Available online at www.sciencedirect.com
SCIENCE DIRECT
Solid State Communications 139 (2006) 87–91
solid state communications
www.elsevier.com/locate/ssc

General compliance transformation relation and applications for anisotropic hexagonal metals

Jian-Min Zhang[a,*], Yan Zhang[a], Ke-Wei Xu[b], Vincent Ji[c]

[a] College of Physics and Information Technology, Shaanxi Normal University, Xian 710062, Shaanxi, PR China
[b] State Key Laboratory for Mechanical Behavior of Materials, Xian Jiaotong University, Xian 710049, Shaanxi, PR China
[c] LIM UMR 8006 ENSAM, 151 bd. de l'Hôpital, 75013 Paris, France

Received 17 May 2006; accepted 21 May 2006 by A.H. MacDonald
Available online 9 June 2006

Abstract

In anisotropic crystals, the compliance (s_{ij}) and the stiffness (c_{ij}) matrices are usually specified in the orthogonal coordinate systems (X_1, Y_1, Z_1), which do not coincide with the crystal axes (X, Y, Z) used commonly, excepting cubic and orthorhombic crystal systems, and must be transformed to an arbitrary orthogonal coordinate system chosen to be convenient for the question. Such a transformation has been done in this paper for hexagonal crystals and a general compliance transformation relation is given. Accordingly, the useful expressions of the Young's modulus $E(hkl)$, Poisson's ratio $\upsilon(hkl)$ and X-ray elastic constants (XREC) $s_1(hkl) = -\frac{\upsilon(hkl)}{E(hkl)}$ and $\frac{1}{2}s_2(hkl) = \frac{1+\upsilon(hkl)}{E(hkl)}$ are also given in terms of the Miller indices of the lattice plane (hkl) in the crystal axes (X, Y, Z) used commonly.

PACS: 62.20.Dc; 62.20.-x; 73.61.At; 68.60.-p

Keywords: A. Metal; A. Thinfilms; D. Mechanical properties; E. X-ray and X-ray spectroscopies

1. Introduction

Metal films have been used extensively in decorative, protective, electronic, magnetic and optical devices and systems. These films usually have strong textures and so anisotropic elasticity [1,2]. The anisotropic elasticity can result in directionally dependent stress and strain energy [3–5], abnormal grain growth and texture transformation in thin metal films [6–10]. In the X-ray diffraction method for determining residual or applied stresses in a polycrystalline specimen, only those grains properly oriented to diffract at each tilt contribute to the diffraction profile. This selectivity implies that the X-ray elastic constants (XREC) $s_1(hkl) = -\frac{\upsilon(hkl)}{E(hkl)}$ and $\frac{1}{2}s_2(hkl) = \frac{1+\upsilon(hkl)}{E(hkl)}$ connecting the lattice strain $\varepsilon = \frac{d(hkl)-d_0(hkl)}{d_0(hkl)}$ to the stresses will vary with the particular set of planes (hkl) chosen for measurement [11]. In bulk materials, isotropic behavior is obtained when the individual crystallites are oriented throughout space with equal directional probability. The resulting macroscopic properties are usually calculated by considering the directionally dependent values averaged over all orientations in space [12].

In anisotropic crystals, however, the elastic compliance constant (in brief, the compliance) (s_{ij}) and/or the elastic stiffness constant (in brief, the stiffness) (c_{ij}) matrices are usually specified in the orthogonal coordinate systems (X_1, Y_1, Z_1), which do not coincide with the crystal axes (X, Y, Z) used commonly, excepting cubic and orthorhombic crystal systems, and must be transformed to arbitrary orthogonal coordinate systems which are chosen to be convenient for the question. Such a transformation has been done in this paper for hexagonal crystals and a general transformation relation is given for compliance from orthogonal coordinate systems (X_1, Y_1, Z_1) to another arbitrary orthogonal system. Emphatic analysis is taken for transformation to laboratory coordinate systems (X_2, Y_2, Z_2) in which the X-ray diffraction is sampled for example and 13 nonzero components s'_{ij} are derived to be dependent only on the polar angle ψ of the normal direction of the plane (hkl) due to the crystallographic Z-axis having the highest six-fold rotation

* Corresponding author. Tel.: +86 29 85308456.
E-mail address: jianm_zhang@yahoo.com (J.-M. Zhang).

0038-1098/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2006.05.026

$$(a_{rt}) = \begin{pmatrix} \dfrac{hL}{\sqrt{h^2+K^2}\sqrt{h^2+K^2+L^2}} & \dfrac{KL}{\sqrt{h^2+K^2}\sqrt{h^2+K^2+L^2}} & -\dfrac{\sqrt{h^2+K^2}}{\sqrt{h^2+K^2+L^2}} \\ -\dfrac{K}{\sqrt{h^2+K^2}} & \dfrac{h}{\sqrt{h^2+K^2}} & 0 \\ \dfrac{h}{\sqrt{h^2+K^2+L^2}} & \dfrac{K}{\sqrt{h^2+K^2+L^2}} & \dfrac{L}{\sqrt{h^2+K^2+L^2}} \end{pmatrix}$$

Box 1.

