Estimation of micromechanical NiAl sintering model parameters from the Atomistic Simulations

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ABSTRACT

Molecular dynamics (MD) [1] and molecular statics (MS) [2] estimation of constitutive parameters for a micromechanical NiAl sintering model [4] is reported in this work. The parameters include surface energy, linear thermal expansion and temperature dependent diffusion coefficients. These parameters define material behavior during sintering and are used in the sintering particle model implemented in the discrete element model [4]. The investigated material, the NiAl intermetallic belongs to novel materials characterized by favourable mechanical properties. Numerous machine elements are fabricated from a pure NiAl powder or from powder mixtures containing the NiAl using the sintering technology. It is well known that sintering is governed by diffusion and therefore diffusive properties are crucial parameters of the micromechanical model of sintering. Numerical estimation of the model parameters by simulations at the lower scale can be a powerful tool alternative to experimental methods.

Molecular statics and dynamics models for NiAl alloy have been created using the embedded-atom method (EAM) potential [3]. Numerical simulations have allowed us to estimate the volume, surface and grain-boundary diffusivity for the B2-NiAl in the 1573 K to 1673 K temperature range. Dependency of the diffusion coefficients on temperature has been determined and validity of the Arrhenius type temperature relation has been assessed. The parameters evaluated numerically have been compared with available experimental data as well as with theoretical predictions obtained with different methods.

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