Equilibrium configurations of crystals

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Contents

1. Introduction
2. A useful construction
3. Subenergy and homogeneous deformation
4. General boundary conditions and the existence of parametrized measures
5. Parametrized measure minima
6. Stable parametrized measure minima
7. Parametrized measure equilibria
8. Some concluding remarks

1. Introduction

The morphology of a crystal may show several phases and these may be altered with changes in its mechanical or thermal environment. For example some crystals may be deformed to consist of several twin related phases. To understand this in the context of thermoelasticity, Ericksen [21-23],[25-31] has derived a stored energy density which shows invariance with respect to change of the crystallographic lattice basis of the material. Such a density is invariant with respect to an infinite discrete group as well as frame indifferent. A body governed by it is rendered highly unstable with respect to certain motions. For example, at a smooth local minimum of energy in a constant temperature heat bath, the Cauchy stress reduces to a pressure, cf. Ericksen [20]. So it seems unlikely that even setting homogeneous boundary conditions leads to a homogeneous extremal.

In this note we wish to determine by direct methods equilibrium configurations under displacement loading conditions. We favor this approach as a means of surmounting the difficulties imposed by the defect structures on the stability of smooth solutions. Our first objective, then, is to calculate the minimum energy of a configuration. An important role in the thermodynamics of the crystal is played by its subenergy, introduced by Ericksen [24] and based in part on a method of Flory [32]. In many