Molecular dynamics study of self-diffusion in stoichiometric B2-NiAl

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ABSTRACT

Molecular statics (MS) [2] and molecular dynamics (MD) [1] study of temperature dependent self-diffusion coefficients in stoichiometric B2-NiAl alloy is reported in this paper. These parameters define material behavior during sintering and are used in the sintering particle model implemented in the discrete element model [4]. The considered material, the NiAl intermetallic belongs to innovative materials characterized by advantageous mechanical properties. Many machine elements are produced from a pure NiAl powder or from powder mixtures containing the NiAl applying the sintering technology. It is well known that sintering is governed by diffusion and for this reason diffusive properties are meaningful parameters of the micromechanical sintering model. Numerical assessment of the model parameters by simulations at the lower scale can be a powerful tool alternative to experimental methods.

Molecular statics and dynamics simulations for B2-NiAl have been carried out using the embedded atom model potential [3]. Numerical calculations have allowed us to estimate the diffusivity for the B2 type NiAl in the ~1200 K to ~1700 K temperature range. Temperature dependence of the diffusion coefficients has been determined and validity of the Arrhenius type temperature equation has been assessed. The parameters evaluated numerically have been compared with available experimental data as well as with theoretical predictions obtained with alternative methods.

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