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A comprehensive lattice-stability limit surface for graphene

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ABSTRACT

The limits of reversible deformation in graphene under various loadings are examined using lattice-dynamical stability analysis. This information is then used to construct a comprehensive lattice-stability limit surface for graphene, which provides an analytical description of incipient lattice instabilities of *all kinds*, for arbitrary deformations, parametrized in terms of symmetry-invariants of strain/stress. Symmetry-invariants allow obtaining an accurate parametrization with a minimal number of coefficients. Based on this limit surface, we deduce a general continuum criterion for the onset of all kinds of lattice-stabilities in graphene: an instability appears when the magnitude of the deviatoric strain γ reaches a critical value γ^c which depends upon the mean normal strain $\bar{\varepsilon}$ and the directionality θ of the principal deviatoric stretch with respect to reference lattice orientation. We also distinguish between the distinct regions of the limit surface that correspond to fundamentally different mechanisms of lattice instabilities in graphene, such as structural versus material instabilities, and long-wave (elastic) versus short-wave instabilities. Utility of this limit surface is demonstrated in assessment of incipient failures in defect-free graphene via its implementation in a continuum finite elements analysis (FEA). The resulting scheme enables on-the-fly assessments of not only the macroscopic conditions (e.g., load and deflection) but also the microscopic conditions (e.g., local stress/strain, spatial location, temporal proximity, and nature of incipient lattice instability) at which an instability occurs in a defect-free graphene sheet subjected to an arbitrary loading condition.

1. Introduction

Limits to reversible deformation – the stress or strain at which elastic-to-inelastic transition takes place in a material – pose fundamental constraints on a material's performance and determine its strength. The limiting stress or strain, in general, depends upon the loading path, and the dependence is often described by means of a phenomenological model termed a limiting (or failure) criterion. Mathematically, a limiting criterion is represented as a surface in stress or strain space, which separates the stable states of reversible deformation from the 'failed' or irreversibly deformed states. For many materials, the limiting criterion is simple enough to be characterized by one or two material constants, which are readily determined from experiments. Examples include the Mises (or Tresca) yield criterion for metals, the Mohr–Coulomb criterion for cohesive-frictional solids (Coulomb, 1776), the Drucker–Prager criterion for pressure-dependent solids (Drucker and Prager, 1952), and the Hoek–Brown criterion for rocks (Hoek and Brown, 1997).

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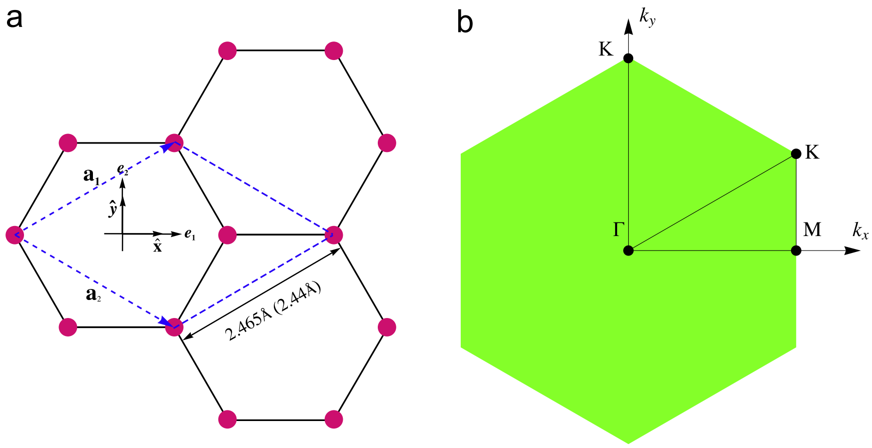

Fig. 1. (a) Graphene lattice with orientations of the material unit vectors – $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ – and the Cartesian unit vectors – $\mathbf{e}_1$ and $\mathbf{e}_2$ – indicated. The dashed blue lines denote the unit cell used in the *ab initio* calculations. The GGA (LDA) value of the lattice parameter is also indicated. The armchair and zigzag directions are along the $\mathbf{e}_1$ and $\mathbf{e}_2$ axes, respectively. (b) Brillouin zone of graphene with high symmetry points and irreducible wedge indicated. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

