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Modelling micro-crack initiation and propagation of crystal structures with microscopic defects under uni-axial tension by discrete element method

Y.C. Chung *, Z.H. Yang, C.K. Lin

Department of Mechanical Engineering, National Central University, Jhong-Li 32001, Taiwan

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ABSTRACT

This paper investigates mechanical behaviour and failure process of a 3D notched plate subjected to uni-axial tension using the discrete element method (DEM). The 3D notched plate consisted of different crystal structures, such as simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC) and hexagonal close-packed (HCP), where constituent spheres were bonded together by contact bond. The inclination angle of the notch ranged from 0° to 90° with an increment of 15°. The aim of this study is to explore the effects of crystal packing and notch inclination angle on the mechanical responses, crack initiation and propagation, and crack paths. The proposed DEM model was first verified for the pre-cracking behaviour by the corresponding FEM calculation, and was confidently used to study the post-cracking behaviour. Numerical results reveal that the crack initiation and propagation of crystal structures depend on the crystal configuration and notch inclination angle. The loading stiffness of the four crystal structures follows the sequence of HCP > FCC > SC > BCC. The stress concentration factor shows a convex profile against notch inclination angle, with the maximum value at the notch inclination angle of 30° and the minimum value at the notch inclination angle of 90°. The SC and BCC crystal structures show a symmetric feature of crack propagation, whilst the FCC and HCP crystal structures exhibit asymmetric characteristics. In such a loading scenario, the crack initiation and propagation in all the four crystal structures are mainly dominated by the tension failure mode.

1. Introduction

The ideal crystal structure has an infinite 3D repetition of identical atoms. However, real crystal structures are limited in size and have some disorder (called defects) in stacking. The microscopic defects can be classified into four kinds (Callister and Rethwisch [1]): (1) point defects (vacancies, interstitials, and impurities); (2) line defects (edge and screw dislocations); (3) planar defects (grain, tilt and twin boundaries, and micro-cracks); and (4) volume defects (voids). These microscopic defects degrade the material strength and greatly affect the mechanical behaviour of the crystal structures subjected to a variety of loading scenarios. Especially when different crystal structures experience some specific stress state, how the micro-cracks initiate and propagate in the crystal structures and how the microstructure influences the macroscopic behaviour are still inadequately understood by far.

Due to the limitation of measurement technology, experimentation approaches may not be appropriate for 3D atom-level observation. Alternatively, computational mechanics of discontinua is currently an essential part of cutting edge research in different fields of solid mechanics. The problem of dynamic fracture in different kinds of materials is still an open issue and continues to be a challenge for researchers. Many researchers have studied this complex problem by means of diverse numerical methods. These numerical methods can be categorized into eight groups: (1) the molecular dynamic (MD) method adopted by Gao [2] and Furuya and Noguchi [3]; (2) the extended finite element method (XFEM) first developed by Belytschko and Black [4]; (3) the mesh-free method proposed by Belytschko et al. [5] and Belytschko et al. [6]; (4) the finite element method (FEM) incorporated with cohesive interface techniques proposed by Xu and Needleman [7]; (5) the dual boundary element method (DBEM) together with fictitious crack model proposed by Aliabadi and Saleh [8]; (6) the discrete element method (DEM) with bonding theory proposed originally by Cundall and Hart [9] and further complemented by Potyondy and Cundall [10]; (7) the combined finite and discrete element method proposed by Munjiza et al. [11] and Rabczuk and Belytschko [12]; and (8) the lattice models proposed by Chiaia et al. [13] and adopted by Kosteski, et al. [14]. Amongst these numerical methods, continuum based methods such as FEM and BEM are restricted to severe element distortion,

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* Corresponding author.
E-mail address: ycchung123@ncu.edu.tw (Y.C. Chung).

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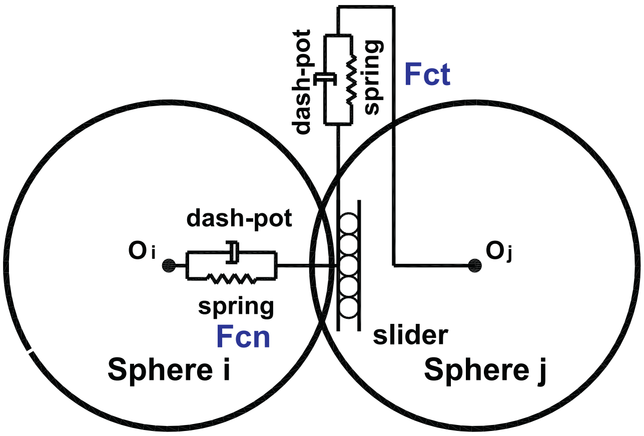


Fig. 1. Linear spring-dashpot model with a frictional slider for non-bonded spheres.

