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Molecular dynamics modeling of deformation and damage behaviour of main structural components of NiAl-Al_2O_3 composite

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ABSTRACT

Intermetallic compound nickel aluminide (NiAl) is a promising material for high-temperature applications, particularly suitable as a bond coat in thermal barrier coatings (TBCs). Moreover, NiAl matrix composite reinforced with alumina (Al_2O_3) particles can be characterized by excellent mechanical and thermal properties as well as high frictional wear resistance. Having in mind their possible industrial application, the deformation and damage behavior is one of the most crucial issues in the context of the durability and long-term performance of NiAl-Al_2O_3 composites. Depending on the microstructural properties of the composite (such as the quality of the interface), a variety of damage modes at the microscopic level has been identified for such materials: reinforcement fracture, matrix/reinforcement interface debonding and matrix cracking [1]. As well as the atomistic properties of each composite component, the density of material defects, the grains orientations and the type of grain boundaries affect the macroscopic mechanical properties significantly [2].

The presented paper is primarily aimed to determine the deformation and damage behavior of individual components of NiAl-Al_2O_3 composite within a molecular dynamics framework. Moreover, an assessment of the strength of individual components in the context of the macroscopic composite strength has been performed. The final goal was to determine the mechanical parameters of individual composite components for upper-scale analysis atomistically. The elastic and strength parameters obtained via molecular dynamics are of primary importance as input data for the micromechanical model.

Simulations of uniaxial tensile, uniaxial compressive and shear tests of single NiAl and Al_2O_3 mono- and polycrystals, and finally NiAl-Al_2O_3 bonding have been performed to evaluate corresponding properties. The effects of crystallographic orientations and atomistic defects (vacancies) in the samples have be studied. It has been shown that atomistic simulations are useful to provide a better understanding of the interface conditions and mechanical properties of matrix and reinforcement mono- and polycrystals as well as matrix-reinforcement bonding.

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