Elastic constants of Mo/V superlattices

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Elastic moduli of Mo, V, and Mo_n/V_n superlattices with $n \leqslant 3$ are calculated in the full-potential linear muffin-tin orbital scheme. No modulation dependence is found for the bulk modulus of the superlattices. Comparisons are made with predictions from continuum models for elastic moduli of layered materials and surprising agreement is found between those and the calculated constants. In the context of elastic anomalies frequently observed for metal superlattices, an estimation employing the Hashin-Shtrikman bounds for composites gives that a softening of Young's modulus up to 30% would be obtained if the disorder at the interfaces were extreme. This suggests that the frequently observed elastic anomalies for small-modulation superlattices is intimately connected with the quality of the interfaces. [S0163-1829(97)01915-2]

I. INTRODUCTION

In the late 1970s to early 1980s, several experimental observations of greatly enhanced elastic moduli in metal superlattices were announced.[1–4] This phenomenon came to be known as the supermodulus effect. The existence of such effects in the investigated superlattices (Cu/Pd, Cu/Ni) was later questioned by Davis *et al.*[5] who examined their elastic properties with more accurate methods and found no great enhancements in the moduli. Nevertheless, elastic anomalies, in the sense of departure from expected average values, of the order of 30–50 % for small superlattice modulation wavelengths are frequently reported.[6–10]

Explanations for these effects have been given in terms of coherency strains,[11] electronic effects due to the folding of the Brillouin zone in the superlattice growth direction,[12] microstructural properties such as changes in the interlayer distances,[13] and effects of disordered interfaces.[14] It has been demonstrated, within specific models for the shape of the Fermi surface,[15] that the Brillouin-zone effects give no significant contributions to the elastic moduli. The same conclusion was drawn in a first-principles calculation of elastic properties of Au/Cr superlattices with respect to modulation wavelength.[16] Furthermore, it is found within continuum elasticity theory[17] that coherency strains in Cu/Ni superlattices only change the biaxial moduli by a few percent and thus also cannot account for the observed magnitudes of the elastic anomalies. It is questionable, however, if continuum theory can give reliable predictions in superlattices with small modulation wavelengths where the interface energetics have a prominent role.[18] Computer simulations employing embedded-atom-method (EAM) potentials[13,14,19] have found anomalies of the order of 50%, primarily connected with the influence of the interfaces—either structural disorder[14] or interface-driven distortions in the interlayer spacings.[13] Similar simulations[20] have also shown *no* anomalies. The situation is thus that, experimentally, elastic anomalies are a real effect in metal superlattices but no consensus exists about the driving mechanism behind them.

Recent developments of full-potential methods in electronic structure calculations of solids have opened up the way for reliable extractions of material elastic constants, in terms of absolute values with respect to experiments. An advantage of the full-potential methods is that they take nonspherical terms of the charge distribution into account, which is crucial for the treatment of anisotropic distortions of lattices. Current calculations of elastic properties of various solids with full-potential methods have been presented[21–24] that show good agreement with experimental results. In this paper, an attempt is made to calculate elastic moduli of a metal superlattice system, Mo/V, within a self-consistent electronic structure scheme—the full-potential linear muffin-tin orbital (FP-LMTO) method, developed by Methfessel.[25] The reason to choose the Mo/V system is that it is extremely well characterized experimentally[26,27] and that accurate elastic data are under way.[28] The calculations are restricted to small modulation wavelengths, i.e., superlattices consisting of at most three layers of each material. For these modulations, possible interface energetics are expected to be most prominent. The calculated moduli are compared to results for layered structures from continuum theory and it is found that the agreement is good. Allowing for disorder at the interfaces, the Hashin-Shtrikman bounds for random two-phase composites give a possible maximum softening of 30% of Young's modulus in these materials.

This paper is organized as follows: in Sec. II, a presentation is made of how the elastic constants are calculated from total energies of the crystals under different distortions. The continuum theory results for effective moduli of composites are also presented, to which the calculated results are compared. In Sec. III, a discussion of the results for the moduli of the constituent metals and the Mo/V superlattices is made. A summary is given at the end.

