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THE USE OF CLASSICAL BEAM THEORY FOR MICRO-BEAMS COMPOSED OF POLYCRYSTALS

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Abstract-Micro-beams, where the transverse dimension of the beam is of the order of microns, are sometimes composed of polycrystals where the average crystal dimension is of the same order as the transverse beam dimension. We show in this paper that classical beam theory can be used to describe the behavior of these micro-beams if the crystals have cubic symmetry. If the symmetry is of lower-order than cubic then the behavior of the micro-beam depends on the internal arrangement of the crystals within the beam. We show, however, that for a particular class of tetragonal crystals (six independent elastic comtants) the classical beam equation may still be used if a local average is introduced. © 1998 Elsevier Science Ltd. All rights reserved.

1. STATEMENT OF PROBLEM

For a homogeneous beam it is shown in any standard textbook on beam theory (Popov *et al.*, 1978) that the governing equation for the displacement $y(x)$ is

$$
d^2/dx^2[(EI) d^2y(x)/dx^2] = q(x).
$$
 (1)

Here the quantity $E I d^2 y(x) / dx^2$ is equal to the bending moment $M(x)$, $q(x)$ is a transverse distributed force, E is Young's modulus and I is the moment of inertia. Referring to Fig. 1 we see that for $\theta = dy/dx \ll 1$ the curvature R is given by the relation $1/R = d\theta/dx = d^2y/dx^2$.

The basic assumption is that the strain e_{xx} is linear over the transverse beam dimension in the y-direction. It has the form

$$
e_{xx} = -y/R. \tag{2}
$$

Assuming next the basic stress-strain relation for an isotropic linear elastic material we find that the stress component τ_{xx} is equal to

$$
\tau_{xx} = E e_{xx} = -E y / R. \tag{3}
$$

We then find the above expression for $M(x)$. In addition, it is assumed that the stress components τ_{yy} and τ_{zz} are zero throughout the beam and the shear components may be neglected.

For a macroscopic beam composed of a polycrystal it is usually assumed that the characteristic size of the smallest transverse dimension of the beam, L_T , satisfies the condition $L_T \gg d$ where *d* is a characteristic grain dimension. The length of the beam, *L*, of course, is much larger than L_T . In this case, on the length scales of interest the beam may be considered to be homogeneous and isotropic. In this paper, however, we are interested in micro-beams where L_T is of order of *d*. The condition $L \gg L_T$ remains true and we

Fig. I. Beam deformation under bending.

continue to assume that the beam is statistically homogeneous in the direction of the beam axis.

When L_T is of order *d* the beam may no longer be considered to be homogeneous in the transverse *y-z* plane. In this paper we show that in spite ofthis transverse inhomogeneity, the standard beam equation given in eqn (1) may still be used if the individual crystals have cubic symmetry. However, if the symmetry is of a lower-order we expect the beam equation to be dependent on the microstructure of the polycrystal within the beam. In Section 3 we discuss the special case of tetragonal crystals where classical beam theory may still be approximately correct if a local average is used. For the case we consider there are six independent elastic constants, but no coupling between the diagonal strain elements and the off-diagonal strain elements in the strain energy function.

2. MICRO-BEAM COMPOSED OF A POLYCRYSTAL OF CUBIC CRYSTALS

2.1. Stress-strain relations along the principal axesfor a crystal with cubic symmetry

When a material is homogeneous and isotropic two constants λ , Lame's constant and μ , the shear modulus are sufficient to define the strain energy function *W*. Here (Love, 1944)

$$
W = (1/2)[(\lambda + 2\mu)[e_{xx} + e_{yy} + e_{zz}]^2 + \mu[e_{xy}^2 + e_{xz}^2 + e_{yz}^2 - 4e_{xx}e_{yy} - 4e_{xx}e_{zz} - 4e_{yy}e_{zz}]].
$$
 (4)

