Discrete Element Method (DEM) to support microstructure design of refractories

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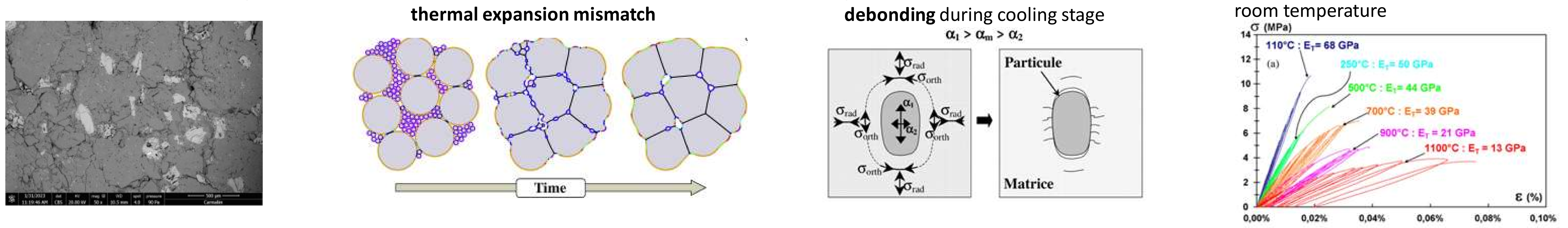
Toughening mechanism in refractory microstructure:

Alumina - aluminum titanate system → expose to thermal cycle introduces **thermal expansion mismatch** → promotion of **microcracks** and **debonding** during cooling stage → shows **non-linear mechanical** response at room temperature



a) b) c) d)

Figure 1: a) Microstructure, b) sintering process, c) thermal damage and d) non-linear mechanical response

Past PhDs studied the influence of

- **Temperature of thermal cycle [1] figure 1d**
- **Percentage of aggregate present [2]**
- **Type of interaction between matrix (Isotropic) and aggregate (Anisotropic) [3] figure 1c**

on **promoting microcracks** in the microstructure to insight on **Thermal Shock Resistance** (TSR)

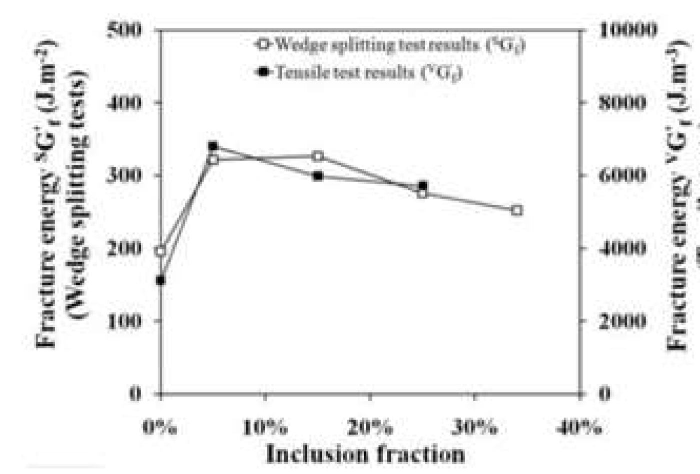


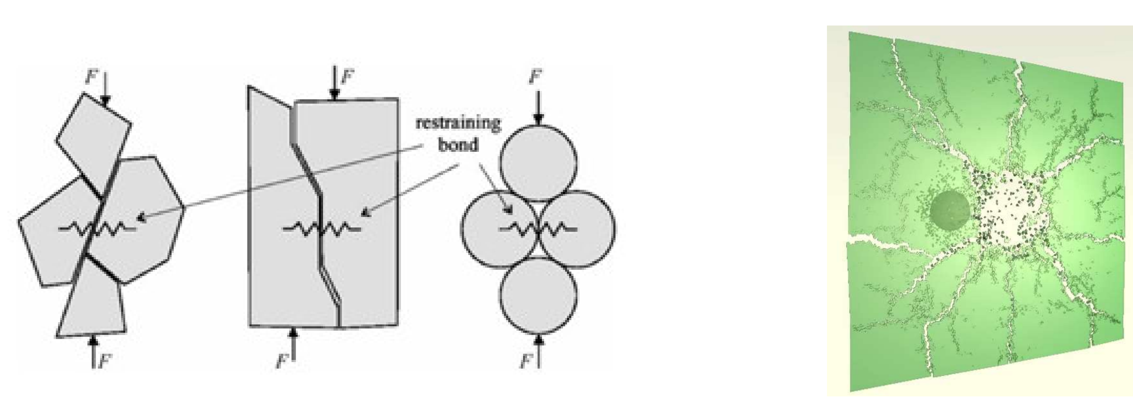
Figure 2: Wedge splitting and tensile test results

