Effective elastic constants of superlattices

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The effective elastic constants of a superlattice composed of layers of orthorhombic symmetry (with principal axes along the superlattice axis) are derived. These results generalize previous determinations for elastically isotropic layers (S. M. Rytov, Akust. Zh. **2**, 71 (1956) [Sov. Phys. Acoust. **2**, 68 (1956)]), but a completely different approach is used.

The derivation of effective elastic constants that describe the properties of a laminated medium in terms of the elastic properties of its constituent layers, is a long-standing problem dating back to at least 1937. Bruggeman[1] first obtained expressions for a superlattice composed of isotropic layers in the long-wavelength regime; his results were later generalized for shorter wavelengths by Rytov[2] using a method based on superposition of waves. Very recent calculations by Nizzoli[3] using this same technique were successful in determining C_{33}, C_{44}, C_{66}, and $C_{11}-C_{12}$ for a superlattice composed of cubic materials. In this case, however, there are six independent constants which should be determined.

Given the current interest in superlattices, many of whose elastic properties are currently being investigated, and since in many cases the properties of the individual layers are far from isotropic, it is convenient to derive effective constants for these more general cases. The general treatment for arbitrary wavelengths described in Ref. 2 is, however, difficult to perform. Here an alternative approach is presented which is valid only for excitation wavelengths longer than the modulation wavelengths.

We consider a superlattice with its axis along the z direction, x and y lying in the plane of the layers. Each layer is assumed to have orthorhombic symmetry with one of its principal axes (z for simplicity) along the superlattice axis. In what follows, σ_{ij}, μ_{ij}, and C_{ij} represent the components of the stress, strain, and elastic constant tensors. Superscripts 1 and 2 refer to the two media and no superscript indicates that it refers to the effective property of the superlattice. If the thicknesses of each layer are d_1 and d_2, respectively, the fraction of each material is defined as $f_j=d_j/(d_1+d_2)$.

Given the assumed symmetry of the layers it can be seen that the diagonal and off-diagonal components of σ and μ do not couple. From the symmetry of the problem it is easy to verify that the following equations must hold:

$$\sigma_{zz}=\sigma_{zz}^1=\sigma_{zz}^2 \ , \tag{1}$$

$$\sigma_{xx}=f_1\sigma_{xx}^1+f_2\sigma_{xx}^2 \ , \tag{2}$$

$$\sigma_{yy}=f_1\sigma_{yy}^1+f_2\sigma_{yy}^2 \ , \tag{3}$$

$$\mu_{zz}=f_1\mu_{zz}^1+f_2\mu_{zz}^2 \ , \tag{4}$$

$$\mu_{xx}=\mu_{xx}^1=\mu_{xx}^2 \ , \tag{5}$$

$$\mu_{yy}=\mu_{yy}^1=\mu_{yy}^2 \ . \tag{6}$$

We then consider the relationship which defines the effective elastic constants; as an example we start with

$$\sigma_{zz}=C_{33}\mu_{zz}+C_{13}\mu_{xx}+C_{23}\mu_{yy} \ . \tag{7}$$

The equivalent expression for medium 1 or 2 can be rewritten as

$$\frac{\sigma_{zz}^i}{C_{33}^i}=\mu_{zz}^i+\mu_{xx}^i\frac{C_{13}^i}{C_{33}^i}+\mu_{yy}^i\frac{C_{23}^i}{C_{33}^i} \ . \tag{8}$$

Adding Eq. (8) multiplied by f_i for $i=1,2$ and using Eqs. (1), (4), (5), and (6) we get

$$\sigma_{zz}\left[\frac{f_1}{C_{33}^1}+\frac{f_2}{C_{33}^2}\right]=\mu_{zz}+\left[\frac{f_1C_{13}^1}{C_{33}^1}+\frac{f_2C_{13}^2}{C_{33}^2}\right]\mu_{xx}+\left[f_1\frac{C_{23}^1}{C_{33}^1}+f_2\frac{C_{23}^2}{C_{33}^2}\right]\mu_{yy} \ . \tag{9}$$

A comparison of the coefficients of μ_{jj} in Eqs. (7) and (9) yields

$$C_{33}=[f_1/C_{33}^1+f_2/C_{33}^2]^{-1} \ , \tag{10}$$

$$C_{13}=\frac{f_1C_{13}^1C_{33}^2+f_2C_{13}^2C_{33}^1}{f_1C_{33}^2+f_2C_{33}^1} \ , \tag{11}$$

$$C_{23}=\frac{f_1C_{23}^1C_{33}^2+f_2C_{23}^2C_{33}^1}{f_1C_{33}^2+f_2C_{33}^1} \ . \tag{12}$$

