Discrete Element Method (DEM): A numerical technique to insight on the role of microcracks on the sustainability of refractory materials

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Abstract

Andalusite and Aluminum titanate are utilized in various industries due to their superior intrinsic properties for thermal shock applications. At the microstructural scale, these materials are identified by their grain crystallinity, such as aluminum titanate, a polycrystalline material with orthorhombic crystals at the microstructure scale. In addition, Aluminum titanate exhibits anisotropic thermal expansion behavior at the microscopic scale. Therefore, these materials exhibit spontaneous microcracking at high temperatures during operational conditions due to CTE mismatch. Moreover, microcracks in the refractory microstructure have led the material to depict a quasi-brittle (non-linear mechanical) behavior under tensile loading. The experimental experts claim that the non-linear macroscopic response of refractory material signifies the toughening of the material. The betterment of the material's fracture toughness contributes to the improvement of its thermal shock resistance. Therefore, simulation of cracking phenomena, including microcracking, branching, or fragmentation, that occurs in brittle or quasi-brittle media has become a topic of research interest. So, the authors propose a simplified and pure polycrystalline model microstructure using the Discrete Element Method (DEM), with Aluminum titanate as a reference material. The study is focused on understanding the role of anisotropy of the grains in a polycrystalline material in promoting debonding or microcracking because of the Coefficient of Thermal Expansion (CTE) mismatch between the grains of the polycrystalline material. In addition, this model involves thermomechanical coupling, crack-closure, and Periodic Boundary Conditions (PBC) to perform thermomechanical simulations such as to predict the dilatometry results, tensile test results, and the fracture mechanism at the microstructural scale of a polycrystalline material. The obtained results are validated using the experimental results regarding mesoscopic thermomechanical quantities (such as CTE, Young's modulus, stress-strain law, etc). In conclusion, the potential advantages of using microcracks engineering for commercial refractory products could be highlighted.

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