- To conclude, there is a strong relationship between the microstructure design and thermomechanical properties of refractory materials ([1],[2] & [3]);
- PhD08 focuses on understanding the influences of **isotropic - anisotropic interaction** in the microstructure to improve TSR using **discrete element method**.

Discrete Element Method:

a) Principles of Discrete Element Method (DEM):

- Elements → **rigid body** that move in 3D space;
- Interaction of elements → preserved by **rheological mechanical** models ex. spring model (figure 2a);
- Each element → **translation** and **rotation** motion → **newton's laws** of motion;
- Explicit technique using **small time** steps.



a) b)

Figure 3: a) Discrete element discretisation with a spring model [4] b) multiple crack growth (granoo website)

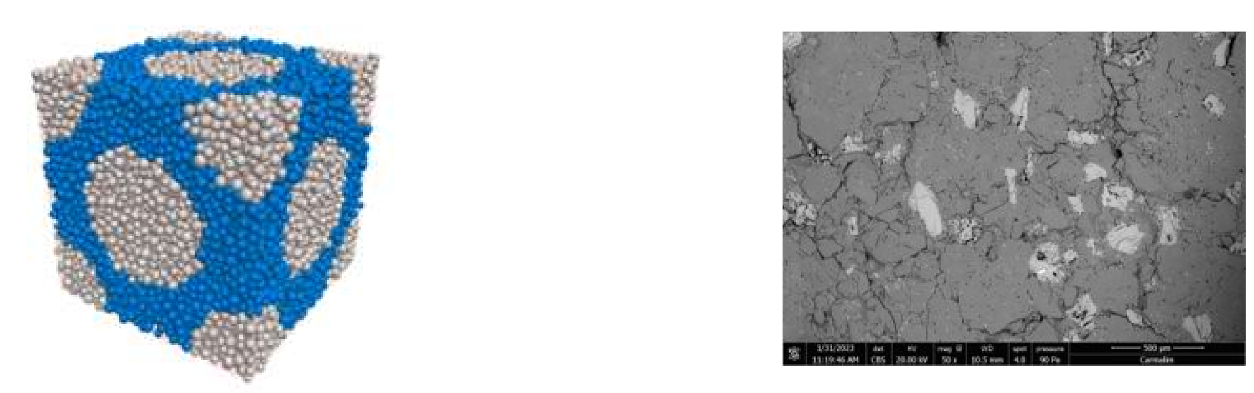
b) Benefits of DEM ([5] & [7]):

- Helps us perform **quasi-brittle** analysis, **multiphysics** and **multiscale** simulation;
- Helps us preserve the realistic natural phenomena's using the **rheology's** (figure 2a);
- Element have **mass** and **geometry** (figure 2a);
- Computationally efficient in **GPU** aspects (figure 2b);
- Multiple **crack** nucleation, propagation, branching and failure (figure 2b).