For cubic symmetry there are three independent constants c_{11} , c_{12} and c_{44} . Here

$$
W = (1/2)c_{11}[e_{xx}^2 + e_{yy}^2 + e_{zz}^2] + C_{12}[e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz}] + (1/2)c_{44}[e_{xy}^2 + e_{xz}^2 + e_{yz}^2].
$$
 (5)

From eqn (5) we find the following stress-strain relations along the principal axes

$$
\tau_{xx} = c_{11}e_{xx} + (1/2)c_{12}[e_{yy} + e_{zz}]
$$

\n
$$
\tau_{yy} = c_{11}e_{yy} + (1/2)c_{12}[e_{xx} + e_{zz}]
$$

\n
$$
\tau_{zz} = c_{11}e_{zz} + (1/2)c_{12}[e_{xx} + e_{yy}]
$$

\n
$$
\tau_{xy} = c_{44}e_{xy}
$$

\n
$$
\tau_{xz} = c_{44}e_{xz}
$$

\n
$$
\tau_{yz} = c_{44}e_{yz}.
$$
\n(6)

2.2. Single crystal alignment within the micro-beam

Let us suppose that a single cubic crystal within the micro-beam is aligned so that the principal axes coincide with the beam axes. In this case if the beam is under pure bending we satisfy eqns (2) and (3) and the conditions $\tau_{yy} = \tau_{zz} = 0$. This yields the expected result

$$
\tau_{xx} = [c_{11} - (1/2)c_{12}^2/(c_{11} + (1/2)c_{12})]e_{xx},
$$

\n
$$
\tau_{xx} = E e_{xx}.
$$
\n(7)

Next let us assume that the principal crystal axes are rotated with respect to the beam axes. The direction cosines are given by α_{ik} , $(i = 1$ is the x-axis, $i = 2$ is the y-axis and $i = 3$ is the z-axis of the principal axes while the *k* index represents the beam axes). We then have

$$
\tau'_{ij} = \alpha_{ik} \alpha_{jm} \tau_{km} \tag{8}
$$

where τ'_{ij} gives the stress components along the principal axes. Writing eqn (6) in terms of the principal axes then gives

$$
\tau'_{xx} = c_{11}e'_{xx} + (1/2)c_{12}[e'_{yy} + e'_{zz}]
$$

\n
$$
\tau'_{yy} = c_{11}e'_{yy} + (1/2)c_{12}[e'_{xx} + e'_{zz}]
$$

\n
$$
\tau'_{zz} = c_{11}e'_{zz} + (1/2)c_{12}[e'_{xx} + e'_{yy}]
$$

\n
$$
\tau'_{xy} = c_{44}e'_{xy}
$$

\n
$$
\tau'_{xz} = c_{44}e'_{xz}
$$

\n
$$
\tau'_{yz} = c_{44}e'_{yz}.
$$
\n(9)

In order to determine the stress-strain relations along the beam axes we substitute τ'_{ij} from eqn (8) in the left-hand side of eqn (9) and a similar expression for e'_{ii} on the righthand side. After manipulation and use of some identities governing sums of the direction cosines we find the same result as that given in eqn (7). That is, independent of the orientation of the principal axes of a cubic crystal [see eqn (5)] the stress-strain relation along the beam axis is the same as that given for an isotropic material. The above result follows from the fact that the constant c_{44} does not enter the calculation and the strains e_{xx} , e_{yy} and e_{zz} all appear in the same manner in the strain energy function. As in the isotropic beam analysis we have assumed here that under pure bending all stress components except τ_{xx} may be neglected in the beam coordinate system.

2.3. Beam equation

If assume that we have a beam made of a single crystal orientated along the beam axis, we may conceptually construct a beam of polycrystals by successively replacing portions of the crystal with crystals of different orientations, until the beam is a polycrystal. Prior to the first replacement the stress field has only a τ_{xx} stress component. As we see from the analysis in Section 2.2 the stress-strain state within the added crystal is the same as it was prior to its addition. Adding successive crystals does not change the stress-strain state and we conclude that the stress-strain state in the beam is exactly the same as it would be for a beam composed of a homcgeneous isotropic material. It thus follows that eqn (I) is the equation governing the displacement $y(x)$ of the micro-beam.

