewicz[1,*], Grzegorz Jurczak[1], Marcin Maździarz[1], Paweł Hołobut[1], Katarzyna Kowalczyk-Gajewska[1], Witold Chromiński[2]

[1]Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland
e-mail: szymon.nosewicz@ippt.pan.pl

[2]Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland

KEYWORDS: *Multiscale modeling, Molecular Dynamics, EBSD reconstruction, NiAl-based materials.*

The presented work proposes a multiscale framework for the numerical/analytical determination of the elastic constants of the intermetallic nickel-aluminate (NiAl) material at the microscopic scale. Molecular dynamics (MD) calculations have been employed to evaluate the stress tensors of a single NiAl monocrystalline body with cubic Pm3m symmetry (B2-NiAl). Moreover, the NiAl amorphous structure was generated and simulated to reproduce the mechanical performance of the grain boundary [1]. The atomistic results were transferred to the upper scale as an input to micromechanical models. Here, the finite element modeling (FEM) was utilized to simulate the elastic behavior of NiAl polycrystalline with special attention to grain anisotropy. The microstructural features of the heterogeneous body were evaluated using electron backscatter diffraction (EBSD) and next generated by Dream3D software, preserving the realistic distributions of grain orientations and grain sizes. The reconstructed NiAl polycrystal was subjected to uniaxial tensile test simulations using FEM to evaluate the effective Young's modulus (E) and Poisson's ratio (μ). The numerical results were confronted with the experimental values of E and μ, indicating a satisfactory agreement with an error of around 7%. To minimize the discrepancy, a modified FEM model was proposed that accounts for the effect of grain boundaries by introducing a weakened phase in the region of crystal bonding. The width of the weakened phase, and as a result its volume fraction, was estimated from SEM images of the NiAl sample, and the elastic properties were obtained from MD simulations of the amorphous structure. With these model assumptions, a nearly perfect correspondence between numerical and experimental results was achieved. Finally, the numerical results were compared with analytical estimates based on the Voigt, Reuss, and Hill bounds, as well as more complex bounds [2]. The analysis assessed the applicability of both numerical and analytical approaches, highlighting their strengths and weaknesses.

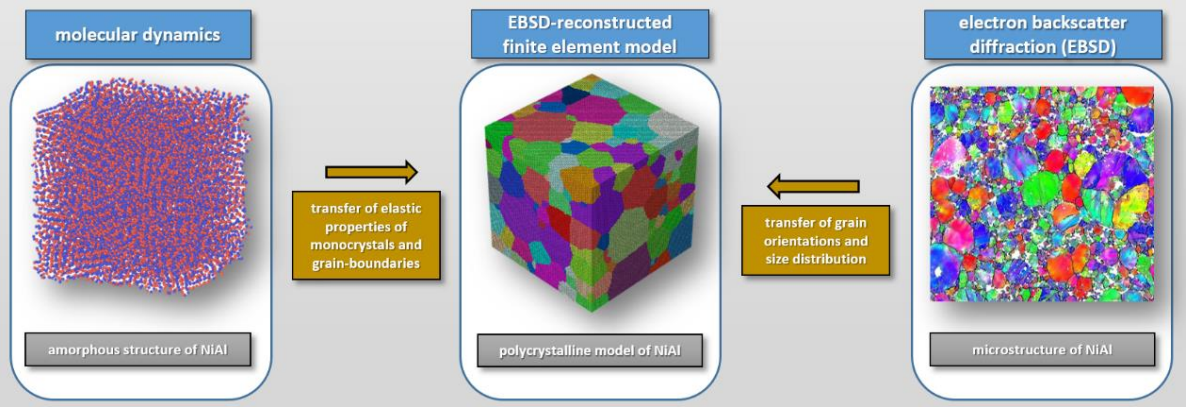

Figure 1. Summary of the multiscale framework.

ACKNOWLEDGEMENT: The authors would like to acknowledge the financial support of the National Science Centre, Poland, under Grant Agreement No. OPUS 2020/37/B/ST8/03907.

[1] Maździarz M., Nosewicz S., Eng. Fract. Mech. **298**, 109953-1-109953-21, 2024. https://doi.org/10.1016/j.engfracmech.2024.109953
[2] Kowalczyk-Gajewska K., Maździarz M., Int. J. Eng. Sci., **157,** 103393-1-21, 2020. https://doi.org/10.1016/j.ijengsci.2020.103393