Introduction
A mesoscopic discrete particle model for simulating fracture and failure of brittle materials is presented. Within the framework of particle dynamics simulations (Discrete Element Method) [1] a macroscopic solid state ceramic tile (typically 10 x 10 x 11 mm$^3$) is modeled as a network of overlapping particles in 2 dimensions (2D). This two-dimensional model version presented here has only three adjustable material parameters but is able to reproduce many salient features of the investigated ceramics under compressive, tensile and shock impact load. Our three model parameters are customized to the typical tensile strength, Young's modulus and the compressive strength of the ceramics under investigation. Using Lennard-Jones type potentials the classic Newtonian equations of motion are integrated and uni-axial quasi-static load simulations are performed. Subsequently, shock load simulations are performed in a standard experimental set-up, the edge-on impact configuration [2,3]. The obtained simulation results are compared with the results of high-speed impact experiments on aluminum oxide ($Al_2O_3$) and silicon carbide ($SiC$) ceramics [4]. Although the model particles have micrometer size we are able to simulate a specimen of macroscopic dimensions. For details, see [4].

Simulation Model
A fundamental requirement for the coarse-grained model is to have very few parameters describing the essential physical behavior of the investigated system. Three basic properties are modeled, namely, first, the resistance to pressure, second, the cohesive forces, and then the microscopic failure.

Resistance Against Pressure
Resistance against pressure is introduced by a Lennard-Jones-type repulsive potential $\phi_{ij}$ which acts on every pair of discs ($ij$) only when $\phi_{ij}(t)$, the mutual distance at time $t$, is smaller than $\phi_{ij}^{0} = \phi_{ij}^0(t)$, the initial separation, of Figure 2. Then for $\phi_{ij} < \phi_{ij}^{0}$:

$$\phi_{ij}(t) = \phi_{ij}^0 \left( \frac{\phi_{ij}(t)}{\phi_{ij}^0} \right)^{12} - 2 \left( \frac{\phi_{ij}(t)}{\phi_{ij}^0} \right)^{6} + 1,$$

whereas for $\phi_{ij} \geq \phi_{ij}^{0}$ the repulsive potential vanishes. The parameter $\phi_{ij}^0$ in Eq. (1) scales the energy density and the prefactor $\phi_{ij}^0$ ensures the correct scaling behavior of the calculated total stress $\sigma_{ij}^0 = \phi_{ij}^{0}/4\pi$ which is independent of $N$, see Figure 3.

Cohesive Potential
The cohesive potential $\phi_{ij}^{coh}$ is modeled by a harmonic function, given that there are no irreversible changes of state when the material is subjected to small external forces. Each pair ($ij$) of discs can thus be visualized as being connected by a spring, the equilibrium length of which equals the initial distance $d_{ij}^0$. Thus, for $\phi_{ij} > \phi_{ij}^{0}$:

$$\phi_{ij}^{coh} = \frac{1}{2} k_{ij} (d_{ij}^0 - d_{ij}^0)^2.$$  

In Eq. (2) $k_{ij}$ (which has dimension [energy/length]) determines the strength of the potential and the prefactor $d_{ij}^0$ ensures proper scaling behavior of the macroscopic response. The total potential $\phi_{ij}$ of our model consequently reads:

$$\phi_{ij} = \phi_{ij}^{coh} + \phi_{ij}^{rep}.$$  

Failure Criteria
Failure is included in our model by introducing two breaking thresholds for the springs with respect to compressive and tensile failure, respectively. A tensile failure criterion is reached when the overlap between two particles vanishes, i.e. when the distance $d_{ij}$ of disc centers exceeds the sum of their radii:

$$d_{ij} > (2R_0).$$  

Failure under pressure load occurs in our model when the actual mutual particle distance is less by a factor $a$ with $0 < a < 1$ than the initial mutual particle distance, i.e. when

$$d_{ij} < a d_{ij}^0.$$  

Note that particle pairs without a spring after pressure or tensile failure still interact via the repulsive potential and cannot move through each other.

Initial Configurations
Using polydisperse particle distributions directly influences characteristic properties of the material, e.g. the coordination number of the starting configuration. In the simple approach chosen here, mono-disperse disks are used and the initial coordination number of the system is adjusted via a compactness or density parameter $\alpha$ as simulation input, see Figure 4.

Crack Initiation and Failure
Uni-axial load simulations are performed until failure in the material occurs. Results of these simulations are displayed in the picture series of Figure 5, which shows the dynamics of crack propagation.

References