II. CALCULATIONAL PROCEDURE

A. Total-energy calculations

The FP-LMTO scheme[25] is used for the calculation of total energies of the materials under different distortions of the lattices. The total energies were calculated in the local density approximation (LDA) based on the von Barth-Hedin parametrization.[30] Since the smallest total energy differences for the lattice distortions are of the order of 10 meV, a relatively large number of **k** points in the irreducible Brillouin

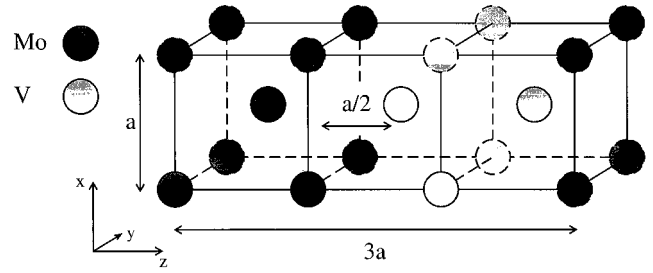

FIG. 1. The unit cell of the Mo_3/V_3 superlattice is shown. The superlattice is coherently grown, i.e., a common lattice constant a, is adopted by both Mo and V. There is also a common distance $a/2$ between layers. The growth direction is along the z axis.

zones (IBZ) has been used in the calculations. For instance, 220 **k** points are required in the Mo_2/V_2 IBZ in order to ensure an accuracy of 0.5 meV in the total energies. When the crystal lattice is deformed, the number of **k** points in the IBZ is recalculated for the new symmetry so that the density of **k** points remains the same. No frozen core approximation was done; all calculations were scalar relativistic in an *spd* basis for the valence electrons where three envelope energies are used. The muffin-tin radii are chosen equally large for each constituent and so as to minimize the interstitial region and the associated numerical inaccuracies.

The lattice symmetries for the equilibrium configurations in the calculations are cubic for Mo, V, and Mo_1/V_1, and tetragonal for the Mo_2/V_2 and Mo_3/V_3 superlattices. The growth direction is taken to be along [001]. The growth of these superlattices is coherent up to 32 layers,[29] i.e., Mo and V adopt a common lattice constant parallel to the interfaces. There might though be an expansion or contraction of the interlayer lattice constants in the growth direction. Experimentally, measurements of lattice parameters of individual layers have been performed for Mo_{10}/V_{18} superlattices,[27] which show that the average lattice parameter in the growth direction differs between Mo and V. In light of the above, total-energy calculations were performed for a variety of tetragonal distortions in Mo_1/V_1 and a variety of tetragonal distortions in Mo_2/V_2 where also the interlayer distances were varied between different layers. None of the tried distortions resulted in lower total energy than the structure depicted in Fig. 1, indicating that such deviations cannot be large in the small-modulation superlattices considered here.

B. Elastic constants

The elastic energy of a crystal under a small deformation can be written as[31]

$$E-E_0=\frac{V_0}{2}\,\lambda_{iklm}u_{ik}u_{lm}, \tag{1}$$

where E_0 and V_0 are the energy and the volume, respectively, of the equilibrium configuration, u_{ik} is the strain tensor, and λ_{iklm} is the elastic modulus tensor. The indices run over the three coordinate directions, x, y, and z, and summation over repeated indices is understood. The strain tensor u_{ik} is to linear order given as

$$u_{ik}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_k}+\frac{\partial u_k}{\partial x_i}\right), \tag{2}$$

where $u_i=r_i'-r_i$ and we have that r_i and r_i' are the coordinates of the atoms before and after the deformation of the crystal, respectively. At most, there are 21 independent components of the elastic modulus tensor λ_{iklm}, but crystal symmetries reduce the number of independent components. For cubic symmetry, there are only three independent moduli. Equation (1) reduces in this situation to

$$E-E_0=\frac{V_0}{2}\,C_{11}(u_1^2+u_2^2+u_3^2)+V_0C_{12}(u_1u_2+u_1u_3+u_2u_3)$$
$$+\frac{V_0}{2}\,C_{44}(u_4^2+u_5^2+u_6^2), \tag{3}$$

where the standard two-index notation $xx=1$, $yy=2$, $zz=3$, $xy=4$, $xz=5$, $yz=6$ is used. The C's here are the (second-order) elastic stiffness constants. The different elastic moduli of interest—the bulk modulus B, the tetragonal shear modulus C', and Young's modulus Y for extension along [001]—are directly related to the stiffness constants as

$$B=\tfrac{1}{3}(C_{11}+2C_{12}),$$
$$C'=\tfrac{1}{2}(C_{11}-C_{12}), \tag{4}$$
$$Y=\frac{9BC'}{3B+C'}.$$

The moduli B, C', and C_{44} are extracted for the cubic crystals by calculating total energies of the crystals for several lattice distortions. The other constants and moduli are then found from the relations in Eq. (4).

