Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 291 (2015) 216–239
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Anisotropic hyperelastic modeling for face-centered cubic and diamond cubic structures

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Received 23 April 2014; received in revised form 27 March 2015; accepted 30 March 2015
Available online 16 April 2015

Abstract

A new hyperelastic model for a crystal structure with face-centered cubic or diamond cubic system is proposed. The proposed model can be simply embedded into a nonlinear finite element analysis framework and does not require information of the crystal structure. The hyperelastic constitutive relation of the model is expressed as a polynomial-based strain energy density function. Nine strain invariants of the crystal structure are directly used as polynomial bases of the model. The hyperelastic material constants, which are the coefficients of the polynomials, are determined through a numerical simulation using the least square method. In the simulation, the Cauchy–Born rule and interatomic potentials are utilized to calculate reference data under various deformation conditions. As the fitting result, the hyperelastic material constants for silicon, germanium, and six transition metals (Ni, Pd, Pt, Cu, Ag, and Au) are provided. Furthermore, numerical examples are performed using the proposed hyperelastic model.

Keywords: Hyperelastic model; Cauchy–Born rule; Face centered cubic; Diamond cubic; Strain invariants; Finite element method

1. Introduction

As global interest of nanoscale devices has greatly increased over the past decade, mechanical analysis that considers the nanoscale effect becomes more important when it comes to designing the nano-electromechanical system (NEMS). Because many nanoscale structures, such as nanowires and nanofilms, are likely to consist of a single crystal material rather than a poly-crystal material, understanding the mechanical behavior of a single crystal structure is essential when constructing the NEMS design. One remarkable feature of a single crystal structure is that the elastic range of the structure is much wider than that of a macroscale structure, which consists of poly-crystals. For an example, a nanowire can elastically stretch more than 5% under tensile loading [1,2], and the magnitude of the equilibrium strain of a nanofilm ranges more than 2% when the thickness of the nanofilm is a few nano-meters [3,4]. Therefore, it is evident that the hyperelastic behavior of a single crystal material is very important when it comes to designing the NEMS.

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http://dx.doi.org/10.1016/j.cma.2015.03.024
0045-7825/

One efficient method when considering the hyperelastic effect of a single-crystal structure is to use CBR, the Cauchy–Born rule [5,6]. The CBR acts as the bridge between the atomistic deformation in a crystal lattice and the macroscopic deformation of the continuum theory. Through the use of CBR, the position of each atom in the deformed configuration can be determined by the macroscopic deformation gradient. If every atomic position of a lattice in a deformed state is known, the tangent modulus of the deformed state can be obtained analytically from the inter-atomic potential function. Many researchers have performed nonlinear finite element analysis when solving nano-scaled structural problems through the use of CBR. Tadmor et al. [7] have used CBR to describe the hyperelastic behavior of local regions in the quasicontinuum method. Utilizing an extension of CBR based on an exponential map, Arroyo and Belytschko [8] proposed hyperelastic membrane models for a carbon nanotube. Park et al. [9] developed a surface Cauchy–Born model to consider the surface effect on nanoscale materials.

However, to implement CBR in a nonlinear finite element analysis procedure as a hyperelastic model is not an easy task. Since pair potentials such as Lennard-Jones [10] and Morse potential [11] functions were introduced, many inter-atomic potentials for crystalline solid structure have been developed and used. However, the use of the simple pair potentials in the CBR is practically limited in nonlinear finite element analysis because many crystal structures generally require complex interatomic potentials rather than simple pair potentials: the embedded-atom method (EAM) potential [12] fully describes metallic bonding of face-centered cubic (FCC) crystals in terms of electron density; Tersoff potential [13] can be used for covalent bonding materials such as silicon, germanium, and carbon; Reactive force field [14] is a bond order based force field that has been developed to consider chemical reactions. Furthermore, in some crystal structures such as diamond and zincblende structures, not all atoms follow transformation rules by the deformation gradient tensor. To describe every atomic position in the deformed state, these structures require additional internal degrees of freedom, which are often called inner displacement or internal displacement [15]: Tang et al. [16] proposed the quasi-continuum method for silicon nanostructures using internal displacement; Park and Klein [17] presented a surface Cauchy–Born model for silicon nanostructures using internal displacement as well. The internal displacement in both works was numerically calculated using an iterative method. As the internal displacements require continuous calculation at each Gauss point for every element in each iteration step, high computing cost is unavoidable. For these reasons, it is needed for crystal structures in finite element analysis to employ a new hyperelastic continuum model which can be an alternative to the CBR.

Over the past several decades, many hyperelastic models have been made to consider large deformation for rubber-like materials and biological soft tissues. For isotropic rubber-like materials, Treloar [18] introduced the simplest hyperelastic form of the Neo-Hookean model, and Mooney [19] and Rivlin [20] presented a new hyperelastic model, the Mooney–Rivlin model, using two invariants of the right Cauchy–Green tensor. Ogden [21] proposed a type of hyperelastic model using principle stretches, which can include the previous two models as special cases. In addition to these models, Yeoh model [22] and Arruda–Boyce model [23] were proposed for isotropic rubber-like materials. For anisotropic hyperelastic materials, Spensor [24] constructed strain energy function using augmented transversely isotropic invariants for fiber-reinforced composites. After his work, many studies were followed for biological soft tissues and fiber-reinforced elastomers [25–30]. To our knowledge, while a lot of hyperelastic models for isotropic and transverse isotropic material have been studied, but a practical hyperelastic model for crystal structures has been rarely reported in the literature.

In this paper, a framework of anisotropic hyperelastic modeling for crystal structures is proposed, and a new hyperelastic model for FCC and diamond cubic crystals is presented. The proposed hyperelastic model is much simpler than the interatomic potentials and can be easily embedded into a nonlinear finite element analysis. A polynomial-based strain energy density function is used to express the hyperelastic constitutive relation. The next section presents the strain energy density function with nine strain invariants which act as the polynomial bases of the function. In Sections 3 and 4, the material constants for FCC and diamond cubic crystals of the hyperelastic model are determined through the use of the least square method, and numerical examples are presented in Section 5 to validate the proposed model.

2. Hyperelastic model for crystal structures

2.1. Strain energy density function

For the hyperelastic isotropic incompressible materials, Treloar [18,31] and Rivlin [32] presented the Neo-Hookean elasticity model to account for large elastic deformation. Mooney [19] and Rivlin [20] proposed a more general form