3. MICRO-BEAM COMPOSED OF A POLYCRYSTAL OF NON-CUBIC CRYSTALS

3.1. Stress-strain relation for a tetragonal polycrystal

In this section we restrict our attention to non-cubic crystals where the strain energy function is of the form

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$$
W = (1/2)c_{11}e_{xx}^2 + c_{12}e_{xx}e_{yy} + c_{13}e_{xx}e_{zz} + (1/2)c_{11}e_{yy}^2 + c_{13}e_{yy}e_{zz} + (1/2)c_{33}e_{zz}^2 + (1/2)c_{44}e_{xz}^2 + (1/2)c_{44}e_{xz}^2 + (1/2)c_{66}e_{xy}^2.
$$
 (10)

Here there are six independent elastic constants. The stress-strain relations are now

$$
\tau'_{xx} = c_{11}e'_{xx} + c_{12}e'_{yy} + c_{13}e'_{zz}
$$

\n
$$
\tau'_{yy} = c_{12}e'_{xx} + c_{11}e'_{yy} + c_{13}e'_{zz}
$$

\n
$$
\tau'_{zz} = c_{13}e'_{xx} + c_{13}e'_{yy} + c_{33}e'_{zz}.
$$
\n(11)

The primes indicate principal axes rotated with respect to the beam axes.

For a particular grain within the polycrystal we substitute eqn (8) into the left-hand side of eqn (11) and a similar expression for the strains into the right-hand side of eqn (11) . Setting $\tau_{yy} = \tau_{zz} = 0$ in the resultant equation we find a relationship of the form

$$
\tau_{xx} = F(c_{11}, c_{12}, c_{13}, c_{33}, \alpha_{ij})e_{xx}
$$
\n(12)

for the stress-strain relation along the beam axis.

Unlike the isotropic or cubic crystal case the proportionality constant between τ_{xx} and e_{xx} is not Young's modulus, but rather a complicated function of four elastic constants and the orientation of the crystal grain relative to the beam axes. Thus, at any cross-section of the beam the stress-strain relation is a function of the transverse coordinates *y* and z. That is, eqn (3) now becomes

$$
\tau_{xx} = -F(y, z, x)(y/R). \tag{13}
$$

The bending moment, M, is found from eqn (13) by integrating the quantity $y_{x_{xx}}$ over the beam cross-section. In eqn (1) we have the constant *EI* where

$$
I = \int_{A} y^2 dA \tag{14}
$$

and *A* is the transverse (yz) cross-section of the beam. Here *EI* is independent of x. For the strain-energy function given in eqn (10) we find for the bending moment *M* the expression

$$
M = [EI]^*(x) d^2 y/dx^2 \tag{15}
$$

where the effective constant $[EI]^*(x)$ at each beam position x, is given by the expression

$$
[EI^*(x) = \int_A F(x, y, z)y^2 dA.
$$
 (16)

The function $\left[ET\right]^{*}(x)$ is a very rapidly varying function on the scale of the beam length *L.* Since the variation depends on the crystal orientation in each transverse section we expect the characteristic scale of variation of $[EI]^*(x)$ in the x-direction to be at most of the order of several grain diameters (Beran *et ai.,* 1996). This would correspond to the characteristic correlation distance over which adjacent grains are correlated in the xdirection.

This rapid variation of $[EI^*(x)]$ is of importance if any measurements are made on the scale of the grain size. If, however, we are only interested in the micro-beam deflection locally averaged over many grain diameters in the x-direction then the function $[EI]^*(x)$ may be replaced by an effective constant $[E]_A$ which is independent of x. We remember that we have assumed that the beam is statistically homogeneous in the x -direction.

