PHYSICAL REVIEW B VOLUME 33, NUMBER 8 15 APRIL 1986

Effective elastic constants of superlattices of any symmetry

M. Grimsditch
Materials Science and Technology Division, Argonne National Laboratory, Argonne, Illinois 60439

F. Nizzoli
Dipartimento di Fisica, Università degli Studi di Modena, I-41100 Modena, Italy

(Received 25 November 1985)

We present a formalism which allows the evaluation of the effective elastic constants of a superlattice composed of layers of arbitrary symmetry.

In a recent article the effective elastic constants in the long wavelength limit of superlattices composed of layers of orthorhombic symmetry with a symmetry axis along the superlattice normal was presented.[1] The approach used there is more restrictive than that used in previous determinations[2–6] in as much as it can only be used in cases where the wavelength of the excitations are longer than the superlattice wavelength, but it does allow more general cases of symmetry to be treated. In Ref. 1 analytical solutions for the case of layers of orthorhombic symmetry were presented and it was stated that for layers of lower symmetry no analytical solutions were found.

Although it was stated in Ref. 1 that the approach used is valid for layers of any symmetry, the method used to solve the resulting equations is not immediately soluble by numerical techniques. Here we present a formalism which enables a numerical evaluation of the elastic constants of a superlattice in terms of the constants of its constituents on which there are no symmetry requirements. We stress that this generalization is more useful than might appear at first sight since it enables the frequently occurring case of layers of cubic symmetry that grow along (111) directions to be treated.

Since the notation used here is only slightly different from that used in Ref. 1, we review it very briefly: viz., C, σ, and μ are the elastic constant, stress, and strain tensors, respectively, in a coordinate system with the z axis along the superlattice normal. The layer materials are labeled 1 and 2 which are also used as subscripts to indicate a given layer. No subscript indicates that we are dealing with a property of the superlattice. The numbers f_1 and f_2 are the fractions of materials 1 and 2 in the superlattice.

The stress and strain of the superlattice can be expressed as a function of the stress and strain of the individual layers by [Eqs. (1)–(6) and (19)–(24) in Ref. 1],

$$\sigma=f_1\sigma_1+f_2\sigma_2\ , \tag{1}$$

$$\mu=f_1\mu_1+f_2\mu_2\ . \tag{2}$$

In each layer the constituent relations are

$$\sigma_i=C_i\mu_i,\quad i=1,2 \tag{3}$$

and the effective elastic constant matrix of the superlattice is defined by

$$\sigma=C\mu\ . \tag{4}$$

Combining Eqs. (1), (2), and (4) we have

$$f_1\sigma_1+f_2\sigma_2=C(f_1\mu_1+f_1\mu_2) \tag{5}$$

which, upon using Eq. (3), can be recast in the form

$$f_1(C_1-C)\mu_1+f_2(C_2-C)\mu_2=0\ . \tag{6}$$

(Note that the 0 matrix is a 3×3 matrix if the four-index notation for C is used and a 6×1 matrix if the two-index notation is used. Here for simplicity we shall use the two-index notation.) Equation (6) could be solved for C if the relationship

$$\mu_1=M\mu_2 \tag{7}$$

were known. Hence we now proceed to evaluate the matrix M. The boundary conditions at the interface between layers are

$$\sigma_1(iz)=\sigma_2(iz),\quad i=x,y,z \tag{8}$$

$$\mu_1(ij)=\mu_2(ij),\quad i,j\neq z \tag{9}$$

which can be written as

$$P_1\mu_1=P_2\mu_2 \tag{10}$$

where

$$P=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{11}$$

From Eqs. (7) and (10)

$$M=P_1^{-1}P_2\ , \tag{12}$$

which can always be evaluated at least numerically. Equations (6) and (12) yield

$$[f_1(C_1-C)M+f_2(C_2-C)]\mu_2=0\ . \tag{13}$$

Since this must hold true for an arbitrary strain μ_2

$$C(f_1M+f_2I)=f_1C_1M+f_2C_2\ , \tag{14}$$

where I is the identity 6×6 matrix. The final expression for the elastic constants of the superlattice is then

$$C=(f_1C_1M+f_2C_2)(f_1M+f_2I)^{-1}\ , \tag{15}$$

which, using M as given by Eqs. (11) and (12), can always be calculated numerically.

This work was supported by the U.S. Department of Energy (Division of Materials Sciences, Office of Basic Energy Sciences, Office of Energy Research), under Contract No. W-31-109-ENG-38 and a travel grant from the North Atlantic Treaty Organization (NATO).

[1]M. Grimsditch, Phys. Rev. B **31**, 6818 (1985).

[2]D. A. G. Bruggeman, Ann. Phys. (Leipzig) **29**, 160 (1937).

[3]S. M. Rytov, Akust. Zh. **2**, 71 (1956) [Sov. Phys.—Acoust. **2**, 68 (1956)].

[4]T. J. Delph, G. Herrmann, and R. K. Kaul, J. Appl. Mech. **45**, 343 (1978).

[5]J. Sapriel, B. Djafari-Rouhani, and L. Dobrzynski, Surf. Sci. **126**, 197 (1983).

[6]F. Nizzoli, in *Proceedings of the 17th International Conference on the Physics of Semiconductors,* edited by J. D. Chadi and W. A. Harrison (Springer-Verlag, New York, 1985), p. 1145.