An Enhanced Bond Model for Discrete Element Method for Heterogeneous Materials

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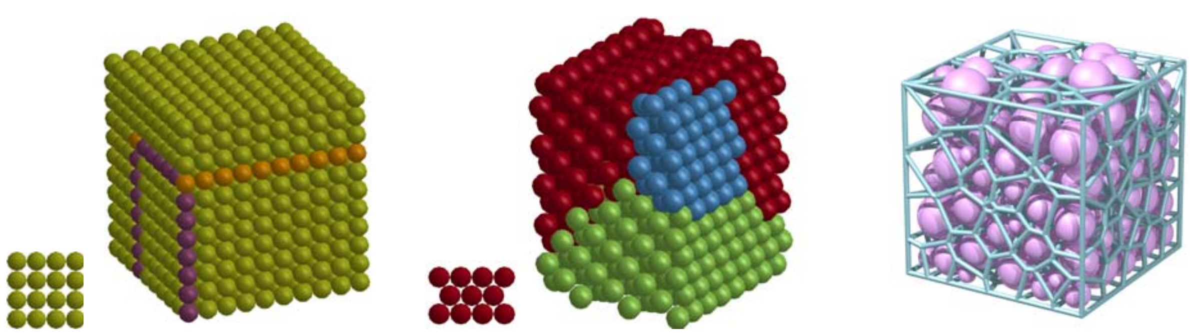
Abstract

The enhanced bond model allows the Discrete Element Method (DEM) to simulate the heterogeneity and discontinuity at the individual particle level at the micro level. The traditional material models at the macro level are applied to each particle independently. This bond model bridges the behaviors of particles at macro and micro levels, and may be used for failure analysis of the homogeneous & heterogeneous materials, including composites, concretes.

Heterogeneous Bond Model for DEM

The new heterogeneous bond model is developed for the discrete spheres as the generalized particle method. The governing equations of the solid mechanics are applied to the solid volume represented by the bonded spheres. The energy conservation laws are also adopted to allow the gaps and introduce the damage between the bonded spheres, as a localized meshless particle method with discontinuity and heterogeneity. The fundamental theory has been reported in the references.

To create a discrete sphere model, the 3-dimensional volume is discretized into many polydisperses. Each polydisperse is further simplified as one sphere element with the same volume placed at the centroid of the volume. Regular models can be created by using cubic or hexagonal lattice unit blocks, and irregular ones by running a packing algorithm, as shown in Fig. 1.



Cubic blocks Hexagonal blocks Generated by Voro++

Fig. 1. Some discrete sphere models

There are three keywords needed for defining the heterogeneous bonds:

1. *ELEMENT_DISCRETE_SPHERE_VOLUME to define the volume of each sphere
2. *DEFINE_DE_HBOND to define the heterogeneous bonds over a set of the discrete sphere elements, which are of different materials.
3. *INTERFACE_DE_HBOND to define the failure criteria for the heterogeneous bonds between the discrete elements of various materials.

The material properties are defined for each PART by using the standard LS-DYNA® material cards. If the discrete elements of multiple parts are bonded together, the failure criteria may be defined for the bonds between the discrete elements of the same material, and those of different materials, respectively. For an example shown in Fig. 2, three parts are included in the heterogeneous bond and there may be up to 6 failure criteria for the different bonds.