Starting with the expression

$$\sigma_{xx}=C_{11}\mu_{xx}+C_{12}\mu_{yy}+C_{13}\mu_{zz} \tag{13}$$

or an equivalent relationship for σ_{yy} it is straightforward although somewhat more complicated to obtain

$$C_{11}=f_1C_{11}^1+f_2C_{11}^2+f_1\frac{C_{13}^1}{C_{33}^1}(C_{13}-C_{13}^1)+f_2\frac{C_{13}^2}{C_{33}^2}(C_{13}-C_{13}^2). \tag{14}$$

Or using Eq. (11) this can be written as

$$C_1=f_1C_{11}^1+f_2C_{11}^2-f_1\frac{(C_{13}^1)^2}{C_{33}^1}-f_2\frac{(C_{13}^2)^2}{C_{33}^2}+\left[\frac{f_1C_{13}^1C_{33}^2+f_2C_{13}^2C_{33}^1}{C_{33}^1C_{33}^2}\right]\left[\frac{f_1C_{13}^1C_{33}^2+f_2C_{13}^2C_{33}^1}{f_1C_{33}^2+f_2C_{33}^1}\right] . \tag{15}$$

One also obtains

$$C_{12}=f_1C_{12}^1+f_2C_{12}^2+f_1\frac{C_{13}^1}{C_{33}^1}(C_{23}-C_{23}^1)+f_2\frac{C_{13}^2}{C_{33}^2}(C_{23}-C_{23}^2) \tag{16}$$

or an equivalent expression (they can be shown to be equal)

$$C_{12}=f_1C_{12}^1+f_2C_{12}^2+f_1\frac{C_{23}^1}{C_{33}^1}(C_{13}-C_{13}^1)$$
$$+f_2\frac{C_{23}^2}{C_{33}^2}(C_{13}-C_{13}^2)\ . \tag{17}$$

C_{13} and C_{23} can be eliminated from Eqs. (16) and (17) using Eqs. (11) and (12). In a similar fashion we obtain

$$C_{22}=f_1C_{22}^1+f_2C_{22}^2+f_1\frac{C_{23}^1}{C_{33}^1}(C_{23}-C_{23}^1)$$
$$+f_2\frac{C_{23}^2}{C_{33}^2}(C_{23}-C_{23}^2)\ . \tag{18}$$

For the shear components, one can write an expression equivalent to Eqs. (1)–(6), i.e.,

$$\sigma_{zy}=\sigma_{zy}^1=\sigma_{zy}^2\ , \tag{19}$$

$$\sigma_{zx}=\sigma_{zx}^1=\sigma_{zx}^2\ , \tag{20}$$

$$\sigma_{xy}=f_1\sigma_{xy}^1+f_2\sigma_{xy}^2\ , \tag{21}$$

$$\mu_{zy}=f_1\mu_{zy}^1+f_2\mu_{zy}^2\ , \tag{22}$$

$$\mu_{zx}=f_1\mu_{zx}^1+f_2\mu_{zx}^2\ , \tag{23}$$

$$\mu_{xy}=\mu_{xy}^1=\mu_{xy}^2\ . \tag{24}$$

In the same manner as described above it is easy to show that

$$C_{44}=[f_1/C_{44}^1+f_2/C_{44}^2]^{-1}\ , \tag{25}$$

$$C_{55}=[f_1/C_{55}^1+f_2/C_{55}^2]^{-1}\ , \tag{26}$$

$$C_{66}=f_1C_{66}^1+f_2C_{66}^2\ . \tag{27}$$

Equations (10)–(12), (15), (16), (18), and (25)–(27) represent the nine independent elastic constants of the superlattice that also has orthorhombic symmetry. All expressions can be shown to have the correct limit when dealing with isotropic layers[2] or with the four known expressions for layers of cubic symmetry.[3]

If the symmetry of the layers is reduced still further Eqs. (1)–(6) and (19)–(24) are no longer independent and cross terms coupling the diagonal and off-diagonal terms appear in Eqs. (7) and (13). In this case there seems to be no simple solution for the effective constants; for particular cases, however, it may be possible to solve the more general equations by iteration or numerically. If this is indeed true the method presented here may prove to be a convenient starting point for superlattices composed of layers of arbitrary symmetry.

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