Computational Materials Science 79 (2013) 284–288

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Nonlinear elastic response of cubic crystals to biaxial strain

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ARTICLE INFO

Article history:
Received 17 April 2013
Accepted 31 May 2013
Available online 13 July 2013

Keywords:
Nonlinear elasticity
Biaxial Poisson's ratio
Biaxial strain
Thin films

ABSTRACT

The biaxial Poissons ratio in the nonlinear elastic theory is an important material parameter. We report here an accurate and efficient means of calculating the nonlinear elastic response of thin, homogeneous films to biaxial strain in arbitrary planes using a continuum-elasticity theory model. The general analytic expressions were derived for the elastic energy and the Poissons ratio under biaxial strain for cubic crystals. The biaxial Poisson's ratio did not remain constants, but showed a linear relationship with strain when second- and third-order elastic constants are considered. The expressions were verified with simulated biaxial Poisson's ratio and elastic energy of copper by density-functional theory calculations for three high symmetry planes.

1. Introduction

The energy associated with elastic distortions plays a major role in the stability of heterostructures [1,2], nanostructures [3], and thin metallic films [4] as well as in the phase stability in metal superalloys [5]. In these structures which are the building blocks of integrated circuits and magnetic disks, large stresses may be present, and nonlinear elastic effects need to be taken into account.

Most of the strain energy is stored in the overlayers that are already bulk-like, and the total strain energy can be estimated by studying the biaxial deformations [6,7] of bulk materials. It has been argued that deviations from bulk elastic behavior play a notable role only in films that are less than several monolayers thick.

It is important to understand nonlinear elastic properties of thin films [8,9], because modeling deformations larger than a few percent that are common in epitaxial and pseudomorphic overlayers, requires going beyond linear elasticity theory. The linear elastic energy and the Poisson ratio under biaxial strain have been previously studied by Hammerschmidt et al. [7]. However, non-linear elastic effects have not been well established.

In this paper, the nonlinear elastic properties of materials with cubic symmetry under biaxial strain were studied in arbitrary planes. The strain tensor was introduced, and the elastic energy and the biaxial Poissons ratio for cubic systems were determined based on continuum-elasticity theory (CET). Finally, the expressions were verified with simulated biaxial Poisson's ratio and elastic energy of copper by density-functional theory (DFT) calculations for three high symmetry planes.

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http://dx.doi.org/10.1016/j.commatsci.2013.05.058

2. Analytical expression for nonlinear biaxial strain-tensor

For a solid body subject to a finite deformation, the configuration of a material point in the system after deformation is represented as $Y = Y(X)$, where X is the initial configuration at the equilibrium state. The deformation gradient is defined by the following expression

$$J_{ij} = \frac{\partial Y_i}{\partial X_j}, \tag{1}$$

where i and j = 1, 2, 3 are the indices of the Cartesian coordinates. Then the Lagrangian strain tensor is defined as follow:

$$\eta = \frac{1}{2}(J^T J - I), \tag{2}$$

where I is the unit matrix. The internal energy is related to the Lagrangian strain through Taylor series expansion in terms of the strain tensor and the expression to the third order is as follow:

$$F(X, \eta_{ij}) = F(X, 0) + \frac{V}{2}\sum_{ijkl} C_{ijkl}\eta_{ij}\eta_{kl} + \frac{V}{6}\sum_{ijklmn} C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} + \dots, \tag{3}$$

where C_{ijkl} and C_{ijklmn} are the second and third order elastic constants (SOECs and TOECs). Often, the symmetries of crystal structures can be used to simplify the expression given above by specifying the strain tensor in the canonical coordinate system of the crystal. The elastic response of a medium under external stress is determined by minimizing the free energy F with respect to the directions with no external stress. The general analytic solutions for the yield of isotropic and one-dimensional (uniaxial) external deformations (Fig. 1a) are the bulk modulus and Poisson ratio, respectively.