Equation (1) is now given by

$$
d^2/dx^2[[EI]_A d^2y(x)/dx^2] = q(x).
$$
 (17)

3.2. Determination of the effective constant [EI].

The constant $[EA]_A$ is quite difficult to determine since it depends on the orientation of the crystals and the correlation between the orientations of adjacent crystals. However, recently Steinberg and McCoy (1996, 1997) have shown that when $[EI^*(x)$ varies rapidly on a scale small compared to L then $[EI]_A$ is given by the following expression:

$$
[EI]_A = 1 / \left[(1/\Delta L) \int_0^{\Delta L} (1/[EI]^*(x)) dx \right],
$$
 (18)

where ΔL is a distance that is large compared to a characteristic grain size, d, but satisfies the condition $\Delta L \ll L$. We note that $[EI]_A$ is not the average of $[EI]^*(x)$, but rather the inverse of the harmonic average.

For $\Delta L \gg d$ the effective constant $[EI]_A$ is also given by the statistical average

$$
[EI]_A = 1/[\overline{1/[EI]^*(x)}],\tag{19}
$$

where the overbar indicates an ensemble average. Since the statistics of the polycrystal are assumed to be homogeneous in the x-direction, the right-hand side of eqn (10) is independent of x. The evaluation of eqn (10) may be done over any beam cross-section and does not require a knowledge of the variation of $[EI]^*(x)$ with x.

The determination of $[EI]_A$ using eqn (19) is a very tedious process that requires an ensemble of beams manufactured in an identical manner. It would be necessary to take a sample micro-beam or many sample micro-beams and analyze a large number of crosssections. In each cross-secticn the orientation of the individual crystals would have to be found as a function of y and z. Once this is done $[E]$ ^{*} can be calculated. Finally $[E]_A$ would be determined from eqn (19) using many sample cross-sections.

A far simpler procedure, and one that is nondestructive, would be to use eqn (17). The beam would be loaded in a simple manner, the displacement $y(x)$ measured at a particular point and $[EI]_A$ found. For better accuracy, $y(x)$ could be measured at several points and a best fit for $[E_1]_A$ determined. The micro-beam could then be used in a desired application with $[EI]_A$ a known quantity.

4. SUMMARY

In this paper it was shown that the equation governing homogeneous beams [eqn (1)] could be used to determine the displacement for micro-beams composed of polycrystals where the individual crystals have cubic symmetry [eqn (5)]. It was further shown that for a class of crystals with lower symmetry [eqn (10)] the governing equation is given by eqn (17) where $[EI]_A$ is defined by eqns (18) and (16).

The constant $\left[ET_A\right]$ is related to the six elastic constants in eqn (10) in a very complex way. It may be determined by an analysis of the micro-beam micro-structure. However, a more direct way would be to load the micro-beam, measure the displacement at one or several points and use eqn (17) to find the relationship between the measured displacement and the constant $[EI]_A$.

We see from the analysis given in this paper, that the effective constant in the beam equation governing a micro-beam composed of a polycrystal is very dependent upon the symmetry properties of the individual crystals. For cubic crystals the equation is the same as for a homogeneous isotropic beam, but for crystals of lower symmetry the constant is dependent upon the way the individual crystals are placed within the beam. Unfortunately, there is no simple relationship between the elastic constants of the individual crystals and the effective constant. Moreover, if displacement measurements are made on the scale of the characteristic crystal size (rather than, as usual, smoothed over a distance large compared to

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this size) then the effective constant is a rapidly varying function of distance in the beam direction.

Finally, we note that we have used a beam theory that neglects the effects of transverse shear. If the shear effects are important then the conclusion that a micro-beam composed of cubic crystals behaves in the same manner as a homogeneous and isotropic beam is not necessarily valid. Before undertaking a more general analysis, however, it is felt that some experimental data must be available on the behavior of micro-beams under controlled conditions.

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