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Twinning mechanism and habit lines in monolayer-thick free-standing graphene: Theoretical predictions☆

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ABSTRACT

Starting from the symmetry breaking stretches of the hexagonal and the rhombohedral graphite viewed as 2-lattices, we study martensite/martensite interfaces (twins) and martensite/austenite interfaces (habit lines) for a monolayer-thick free-standing graphene sheet. We do that by adopting the theoretical framework of Bhattacharya and James (1999). The outcome of our analysis consists of inequalities that should be satisfied by the components of the symmetry breaking stretches in order the twinning equation to have a solution. We also evaluate the vector describing the twin interface and the habit line. This is done for some specified film orientation and for the first breaking of symmetry for hexagonal and rhombohedral graphite which leads to orthorombic and face-diagonal monoclinic configurations, respectively. In 2 dimensions, this transformation corresponds to the hexagonal to rhombic phase transition for graphene. The second symmetry breaking for both the hexagonal and the rhombohedral graphite results to the triclinic configuration and corresponds, in 2 dimensions, to the hexagonal to oblique transformation for graphene. For the second symmetry breaking, we only report inequalities that should be satisfied by the components of the symmetry breaking stretches in order the twinning equation to have a solution, for some specific cases. Constraints necessary for the formation of tunnels and tents are also included in our analysis. Connection with what one may expect to see during experiments or when using molecular calculations is done using some representative figures.

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1. Introduction

A martensitic phase transformation is a first-order, diffusionless solid to solid phase transformation (Bhattacharya, 2004; Pitteri & Zanzotto, 2003). Thus, during this transformation the material remains a solid. The characterization first or second order pertain to the continuity of the lattice parameters during the change. When the lattice configuration changes abruptly at the transition we speak about a first-order phase transition. When the change is continuous near and at the transition we speak about a second-order phase transition. During a martensitic phase change there is no change in the relative position

☆ This work is dedicated to the memory of P.S. Theocharis (1921–1999). I thank the Academy of Athens for honoring me with the P.S. Theocharis award on Mechanics which is given biennially to the best paper on Mechanics. The paper selected for the period 2012–2014 is Sfyris, Sfyris, and Galiotis (2014) co-authored by D. Sfyris, G.I. Sfyris and C. Galiotis. P.S. Theocharis was an exceptional scholar who had a tremendous impact on the Greek mechanics community and shaped the thought of all of us.

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of the atoms: the transition is diffusionless. Essentially, there is no rearrangement of atoms and one can obtain one structure from a deformation of the other. If there is only one control parameter, e.g. the temperature, the lattice has one structure at high temperature and a different one at low temperature. The high temperature phase is called the austenitic phase (or the austenite), while the low temperature phase is called the martensitic phase (or the martensite).

Generalizations of the classical theory of elasticity to take into account martensitic phase changes begin with the theories of Ericksen (1970, 1979) and Parry (1978, 1976). These authors provide a means for extending the framework of nonlinear elasticity to cover cases where symmetry of a crystalline material changes due to loading or changes of temperature. For the particular class of martensitic transformations, one should confine himself to weak transformation neighborhoods (Pitteri, 1984b). These are neighborhoods in the space of admissible metrics and limit the symmetry breaking procedure according to the scheme: symmetry can only reduce to one of its subgroups. Thus, the martensite should have crystallographic symmetry which is a subgroup of the crystallographic symmetry of the austenite. Confinement to weak transformation neighborhoods guarantees also the uniqueness of the austenitic phase (Bhattacharya, 2004). An energy that describe austenite-martensite changes has mutliple minima. The location of the wells are related to the crystal structure of the austenitic and the martesnitic phase.

A very important class of non-homogeneous energy minimizing deformations is twins in martensite (Ball & James, 1987, 1992; James, 1981). A twin is built up of two homogeneous portions of the same crystal species oriented with respect to one another by a rotation. The homogeneous portions of the material are called variants of the martensite. More complex arrangements of the variants of the martensitic phase are called microstructure (Bhattacharya, 1991, 1992, 2004). Some examples of microstructure are the wedge-like microstructure as well as the case where twins appear within twins as a consequence of loading and/or heating/cooling. From the physical point of view microstructure is a consequence of the multiwell structure of the energy. If the applied boundary conditions correspond to the average value of some of the wells, then the material prefers to make a mixture of different wells (Bhattacharya, 2004).