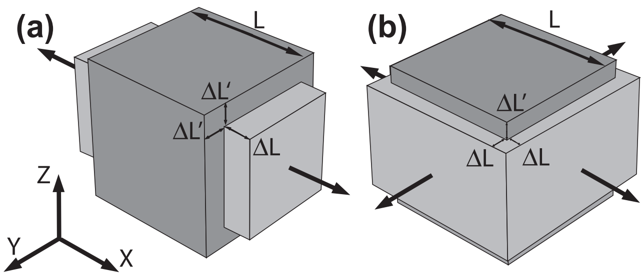

Fig. 1. Schematic diagram to illustrate the uniaxial and biaxial strains. The dark gray cube is unstrained with side length L, and the light gay is strained. (a) Expanded along the x direction by L due to an externally applied uniaxial tension, and contracted in both y and z directions by L', and the uniaxial Poisson ratio is defined as $v = \Delta L'/\Delta L$. (b) Expanded along the x and y direction by L due to an externally applied biaxial tension, and contracted in z directions by L', and the biaxial Poisson ratio is also defined as $v = \Delta L'/\Delta L$.

A biaxial Poisson ratio can be defined for isotropic two-dimensional deformations (Fig. 1b). Similar to the uniaxial case, the elastic relaxation upon biaxial strain in a plane (hkl) can be given in an orthogonal coordinate system with two perpendicular axes (e_1, e_2) in the strain-plane (hkl) and a third (e_3) along the [hkl] direction. The relation to the canonical coordinates can be given by a matrix $T = (e_1, e_2, e_3)^{-1}$. The biaxial Lagrange strain tensor $\eta_\parallel$ in this coordinate system [7] is

$$\eta_\parallel = \begin{bmatrix} \xi & 0 & 0 \\ 0 & \xi & 0 \\ 0 & 0 & -\kappa\xi \end{bmatrix}, \tag{4}$$

where ξ is a nonzero strain component, κ is the biaxial Poissons ratio. The strain tensor $\eta_\parallel$ can be inserted into the expression for the free energy (Eq. (3)) after transforming $\eta_\parallel$ from the coordinate system of the deformation to the canonical coordinate system of the crystal.

This is advantageous as it allows using the well-known structure-specific expressions of the free energy in canonical coordinates. The matrix T transforms the strain tensor $\eta_\parallel$, expressed in terms of $\{e_1, e_2, e_3\}$ to the corresponding strain tensor η in canonical coordinates $\{e_x, e_y, e_z\}$. This yields the free energy

$$F(\eta) = F(T\eta_\parallel T^T). \tag{5}$$

Together with the structure-specific free energy and the values of the elastic constants, Eq. (5) allows us to calculate the elastic response upon biaxial strain in arbitrary planes by determining the minimum of the elastic energy with respect to the biaxial Poisson ratio:

$$\frac{\partial}{\partial \kappa} F(\eta) = 0. \tag{6}$$

Hence, whenever the terms Poissons ratio or biaxial Poissons ratio are used, they actually refer to the engineering Poissons ratio which is represented by engineering strain.

$$\varepsilon_\parallel = \eta_\parallel - \frac{1}{2}\eta_\parallel \cdot \eta_\parallel \tag{7}$$

The engineering biaxial Poissons ratio is expressed as follow [10]:

$$v \equiv -\frac{\varepsilon_\perp}{\varepsilon_\parallel} = \frac{\kappa^2 \cdot \xi + 2\kappa}{2 - \xi}. \tag{8}$$

With this scheme Marcus et al. derived the elastic energy of cubic systems upon biaxial strain analytically for low-index planes and numerically for several high-index planes [11]. Without loss of generality, an orthonormal deformation coordinate system that allows easy derivation a general transformation matrix T, similar to that used by Lee [12,13], can be chosen:

$$\begin{aligned} e_1 &= e_2 \times e_3, \\ e_2 &= \frac{1}{\sqrt{h^2l^2 + k^2l^2 + 4h^2k^2}} \cdot \begin{bmatrix} kl \\ hl \\ -2hk \end{bmatrix}, \\ e_3 &= \frac{1}{\sqrt{h^2 + k^2 + l^2}} \cdot \begin{bmatrix} h \\ k \\ l \end{bmatrix}. \end{aligned} \tag{9}$$