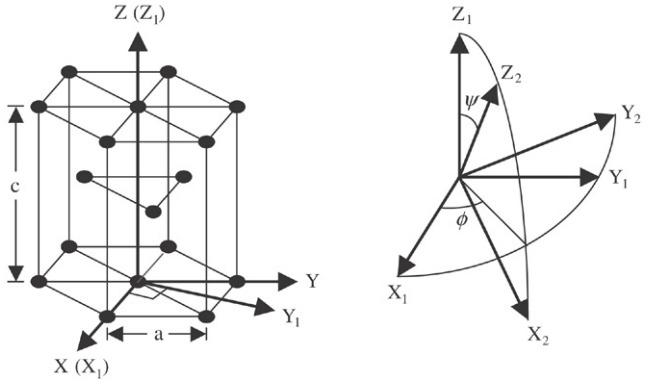

Fig. 1. Coordinate systems of crystal axes (X, Y, Z), orthogonal coordinate systems (X_1, Y_1, Z_1) and laboratory coordinate systems (X_2, Y_2, Z_2).

symmetry. Accordingly, the useful expressions of the Young's modulus $E(hkl)$, Poisson's ratio $\upsilon(hkl)$ and XREC $s_1(hkl) = -\frac{\upsilon(hkl)}{E(hkl)}$ and $\frac{1}{2}s_2(hkl) = \frac{1+\upsilon(hkl)}{E(hkl)}$ are also given in terms of the Miller indices of the lattice plane (hkl) in the crystal axes (X, Y, Z) used commonly.

2. General compliance transformation relation

For writing out tensors or matrices which represent the compliance or stiffness of hexagonal systems, as shown in Fig. 1 (left), we use orthogonal coordinate systems (X_1, Y_1, Z_1) instead of crystal axes (X, Y, Z) used commonly. The axis Y_1 is in the X, Y plane at 90° and 30° to X and Y respectively. Another laboratory coordinate systems (X_2, Y_2, Z_2) shown in Fig. 1 (right), in which diffraction is sampled for example, is defined such that Z_2 is in the normal direction of the lattice plane (hkl) (noted with Miller indices in crystal axes (X, Y, Z)) whose lattice plane distance $d(hkl)$ is measured by X-ray diffraction.

As shown in Fig. 1 (right), the transformation matrix (a_{rt}) from the orthogonal coordinate systems (X_1, Y_1, Z_1) to laboratory coordinate systems (X_2, Y_2, Z_2) can be obtained through the following two rotations, one by an angle ϕ about the Z_1 axis, and the other by ψ about the Y_2 axis

$$(a_{rt}) = \begin{pmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\psi\cos\phi & \cos\psi\sin\phi & -\sin\psi \\ -\sin\phi & \cos\phi & 0 \\ \sin\psi\cos\phi & \sin\psi\sin\phi & \cos\psi \end{pmatrix}. \quad (1)$$

For the (hkl)-plane, the transformation matrix (a_{rt}) can be expressed as the equation given in Box 1; where $K = \frac{h+2k}{\sqrt{3}}$, $L = \frac{a}{c}l$, a and c are lattice constants of the hexagonal metal as shown in Fig. 1 (left).

In laboratory coordinate systems (X_2, Y_2, Z_2), the basic equation relating stress σ_{kl} to strain ε_{ij} is the generalized form of Hooke's Law [13]

$$\varepsilon_{ij} = s'_{ijkl}\sigma_{kl} \quad (i, j, k, l = 1, 2, 3) \quad (2)$$

where s'_{ijkl} are the compliances in laboratory coordinate systems (X_2, Y_2, Z_2) and can be transformed from the compliances s_{mnop} in orthogonal coordinate systems (X_1, Y_1, Z_1)

$$s'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}s_{mnop}. \quad (3)$$

It is worth noting that this equation typifies 81 equations each with 81 terms on the right-hand side, making a total of $81 \times 81 = 6561$ terms in all.

The symmetry of s_{mnop} (or s'_{ijkl}) in the first two and the last two suffixes, that is $s_{mnop} = s_{nmop} = s_{mnpo}$, makes only 36 of the 81 components s_{mnop} (or s'_{ijkl}) independent and it is possible to use the matrix notation. The first two suffixes are abbreviated into a single one running from 1 to 6, and the last two can be abbreviated in the same way, according to the following scheme

Tensor notation:	11	22	33	23, 32	31, 13	12, 21
Matrix notation:	1	2	3	4	5	6.

At the same time factors of 2 and 4 are introduced as follows

$s_{mnop} = s_{ij}$ when i and j are 1, 2 or 3
$2s_{mnop} = s_{ij}$ when either i or j are 4, 5 or 6
$4s_{mnop} = s_{ij}$ when both i and j are 4, 5 or 6.

The components of the stress and the strain tensors are also written in a single suffix running from 1 to 6

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix} \quad (4)$$

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \varepsilon_1 & \frac{1}{2}\varepsilon_6 & \frac{1}{2}\varepsilon_5 \\ \frac{1}{2}\varepsilon_6 & \varepsilon_2 & \frac{1}{2}\varepsilon_4 \\ \frac{1}{2}\varepsilon_5 & \frac{1}{2}\varepsilon_4 & \varepsilon_3 \end{bmatrix}. \quad (5)$$