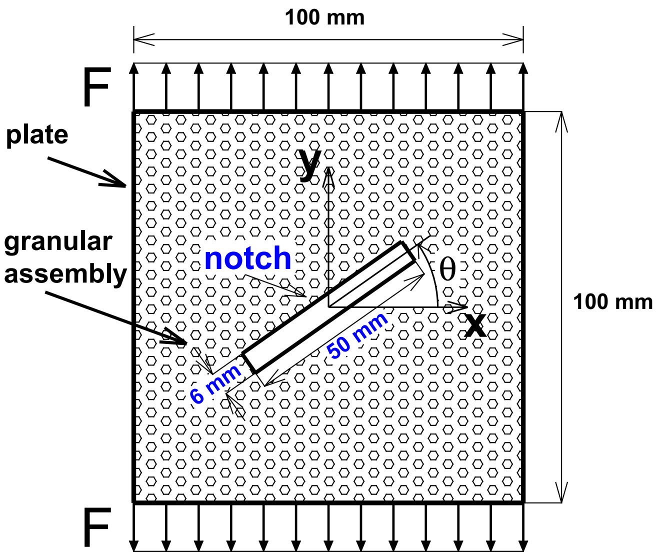
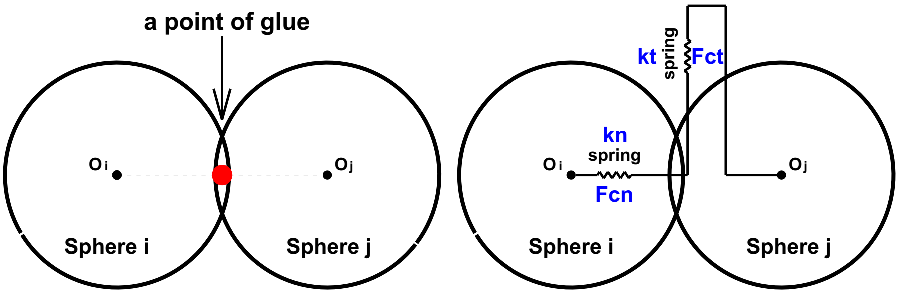


Fig. 4. Schematic illustration of a plate made of different crystal structures.

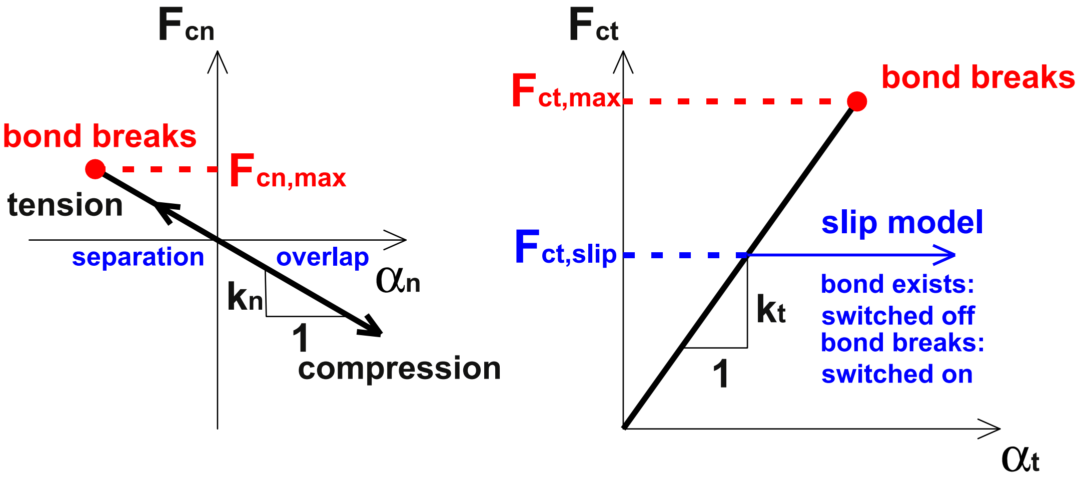
frequent re-meshing, and the need for continuum constitutive models (Tavarez and Plesha [15]), so applying them to the problems with severe damage is still a challenge. On the contrary, DEM (Cundall and Strack [16]) has shown to be a powerful, versatile and natural numerical tool for modelling the behaviour of particulate media, and also very suitable for exploring the micro-mechanics at the particle level. Equipped with appropriate bonded-particle models (BPM) (Potyondy and Cundall [10]), DEM also provides a promising way to model solid damage problems, giving a seamless transition from solid phase to particulate phase.

Vesga et al. [17] investigated the failure behaviour of a plate with an inclined notch subjected to uni-axial compressive loading using 2D



(a) (b)

Fig. 2. Contact-bond model for bonded spheres: (a) schematic of contact bond; (b) linear spring model.



(a) (b)

Fig. 3. Force-displacement relation for contact-bond model: (a) normal force; (b) shear force.