This defines the transformation matrix T, which allows us to transform the strain tensor from the coordinate system of the deformation to canonical coordinates

$$\eta = -\frac{\xi}{h^2 + k^2 + l^2} \begin{bmatrix} h^2\kappa - k^2 - l^2 & kh(\kappa+1) & hl(\kappa+1) \\ hk(\kappa+1) & -h^2 + k^2\kappa - l^2 & kl(\kappa+1) \\ hl(\kappa+1) & kl(\kappa+1) & -h^2 - k^2 + l^2\kappa \end{bmatrix}. \tag{10}$$

Note that the cubic symmetry of the crystal lattice enters the transformation matrix in the definition of the orthonormal deformation coordinate system in Eq. (9). In this way, the canonic representation of the strain tensor as given in Eq. (10) holds only for materials with cubic symmetry.

In the case of the cubic system, the elastic energy and the Poisson's ratio for the (hkl) plane can be derived analytically. With the elastic energy of Eq. (3) and the canonic strain tensor of Eq. (10), the elastic response of a system with cubic symmetry can be obtained by minimizing the elastic energy with respect to the biaxial Poisson's ratio κ according to Eq. (6). The resulting Poisson ratio and elastic energy upon biaxial strain in the (hkl) plane depend only on the elastic constants and the orientation,

$$\begin{aligned} \kappa_{(hkl)} = {} & [2mC_{12} + 2n(C_{11} + C_{12} - 2C_{44})]B \\ & + \frac{p^2}{2}B^3 \left\{ \begin{array}{l} [q - rp - m(m-n)](C_{11} + 2C_{12})^2 \\ +4[(m-n)C_{12} - 2nC_{44}]^2 \end{array} \right\} C_{111}\xi \\ & + \frac{p^2}{2}B^3 \left\{ \begin{array}{l} (6n^2 - 5mn + 2m^2 - 9rp)(C_{11} + 2C_{12})^2 \\ -8[(m-n)(C_{12} + 2C_{11}) + 6C_{44}n][(m-n)C_{12} - 2C_{44}n] \end{array} \right\} C_{112}\xi \\ & + p^2B^3 \left\{ \begin{array}{l} [(m-n)C_{11} + 4nC_{44}]^2 + (rp - s)C_{11}^2 \\ +4(3rp - n^2)(C_{11} + C_{12})C_{12} \end{array} \right\} C_{123}\xi \\ & + 2p^2B^3 \left\{ \begin{array}{l} (9rp - 2mn)(C_{11} + 2C_{12})^2 + 8(m-n)nC_{12}^2 \\ -4(2rp + s - mn)C_{11}C_{12} - 8n^2(C_{11} + 2C_{12})C_{44} \end{array} \right\} C_{144}\xi \\ & + 2p^2B^3 \left\{ \begin{array}{l} (3rp - mn + 6s)C_{11} \\ +2(np^2 - 9pr + 2mn)C_{12} - 16n^2C_{44} \end{array} \right\} (C_{11} + 2C_{12})C_{155}\xi \\ & + 24p^3B^3r(C_{11} + 2C_{12})^2C_{456}\xi, \end{aligned} \tag{11}$$

where,

$$\begin{aligned} m &= h^4 + k^4 + l^4 \\ n &= h^2k^2 + h^2l^2 + l^2k^2 \\ p &= h^2 + k^2 + l^2 \\ q &= h^8 + k^8 + l^8 \\ r &= h^2k^2l^2 \\ s &= h^4k^4 + h^4l^4 + k^4l^4 \\ B &= \frac{1}{mC_{11} + 2n(C_{12} + 2C_{44})} \end{aligned}$$

We have chosen $\kappa > 0$ for a normal solid. The solution with a positive square root corresponds to a negative κ so it is discarded in Eq. (11). The analytical expressions above provides an efficient