Another very important manifestetion of microstructure is the formation of austenite/martensite interfaces (habit planes). These interfaces are not commonly observed in most martensitic materials (Bhattacharya, 2004). Instead one observes an interface separating austenite from variants of martensite. A typical example is the austenite/martensite interface in cooper-aluminum-nickel (Bhattacharya, 2004).

The mathematical framework for treating twins in a bulk material is given in the fundamental work of Ball and James (1987, 1992). These authors lay down a solid mathematical framework where twins need not be known a priori; they are the outcome of the theory provided one knows the transformation matrices from the austenite to the martensite. This theory has been successfully applied to treat twin and habit plane microstructure for the tetragonal to monoclinc transformation in zirconia (Simha, 1997), wedge microstructure (Hane, 1999) and more complex microstructure for the cubic to tetragonal transition (Hane & Shield, 1998). An excellent book by Bhattacharya (2004) and a review article by James and Hane (2000), collect all necessary material and provide valuable references on the topic.

The thin film theory of martensite is presented by Bhattacharya and James (1999). These authors start from three dimensional nonlinear elasticity and derive a theory for single crystal thin films as a Cosserat membrane theory with one Cosserat vector field. They also provide the mathematical framework for evaluating twins and habit lines for thin films knowing only the symmetry breaking stretches of the bulk material. More specifically, Proposition 5.1 of Bhattacharya and James (1999) gives the general methodology for studying twinning on a thin film starting from the symmetry breaking stretches of the bulk material. These authors (Bhattacharya & James, 1999) infer that thin films can undergo a richer class of deformations compared to their bulk counterparts which makes microstructure formation more possible for thin films and conclude that there are many material's and film's orientations where the austenite can form an exact interface with a single variant of the martensite.

Since such interfaces can be used as hinges, because they are compatible with a one-parameter family of rotations, Bhattacharya and James (1999) examined if they can be arranged in a specified manner. Such a line of thought led them to study tent and tunnel formation as energy minimizing deformations which may be used for microactuators and apply this theory to some representative materials such as $Ni_{50}Ti_{50}$, Ni_2MnGa, $Ni_{64}Al_{36}$. They also provide constraints the components of the symmetry breaking stretches of the bulk material should satisfy in order martensite/austenite interfaces to exist for the cubic to tetragonal, cubic to orthorombic, and cubic to monoclinic transformations for different film orientations. Their theory is used to study tents and tunnels in Ni_2MnGa, $PbTiO_3$ and Cu-Zn-Al (Bhattacharya, DeSimone, Hane, James, & Palmstron, 1999) and also for the quasiconvexification problem of the two-well and the four-well problem (Bhattacharya & Dolzmann, 2000, 2001).

The analysis in the present work is guided by the thin film framework of Bhattacharya and James (1999) and aims to find conditions for having twins (martensite/martensite interfaces) as well as habit lines (martensite/austenite interfaces) for a monolayer-thick free-standing graphene sheet. Since Proposition 5.1 of Bhattacharya and James (1999) uses the symmetry breaking stretches of the bulk material to infer whether twinning is possible for the thin film, the starting point of our analysis is graphite, which is the bulk material from which graphene can be exfoliated by the micromechanical cleavage method or the Scotch tape method (Novoselov, 2011). Graphite has two stackings: hexagonal and rhombohedral graphite. As a 2-lattice hexagonal graphite belongs to type 27 of the classification of Fadda and Zanzotto (2001). For the special ratio $c/a = 1.633$ of its lattice parameters the hexagonal 2-lattice gives the well known hexagonal closed pack (h.c.p.) structure while for a generic value of the c/a it is usually called a deformed h.c.p. structure (Fadda & Zanzotto, 2001). Rhombohedral

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