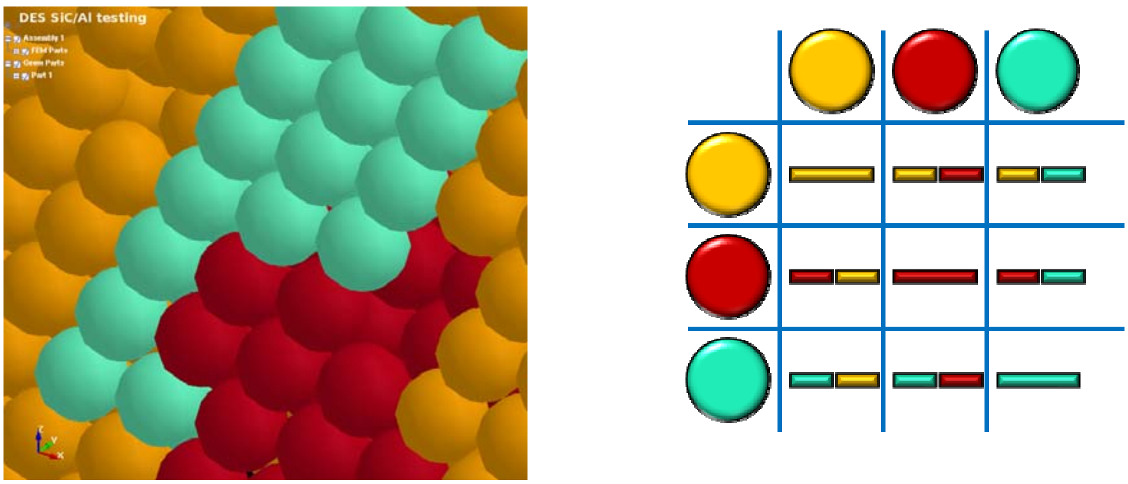
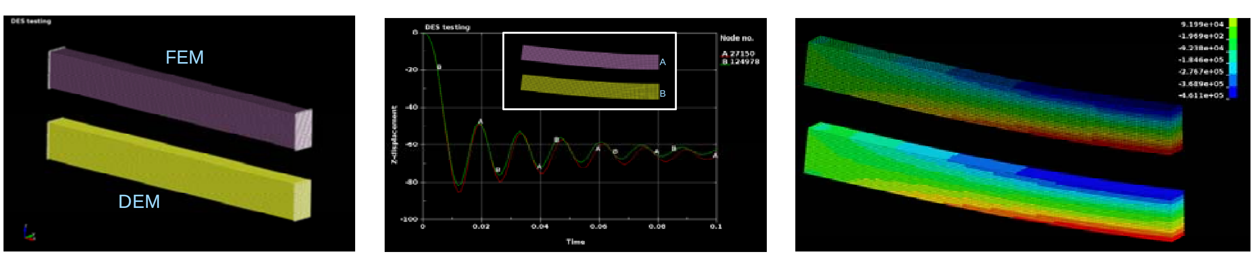


Fig. 2. The heterogeneous bonds over three kinds of the discrete elements

Numerical Examples

The first example is to simulate a simply-supported beam under a uniform body force by using both FEM & DEM. The symmetric boundary conditions are applied to the nodes at the middle plane straightforwardly without any other treatments. The numerical results in Fig. 3 show the agreements between the FEM and DEM.