In crystalline materials that are free from lattice imperfections, the limit to elastic deformation sets an upper bound on the material strength (Macmillan, 1983). This upper bound, termed the ideal strength, depends on the intrinsic nature of bonding between atoms in the material. Because of the various types of lattice defects, such as dislocations, grain boundaries, interstitial impurities, and voids which normally exist in materials (Minor et al., 2006; Suresh and Li, 2008), most conventional materials are irreversibly deformed at stress-levels well below the ideal strength. However, in recent years, advancements in nanotechnology have enabled fabrication and growth of defect-free nano-crystals in which mechanical failure indeed occurs upon reaching stress levels near the ideal strength (Lee et al., 2008; Rasool et al., 2013; Jang et al., 2012; Chuang and Sansoz, 2009; Sansoz et al., 2013).

Graphene, an atomic monolayer comprising a hexagonal network of covalently bonded C-atoms, is a representative example of such materials (see Fig. 1). Experimental studies have shown that defect-free, single-crystalline graphene can sustain near-ideal-strength stresses while remaining within the reversible regime of deformation (Lee et al., 2008; Rasool et al., 2013). Beyond the limit of elastic deformation, the fate of the material is determined by a strength-limiting mechanism such as incipient plasticity or crack-initiation. Since, in the absence of lattice-imperfections, a strength-limiting mechanism can only be activated by a lattice-instability (Born, 1940; Li et al., 2002; Liu et al., 2007; Liu et al., 2010), the incipient failure of a defect-free crystalline material is intrinsically related to the loss of internal lattice-stability. The point at which the loss of lattice-stability occurs is called the *lattice-stability limit*, and it varies from loading path to path. Further, the dependence of the lattice-stability limit on the loading condition in crystalline materials is generally too complex to be adequately characterized by one or two parameters.

Individually, lattice-instabilities of all kinds can be assessed via the lattice-dynamical stability analysis (see Born and Huang, 1954; Hill, 1962), which asserts that a necessary and sufficient criterion for an ideal crystal under arbitrary uniform loading to be stable is that it exhibits stability with respect to bounded perturbations of all wavelengths. Integration of the lattice-dynamical stability analysis with a continuum analysis scheme such as FEA would be ideal for failure analysis of defect-free graphene crystals. This could enable assessment of incipient failures and ideal strength of graphene, under arbitrary loading conditions at realistic length-scales and slow enough loading rates, directly in a continuum-level simulation. However, stability analysis based on lattice-dynamics requires carrying out an elaborate sequence of computationally expensive steps that cannot be treated within the confines of an analytical framework, making it difficult to integrate the lattice-dynamical stability analysis into a continuum scheme. Therefore, there remains a need for a general continuum criterion that could describe the onset of instability (of any kind) in graphene under an arbitrary state of deformation.

The aim of this work is to construct a comprehensive lattice-stability limit surface, which constitutes an analytical parametrization of incipient lattice instabilities of *all kinds*, over the space of all homogeneous deformations, in terms of stress/strain. There are two main difficulties in obtaining such a parametrization: First, crystalline materials are intrinsically anisotropic, so material response, including lattice-stability limit, varies with orientation (Neumann and Meyer, 1885). Secondly, two fundamentally different types of lattice-instabilities govern strength-limiting mechanisms under different loading conditions (Marianetti and Yevick, 2010; Clatterbuck et al., 2003; Clatterbuck, 2003): a long-wave (or elastic) instability and a short-wave (or soft mode) instability. The condition for onset of an elastic instability can be parameterized in terms of strain via acoustic tensor analysis (see Kumar and Parks, 2014 for details), whereas the short-wave instabilities are much more complex since there is no continuum framework for parametrization of limiting conditions governing the onset of short-wave instabilities.

The proposed parametrization, in order to overcome the above-mentioned difficulties, employs interpolation of the lattice-stability limits of graphene, corresponding to some representative homogeneous deformation modes, in the basis of