Modeling of materials with a cubic crystal structure using the Deformable Discrete Element Method

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ABSTRACT

Many materials have a cubic crystal structure, which can be simple cubic (SC), found in polonium, body-centered cubic (BCC), e.g. in iron, chromium and tungsten, or face-centered cubic (FCC), e.g. in aluminum, copper and nickel. Simulation of the behavior of polycrystals or composites of cubic materials, or estimation of their effective mechanical properties by numerical homogenization, requires an adequate computational model of a single crystal, reflecting its internal cubic symmetry. Standard models of this kind are provided by the Finite Element Method (FEM), with FEM packages routinely handling finite elements with cubic material properties. In the present work, we investigate an alternative approach, based on the Discrete Element Method (DEM) and its extension, the Deformable Discrete Element Method (DDEM) [1], which may be advantageous in some applications.

In a DEM model of a solid, a material volume is filled with DEM particles (spheres) which are bound together by cohesive forces. The material is in effect represented by a network of beams, whose geometry and mechanical parameters can be adjusted. The advantage of DEM over FEM is its more natural handling of mechanisms like crack propagation, represented in DEM by sphere debonding, while, on the downside, DEM can be less precise and computationally more expensive in some situations. In the case of a cubic material, the beam network needs to produce an average cubic response. This can be achieved by using a random packing of DEM particles with cubic material properties [2] or by a cubic-symmetric packing of isotropic particles. We focus on the second approach, limiting ourselves to investigating elastic properties only. We demonstrate the inherent limitations of the standard DEM with regard to modeling highly anisotropic crystals like the BCC-structured intermetallic NiAl, whose Zener ratio is approximately four. We finally show that, in principle, DDEM allows the modeling of all cubic materials in the linear-elastic regime. We discuss possible extensions and micromechanical applications of these results.

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