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Modeling of single crystals and polycrystals of NiAl using the Deformable Discrete Element Method

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Many important materials are polycrystals with a cubic crystal structure. Examples are aluminum and copper with the face-centered cubic (FCC) structure, iron and chromium with the body-centered cubic (BCC) structure, as well the BCC intermetallic NiAl which is the main focus of this study. A widespread way of modeling such materials at the microscale is by using the Finite Element Method (FEM). In the present work, an alternative approach based on the Discrete Element Method (DEM) is employed instead. Both methods have advantages and disadvantages, with FEM being potentially less computationally intensive and more accurate in some applications, while DEM being better adapted to handling discontinuous phenomena like fracture.

A DEM model is created by filling a given volume with spherical particles of the same or different sizes and bonding adjacent ones together by cohesion. The effective properties of the ensemble are calibrated by adjusting stiffness parameters of the inter-particle bonds. A single crystal of cubic symmetry can be modeled by using either a random-dense packing of DEM particles or a cubic-symmetric periodic one, both having a cubic-symmetric distribution of bond stiffness coefficients. The second approach is followed in this work, since the first one faces difficulties reproducing properties of highly anisotropic crystals like NiAl. The simple cubic (SC) arrangement of particles is adopted, with deformable DEM (DDEM) particles used instead of standard ones [1] – a change which increases the range of values of effective parameters that can be obtained. In particular, it allows easy representation of the elastic properties of NiAl crystals.

The transition to the polycrystal is made by subdividing a representative volume into grain sub-volumes and filling them with SC patterns of DDEM particles at different orientations, corresponding to EBSD test results. It is ensured that proper attachment conditions at the grain boundaries are created, where SC patterns of different orientations meet. The results of simulations for NiAl in the linear-elastic regime are presented and discussed in connection with future tests of larger deformations leading to grain-boundary fracture.

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REFERENCES

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