In order to extract C' and C_{44}, the same lattice distortions as in Alouani, Albers, and Methfessel[22] were made. Making a (volume-conserving to linear order in strain) tetragonal distortion as $2u_1=2u_2=-u_3=u$; $u_4=u_5=u_6=0$, where u_3 is along the growth direction of Mo_1/V_1, it is obtained from Eq. (3),

$$\Delta E(u)=E-E_0=\frac{3V_0}{4}\,u^2(C_{11}-C_{12}), \tag{5}$$

from which $(C_{11}-C_{12})=2C'$ is extracted by making a polynomial fit to $\Delta E(u)$. (Alternatively, one may use Andersen's force theorem[33] and express the total energy difference under deformation in order to obtain the shear modulus of crystals.[34,35]) A distortion $u_4=u$ will, in a similar fashion, give C_{44}. Energy differences $\Delta E(u)$ have been calculated for u's in the range ± 0.02–0.06. The odd powers in the polynomial fits are kept in order to ensure that pressure terms due to possible deviations from the equilibrium configuration are not neglected. It is noticed that the linear term is very small, indicating that we indeed are close to one equilibrium configuration.

There exists different methods to give error estimates for the extracted elastic constants from polynomial fits. They can be based on the change of the extracted values with polynomial order[21,22] or statistical goodness-of-fit analyses.[24] The latter procedure is followed here in order to judge which polynomial fit is more appropriate. The error estimates in C'

and C_{44} are then given by a $\chi^2(N)$ analysis, where N is the polynomial order. The error estimates of the related C_{11} and C_{12} constants indicate the maximum deviation of these constants given the errors in C'.

Only the bulk modulus for the ''larger'' superlattices is calculated. It is expected that electronic and interface effects on the elastic constants would show in any modulus. Some precaution is needed when speaking about an overall bulk modulus for superlattices. B is calculated by applying a uniform strain in all directions and in all layers, which corresponds to a volume change under preserved lattice symmetry. A uniform strain will, in the case of an inhomogeneous structure, not generally correspond to a uniform stress field. This has the consequence that, if we want to measure (or define) an overall bulk modulus from the energy change associated with a uniform pressure, we will find that the crystal may change its shape. The definition of B as the second derivative of the total energy upon symmetry-preserving compression is here nevertheless retained. It is exact for the cubic lattices and an upper bound[36] for the bulk modulus of the tetragonal superlattices. The bulk modulus B is hence given by

$$B = V_0 \frac{\partial^2 (E - E_0)}{\partial V^2}, \tag{6}$$

where V is the volume of the crystal under a uniform and isotropic deformation. The energy differences $(E - E_0)$ are calculated for six or seven different crystal volumes and fitted to the equation of state,[37]

$$E(V) - E_0 = \sum_{n=2}^{M} a_n \left[1 - \left(\frac{V}{V_0} \right)^{-(2/3)} \right]^n, \tag{7}$$

where E_0 is the equilibrium total energy of the crystal. The order, M, of the polynomial is determined as before by a $\chi^2(N)$ analysis. The bulk modulus is then found from differentiation of Eq. (7).

C. Moduli from continuum elasticity considerations

Within linear continuum elasticity theory, it is possible to derive expressions for the elastic response of composite materials. Results are here listed for bounds for the overall elastic moduli of a two-phase composite and exact expressions for elastic constants of laminates, or superlattices, which is a special case of a two-phase composite. The calculated results will be compared to the continuum predictions.

In order to relate the calculated values of effective elastic constants in Mo/V with results from continuum elasticity theory, we will follow Grimsditch and Nizzoli and Kim *et al.*[38–40] and give the expressions for the effective elastic constants and moduli in terms of the constituent's elastic constants. These expressions do not take coherency strains into account, for which higher-order elastic stiffness constants would be needed. Such effects are shown to be small.[17,18]

