

THE FLEXING OF LOCALLY ISOSTATIC PERIODIC STRUCTURES

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Summary Many natural crystal structures, in particular zeolites, can be modelled as simple pin-jointed structures which are locally isostatic, where the number of structural constraints are equal to the number of structural freedoms. Guest and Hutchinson [1] showed that such structures must have mechanisms that will allow the structure to deform, and it is conjectured that these mechanisms are responsible for some of the unexpected properties of zeolites, for instance having a negative coefficient of thermal expansion.

In fact, many repetitive locally isostatic structures have many additional mechanisms beyond those predicted by Guest and Hutchinson [1]. This paper will explore the infinitesimal mechanisms associated with some simple two-dimensional structures, such as the kagome and roman mosaic structures. In particular, the paper will examine which of the mechanisms extend to finite mechanisms that might lead to the large-scale deformation of the structure.

INTRODUCTION

Zeolites are industrially important crystal structures, mainly made up of silicon and oxygen. Internally, they primarily consist of SiO_4 tetrahedra that are joined at corner oxygen atoms in such a way that large internal pores remain. From a structural perspective, the SiO_4 tetrahedra form relatively rigid components, while the Si-O-Si bonds are relatively flexible. Thus a good simplifying model is to consider zeolites as consisting of rigid tetrahedra, connected at their corners through spherical joints. Such a structure is locally isostatic [2], where the number of structural constraints are equal to the number of structural freedoms. Guest and Hutchinson [1] showed that such structures must have at least three mechanisms that will allow the structure to deform, and it is conjectured that these mechanisms are responsible for some of the unexpected properties of zeolites, for instance having a negative coefficient of thermal expansion.

This paper will explore the 2D analogue of the zeolite model: repetitive structures which consist of rigid triangles, connected through pin-joints at their corners. Understanding the behaviour of such structures might provide a key to understanding some of the unusual properties of zeolites.

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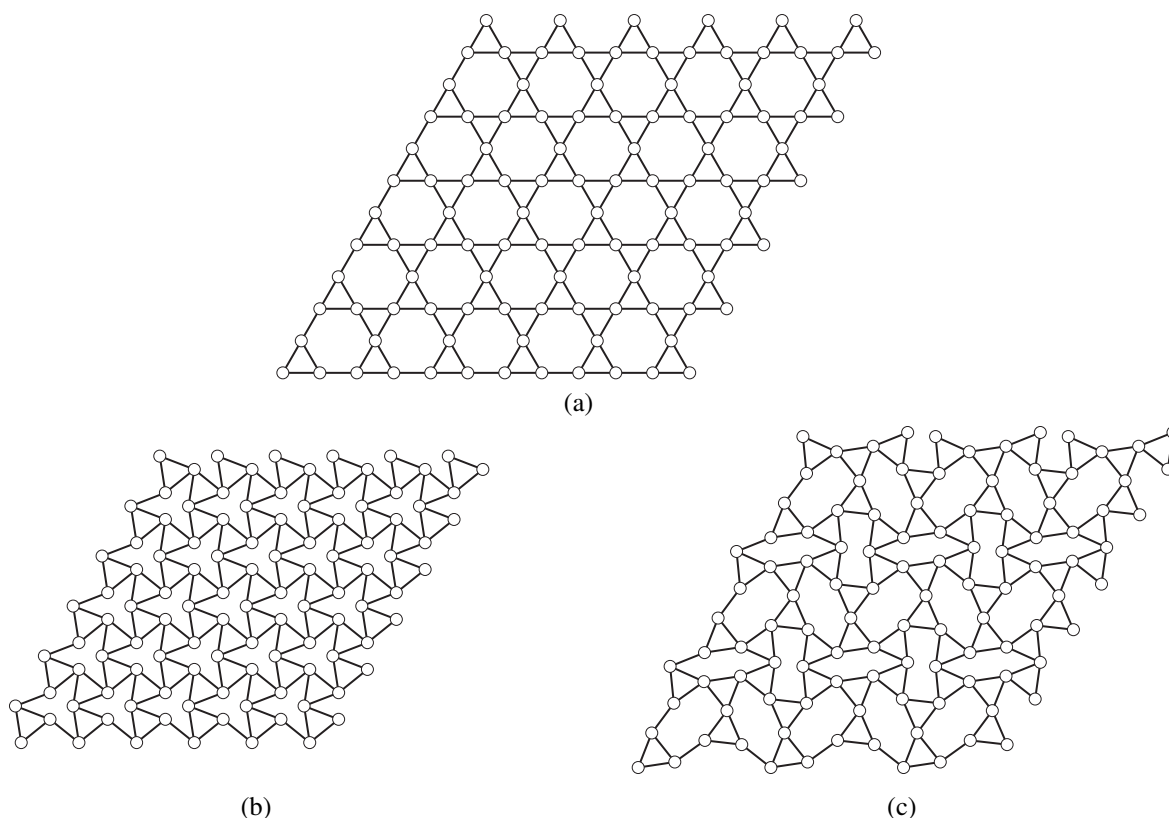


Figure 1. (a) Part of a repetitive kagome lattice; (b) a fully repetitive finite mechanism of the lattice; (c) another finite mechanism, where the pattern of deformation repeats over a longer unit period than seen in (b).

