Modeling of NiAl crystals using the Deformable Discrete Element Method

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Abstract: NiAl is an intermetallic alloy with many favorable physical properties which make it an attractive material for modern industrial applications. NiAl has the BCC crystal structure and the resulting cubic anisotropy. Its properties have been the subject of numerous experimental and theoretical investigations, as well as simulations using the methods of molecular dynamics. Mechanical modeling of larger NiAl assemblies like polycrystalline NiAl or NiAl-based composites can be done using the Finite Element Method (FEM). An alternative approach, which is the subject of this research, is to employ the Discrete Element Method (DEM), with the DEM spheres which form the material being held together by cohesive forces. DEM offers both advantages, such as easy handling of various kinetic mechanisms like crack propagation, and disadvantages, stemming from its intrinsic beam-network representation of the material. The major difficulty which arises when modeling NiAl crystals in DEM is to reproduce NiAl's cubic symmetry with its relatively high Zener ratio of around 4. This can neither be achieved in standard DEM by arranging spheres in the RC, FCC or BCC structures, nor by using random dense packings in a modified DEM, where the spheres' stiffness varies angularly in a cubic-symmetric fashion. The mechanical properties of NiAl, and possibly other high-anisotropy materials, can be reproduced by resorting to the Deformable Discrete Element Method. The present work explains how this can be achieved and discusses some aspects of the approach, with a view to future plans for modeling damage in NiAl polycrystals.

Keywords: NiAl crystal, cubic anisotropy, Deformable Discrete Element Method, numerical modeling, mechanical properties.

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