In the present special case of superlattices composed of equally thick layers of cubic materials, the superlattice has tetragonal symmetry and will be characterized by the following six independent elastic constants:

$$\begin{aligned}
C_{33}^{\text{eff}} &= \frac{2 C_{11}^{\text{Mo}} C_{11}^{\text{V}}}{C_{11}^{\text{Mo}} + C_{11}^{\text{V}}}, \\
C_{66}^{\text{eff}} &= \frac{C_{44}^{\text{Mo}} + C_{44}^{\text{V}}}{2}, \\
C_{13}^{\text{eff}} &= \frac{C_{11}^{\text{Mo}} C_{12}^{\text{V}} + C_{11}^{\text{V}} C_{12}^{\text{Mo}}}{C_{11}^{\text{Mo}} + C_{11}^{\text{V}}}, \\
C_{44}^{\text{eff}} &= \frac{2 C_{44}^{\text{Mo}} C_{44}^{\text{V}}}{C_{44}^{\text{Mo}} + C_{44}^{\text{V}}}, \\
C_{11}^{\text{eff}} &= \frac{C_{11}^{\text{Mo}} + C_{11}^{\text{V}}}{2} - \frac{(C_{12}^{\text{V}} - C_{12}^{\text{Mo}})^2}{2(C_{11}^{\text{Mo}} + C_{11}^{\text{V}})}, \\
C_{12}^{\text{eff}} &= \frac{C_{12}^{\text{Mo}} + C_{12}^{\text{V}}}{2} - \frac{(C_{12}^{\text{V}} - C_{12}^{\text{Mo}})^2}{2(C_{11}^{\text{Mo}} + C_{11}^{\text{V}})},
\end{aligned} \tag{8}$$

Here, C^{Mo} and C^{V} denote the respective elastic constants of the constituent metals. It is recalled that the z $(=3)$ direction is always along the growth axis.

The effective bulk modulus of the superlattice may be expressed in terms of its effective elastic constants. For a material with tetragonal symmetry and under a constant-strain condition, this relation is

$$B^{\text{eff}} = \frac{2}{9} \left(C_{11}^{\text{eff}} + C_{12}^{\text{eff}} + 2 C_{13}^{\text{eff}} + \frac{C_{33}^{\text{eff}}}{2} \right). \tag{9}$$

The expressions for the effective elastic constants from Eq. (8) are inserted into Eq. (9). In order to obtain a manageable relation in terms of the constituent bulk moduli, the resulting expression is reformulated in terms of B^{Mo} and B^{V}. These moduli are, as before, given by $B = \frac{1}{3}(C_{11} + 2C_{12})$ and, finally, the following is obtained:

$$B^{\text{eff}} = \frac{1}{2} (B^{\text{Mo}} + B^{\text{V}}) - \frac{(B^{\text{V}} - B^{\text{Mo}})^2}{2(C_{11}^{\text{Mo}} + C_{11}^{\text{V}})}. \tag{10}$$

There also exist *bounds* derived within continuum elasticity theory for multiphase materials. Such bounds will be used here, expressed for a two-phase composite of Mo and V with 50-50 composition, in connection with discussions of effects of disorder at the interfaces. The Hashin-Shtrikman bounds[41] for bulk and shear moduli (B and μ) of multiphase materials are derived from variational principles of the elastic energy. For a two-phase composite that is macroscopically quasihomogeneous and quasiisotropic, they read (taken from Laws[42])

$$B_{\text{min}} = B_{\text{V}} + \frac{\frac{1}{2}(B_{\text{Mo}} - B_{\text{V}})(B_{\text{V}} + B_l)}{B_{\text{Mo}} + B_l - \frac{1}{2}(B_{\text{Mo}} - B_{\text{V}})},$$

TABLE I. Elastic moduli in Mbar and equilibrium lattice constant in a.u. of bcc Mo calculated in the present work are presented and compared to experiments and other theoretical calculations. The FP-LMTO calculations are by Alouani, Albers, and Methfessel (Ref. 22) and the LMTO-ASA calculations are by Tang, Zhang, and Xi (Ref. 32) and Dacorogna, Ashkenazi, and Peter (Ref. 34). The experimental values for the elastic moduli are from Katahara, Manghnani, and Fisher (Ref. 45), and the equilibrium lattice constant is taken from Ashcroft and Mermin (Ref. 49).