Problem Statement:

a) Example of microstructure of interest: Alumina - aluminum titanate system

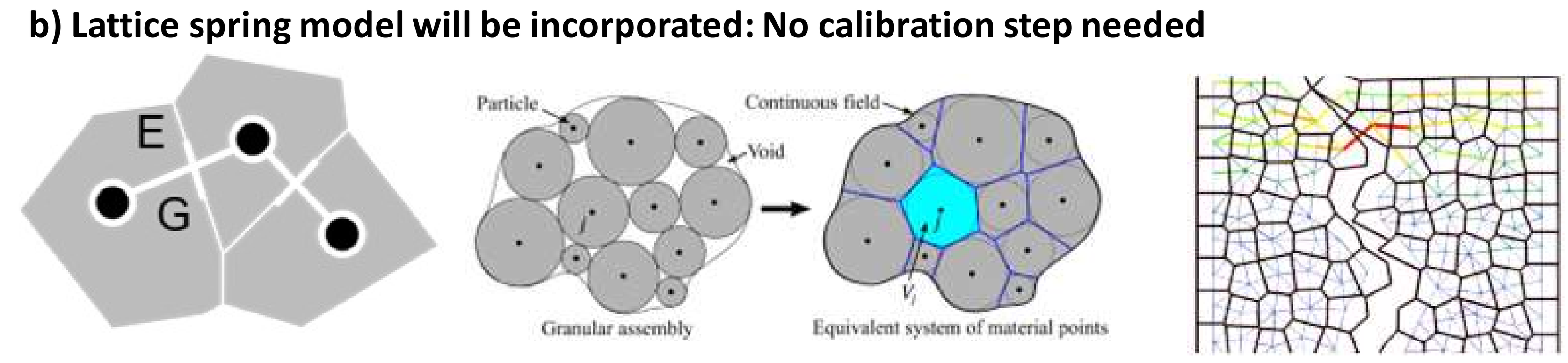
- **Matrix:** Alumina with **isotropic** nature;
- **Inclusion/aggregate:** aluminum titanate with huge **anisotropic** nature.



a) b)

Figure 4: Model Material a) bi-phase system [5], b) real microstructure [6]

b) Lattice spring model will be incorporated: No calibration step needed

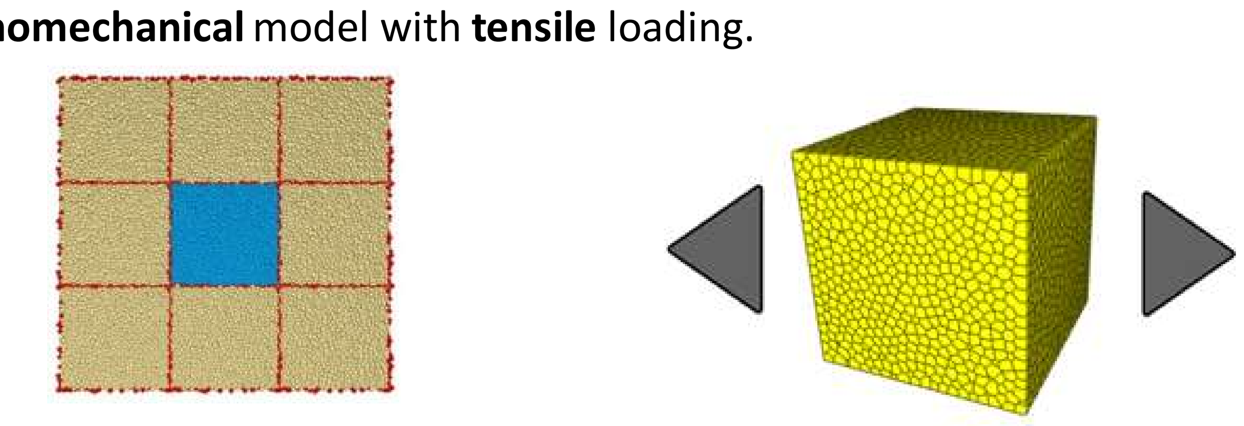


a) b) c)

Figure 5: Lattice spring model a) 2D view [7], b) discretisation [8] and c) clear visibility of crack surface [7]

c) Boundary Conditions (BC), material routine and loading:

- **Free** and **periodic** BCs (figure 5);
- Material routine: **Elastic** and **Fracture** model (Mode I);
- **Thermomechanical** model with **tensile** loading.



a) b)

Figure 6: BCs incorporates a) free and b) periodic boundaries [1]

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Beneficiaries