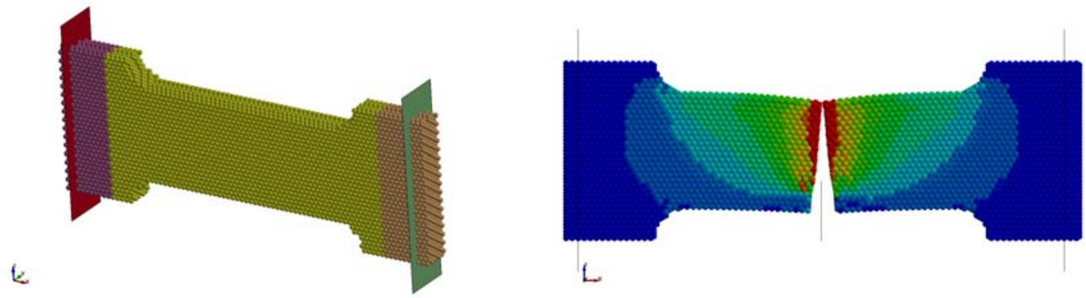
FEM & DEM models of a beam

Z-Displacement at the middle plane

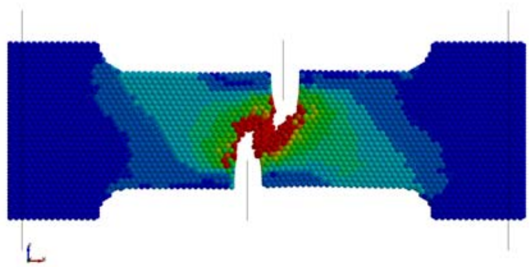
Tension stress distribution

Fig. 3. Comparison between the FEM and DEM

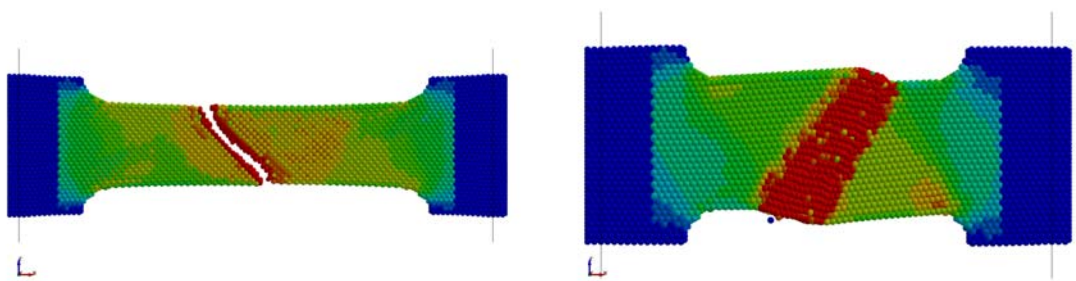
The second example is a test specimen under tension. The plastic material model is used (MAT_224). Crack initialization and propagation are simulated with various pre-notched settings.



DEM Model | with a single-edge crack



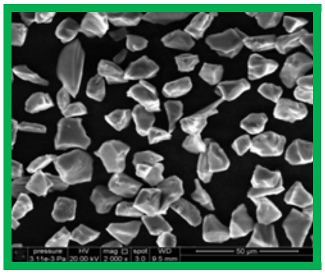
with a double-edge crack | with an inclined crack



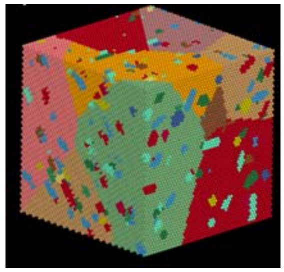
large plastic deformation without pre-cracks | under compression without pre-cracks

Fig. 4. Crack initialization and propagation in a specimen

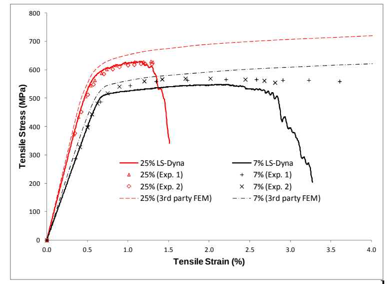
The third example is to simulate a cube of a SiC particle reinforced metal-matrix composite under tension. The size, shape and distribution of the SiC particles are obtained from the microstructure by SEM. The average size of the SiC particle is 13 micrometers. Four failure criteria are defined for the heterogeneous bonds between: a) two spheres of the Al matrix; b) one sphere of the Al matrix and another one of the SiC particle; c) two spheres of one same SiC particle; d) two spheres of two different SiC particles. The Young's modulus and the tensile strength are determined from the numerical loading displacement curve, and compared to the experimental results. The errors are within 5%. The third-party FEM results are also shown in Fig. 5 in which the tensile strength cannot be determined.



Actual micro-structure by SEM [Su, et al (2014)]



DEM Model at the middle plane



Results by LS-DYNA and 3rd party FEM [Su, et al (2014)]

Fig. 5. A DEM analysis of a SiC/Al Metal Matrix Composite under tension

References

Han, Z. D.; Atluri, S. N. (2014a): Eshelby Stress Tensor T: a Variety of Conservation Laws for T in Finite Deformation Anisotropic Hyperelastic Solid & Defect Mechanics, and the MLPG-Eshelby Method in Computational Finite Deformation Solid Mechanics-Part I. CMES: Computer Modeling in Engineering & Sciences, vol. 97, no. 1, pp. 1-34.

Han, Z.D. and Atluri, S.N. (2014b): On the (Meshless Local Petrov-Galerkin) MLPG-Eshelby Method in Computational Finite Deformation Solid Mechanics – part II. CMES: Computer Modeling in Engineering & Sciences, vol 97, no. 3, pp. 199-237.

Su, Y.S.; Ouyang Q.B.; Zhang, W.L.; Li, Z.Q.; Guo, Q.; Fan, G.L.; and Zhang, D. (2014): Composite Structure Modeling and Mechanical Behavior of Particle Reinforced Metal Matrix Composites. Materials Science & Engineering A 597, pp. 359-369

Voro++: http://math.lbl.gov/voro++/