Mo	a_0	B_0	C'	C_{11}	C_{12}	C_{44}
Present work	5.83	2.61±0.03	1.80±0.03	5.01±0.07	1.41±0.05	1.02±0.03
FP-LMTO (Ref. 22)	5.97	2.55	1.39	4.40	1.62	1.39
LMTO-ASA (Ref. 32)	5.86	2.92	2.045	5.6	1.51	
LMTO-ASA (Ref. 34)			2.47			
Expt. (Ref. 49)	5.95					
Expt. (Ref. 45)		2.63	1.52	4.65	1.62	1.09

$$B_{\max}=B_{\mathrm{V}}+\frac{\frac{1}{2}\,(B_{\mathrm{Mo}}-B_{\mathrm{V}})(B_{\mathrm{V}}+B_h)}{B_{\mathrm{Mo}}+B_h-\frac{1}{2}\,(B_{\mathrm{Mo}}-B_{\mathrm{V}})},$$

$$\mu_{\min}=\mu_{\mathrm{V}}+\frac{\frac{1}{2}\,(\mu_{\mathrm{Mo}}-\mu_{\mathrm{V}})(\mu_{\mathrm{V}}+\mu_l)}{\mu_{\mathrm{Mo}}+\mu_l-\frac{1}{2}\,(\mu_{\mathrm{Mo}}-\mu_{\mathrm{V}})}, \tag{11}$$

$$\mu_{\max}=\mu_{\mathrm{V}}+\frac{\frac{1}{2}\,(\mu_{\mathrm{Mo}}-\mu_{\mathrm{V}})(\mu_{\mathrm{V}}+\mu_h)}{\mu_{\mathrm{Mo}}+\mu_h-\frac{1}{2}\,(\mu_{\mathrm{Mo}}-\mu_{\mathrm{V}})},$$

where

$$B_l=\tfrac{4}{3}\mu_{\mathrm{low}},$$

$$B_h=\tfrac{4}{3}\mu_{\mathrm{high}}, \tag{12}$$

$$\mu_l=\frac{3}{2}\left(\frac{1}{\mu_{\mathrm{low}}}+\frac{10}{9B_{\mathrm{low}}+8\mu_{\mathrm{low}}}\right)^{-1},$$

$$\mu_h=\frac{3}{2}\left(\frac{1}{\mu_{\mathrm{high}}}+\frac{10}{9B_{\mathrm{high}}+8\mu_{\mathrm{high}}}\right)^{-1}.$$

The subscripts high and low refer to the greater and lesser, respectively, of the constituent's moduli. The question is how to choose a representative shear modulus μ for each phase. For cubic materials, there are two shear moduli: C' and C_{44}. If phases in the composite are randomly oriented, we will have a representative shear modulus μ in each phase, which is some average between C' and C_{44}. Hashin and Shtrikman[41] have given expressions for bounds of the average μ in polycrystalline materials of cubic symmetry. As an example, the bounds for the average shear modulus of Mo in a polycrystalline sample are given as

$$\mu_{\min}^{\mathrm{Mo}}=C_{44}^{\mathrm{Mo}}+3\left(\frac{5}{C'^{\mathrm{Mo}}-C_{44}^{\mathrm{Mo}}}-4\beta_1\right)^{-1}, \tag{13}$$

$$\mu_{\max}^{\mathrm{Mo}}=C'^{\mathrm{Mo}}+2\left(\frac{5}{C_{44}^{\mathrm{Mo}}-C'^{\mathrm{Mo}}}-6\beta_2\right)^{-1},$$

where

$$\beta_1=-\frac{3(B^{\mathrm{Mo}}+2C_{44}^{\mathrm{Mo}})}{5C_{44}^{\mathrm{Mo}}(3B^{\mathrm{Mo}}+4C_{44}^{\mathrm{Mo}})},$$

$$\beta_2=-\frac{3(B^{\mathrm{Mo}}+3C'^{\mathrm{Mo}})}{5C'^{\mathrm{Mo}}(3B^{\mathrm{Mo}}+4C'^{\mathrm{Mo}})}. \tag{14}$$

By calculating minimum and maximum values for the respective representative shear moduli of Mo and V, the highest and lowest values obtained can be inserted into Eqs. (11) and (12) in order to obtain upper and lower bounds, respectively, for a two-phase composite of Mo and V.

III. RESULTS AND DISCUSSION

A. Elastic moduli of Mo and V

Three independent elastic moduli of bcc Mo and V have been calculated, the bulk modulus B, the tetragonal shear modulus C', and the trigonal shear modulus C_{44} following the procedure described in Sec. II. From these moduli, C_{11} and C_{12} are derived according to Eq. (4).

