Abstract

'Locally isostatic' frameworks are periodic bar-joint frameworks, which on average have the same number of constraints as degrees of freedom. An important class of minerals, zeolites, can be modelled as 3D locally isostatic frameworks. Zeolites are widely used in oil-refining, water purification, air pollution control and ion exchange. However, the underlying kinematic properties of zeolites are not yet well understood. There are many different hypothetical zeolites, whereas only about 50 types of zeolites are found in nature. This study provides some insights into the kinematic properties of zeolites through studying 2D 'zeolite-like' frameworks: kagome lattice and Roman mosaic net.

The core of this study concerns periodic bar-joint framework. Previous work has described a predictor-corrector method, which finds configurations along a finite path. This study extends the predictor-corrector method to adapt configurations that have more than one path and to work for periodic structures. Two other new techniques are introduced in this study; a 'path description method' that describes a continuous finite kinematic path by a single configuration; and a 'path projection technique' that provides an overview to all the finite kinematic paths of a framework.

This work mainly studies two classic examples of locally isostatic frameworks in 2D: the kagome lattice and Roman mosaic net. The two frameworks are studied in different sizes of repetitive 'unit cell': from the smallest repeatable part, gradually increased to a size up to 25 times larger (the sizes increase in both dimensions). According to Maxwell's rule, 2D locally isostatic frameworks are guaranteed to have one degree of freedom regardless the size of unit cell. This corresponds to a single finite kinematic path. However, this study found some configurations with many more finite kinematic paths, and an increase of kinematic freedom – these are often associated with highly symmetric configurations. At these 'singular' configurations, the compatibility or rigidity matrix describing the first-order effect of the constraints is rank-deficient. In order to give further insight, the kinematic properties of perturbed cases and 'added-bar' cases are also studied.

Results suggest that configurations with some symmetry have more degrees of kinematic freedom. Notably, some two-fold symmetric configurations have increased kinematic freedoms, and their corresponding states of self-stress are two-fold anti-symmetric. This result is found in both kagome lattice and Roman mosaic net. A symmetry-extended counting rule that uses Group Representation Theory is applied to give a symmetry insight for the mechanisms and states of self-stress. The study finds that different choices of symmetry cell structure for an identical configuration could have different characters after symmetry operations. This depends on the location of two-fold rotation centres: if no two-fold rotation centres are located on the joints, the compatibility matrix has the minimum rank, thus the framework has the greatest kinematic freedom.

Key words: periodic bar-joint frameworks, locally isostatic, kinematic paths, mechanisms, states of self-stress, symmetry