

An Analytical and Numerical Investigation of
Auxeticity in Cubic Crystals and Frameworks

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Abstract

Negative Poisson's ratio, or auxetic, materials present the possibility of designing structures and components with tailored or enhanced mechanical properties.

This thesis explores the phenomenon of auxetic behaviour in cubic crystals using classical and quantum modelling techniques and assesses the validity of these techniques when predicting auxetic behaviour in cubic elemental metals. These techniques are then used to explore the mechanism of this behaviour.

The findings of the atomistic modelling are then used as a template to create networks of bending beams with tailored Poisson's ratio behaviour.

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