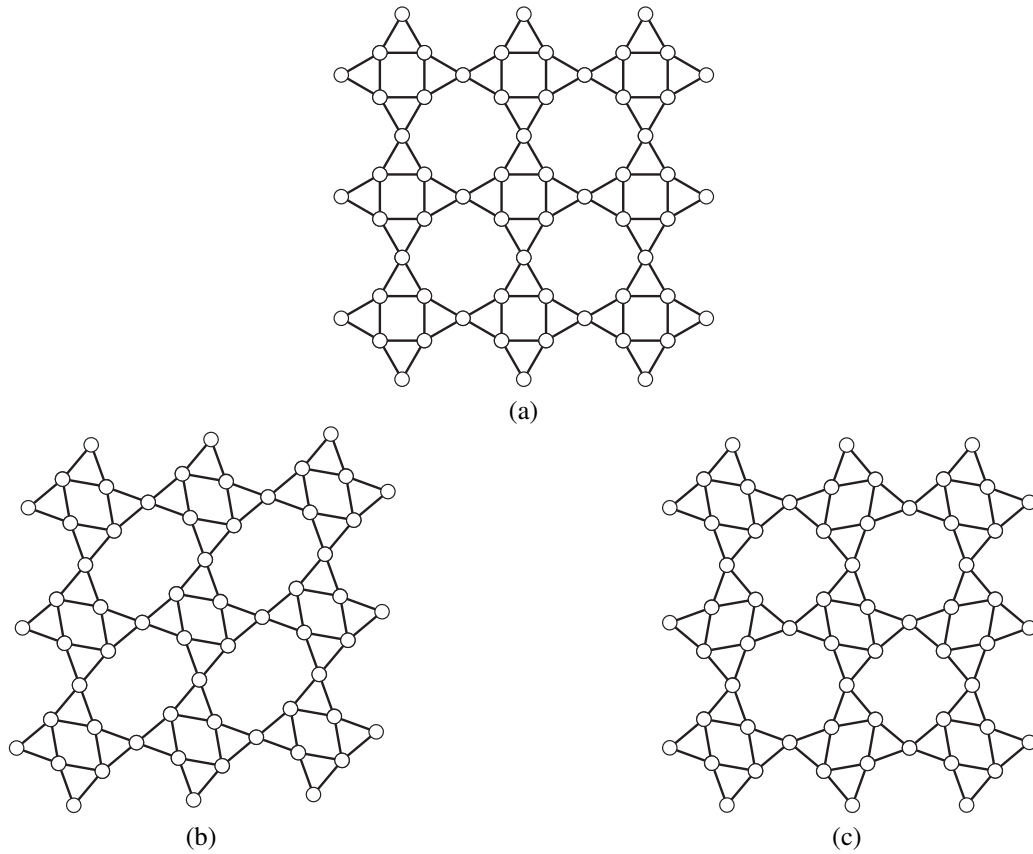


Figure 2. The present figure mirrors the layout of Figure 1:(a) part of a repetitive ‘roman mosaic’ lattice; (b) a fully repetitive finite mechanism of the lattice; (c) another finite mechanism, where the pattern of deformation repeats over a longer period than seen in (b).

TWO-DIMENSIONAL STRUCTURES

We will consider two examples of repetitive structures that are made up of pin-jointed corner-sharing triangles, the ‘kagome’, shown in Figure 1(a), and the ‘roman mosaic’ model shown in shown in Figure 2(a). In both cases, we will consider the structure as a pin-jointed bar model. For the two-dimensional case, there is guaranteed to be a single fully repetitive mechanism [1], and this is shown for the two examples in Figure 1(b) and Figure 2(b). In fact these highly symmetric structures turn out to have many more infinitesimal mechanisms, as was comprehensively explored for the kagome case by Hutchinson and Fleck [3]. However the question remains, which of these infinitesimal mechanisms will extend to a finite mechanism, and actually provide a flex by which the structure might undergo large deformations? Both example structures have many additional such flexes, as are shown in Figure 1(c) and Figure 2(c). The presentation will explore how this question might be answered.

References

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