The elastic moduli and equilibrium lattice constants of Mo and V are shown in Tables I and II, separately. It is

TABLE II. Listed are elastic moduli in Mbar and equilibrium lattice constant in a.u. of bcc V calculated in the present work. Comparisons are made to experiments and other theoretical calculations. The FP-LMTO calculations are by Paxton, Methfessel, and Polatoglou (Ref. 46) and the LMTO-ASA calculations are by Dacorogna, Ashkenazi, and Peter (Ref. 34).

V	a_0	B_0	C'	C_{11}	C_{12}	C_{44}
Present work	5.48	1.92±0.03	0.90±0.01	3.12±0.04	1.32±0.03	0.30±0.03
FP-LMTO (Ref. 46)	5.60	2.00				
LMTO-ASA (Ref. 34)			0.44			
Expt. (Ref. 49)	5.71					
Expt. (Ref. 45)		1.57	0.55	2.31	1.20	0.43

found that the calculated equilibrium lattice constants of Mo and V are $a_0=5.83$ a.u. and $a_0=5.48$ a.u., respectively. This represents an underestimation of 2% and 4%, correspondingly, compared to the experimental values. These values are also lower than the values obtained from nonrelativistic calculations,[22,43] which is not unexpected, since it has been demonstrated that scalar-relativistic effects tend to ''shrink'' the core radius.[44] The calculated bulk modulus of bcc Mo agrees with the experimental results of Ref. 45 and also with the FP-LMTO calculations of Alouani, Albers, and Methfessel.[22] The bulk modulus for V is overestimated with respect to experiments with about 20% but is in agreement with FP-LMTO calculations of Paxton, Methfessel, and Polatoglou.[46] This larger discrepancy for V in the bulk and subsequent moduli is believed to be due to the neglect of magnetic effects[23] and the larger underestimation of the volume with respect to experiments. Comparing the calculated constants of Mo and V to experiments, we notice that, for both materials, good agreement is obtained for C_{44} but C' differs with ~18% in Mo and as much as ~60% in V. Comparing with other calculations of C' of Mo, performed within the LMTO-ASA (atomic sphere approximation) scheme,[34] and the Ewald corrected LMTO-ASA scheme,[32] it is noticed that the FP-LMTO scheme gives results closer to experiments.

B. Elastic moduli of Mo_n/V_n

The elastic moduli of Mo_1/V_1 are displayed in Table III. No experimental results have been found for this material. The calculated results are compared to continuum theory predictions obtained from Eq. (8), for the elastic stiffness constants of Mo_n/V_n. It is recalled that the $C^{\rm eff}$ are derived for the tetragonal symmetry of Mo_n/V_n. In the special case $n=1$ here, the symmetry is cubic and imposes the restriction that the strain should be uniform. The analytic effective elastic moduli for the laminate that reflect such conditions are $C_{11}^{\rm eff}$, $C_{12}^{\rm eff}$, and $C_{66}^{\rm eff}$. The notation $C_{126}^{\rm eff}$ in Table III is used to refer to $C_{11}^{\rm eff}$, $C_{12}^{\rm eff}$, and $C_{66}^{\rm eff}$ in Eq. (8). The remaining effective elastic constants from Eq. (8) are also displayed, denoted as $C_{134}^{\rm eff}$, which refers to $C_{33}^{\rm eff}$, $C_{13}^{\rm eff}$, and $C_{44}^{\rm eff}$ in Eq. (8). Agreement is noted between the calculated elastic constants for Mo_1/V_1 and the $C_{126}^{\rm eff}$—the corresponding effective elastic constants from continuum results for layered materials. The exception is C_{44}, which agrees with the constant-strain result $C_{44}^{\rm eff}$ in Eq. (8). There is also very good agreement between the calculated bulk modulus and the result for B_0 from Eq. (10).

The equilibrium lattice constants and bulk moduli of the Mo_n/V_n superlattices are shown in Table IV. An increase in equilibrium lattice constant of the Mo_n/V_n with superlattice periodicity Λ is noticed. This may be connected with the amount of charge transfer across the Mo/V interface, which is also manifested in the Fermi energy increase with Λ in these materials.[47] The bulk modulus of the Mo_n/V_n superlattices with $n=1$–3 is stable at ~2.25 Mbar and seems unaffected by the (small) volume variation of the crystals. It is also in good agreement with the continuum theory result, $B_0=2.23\pm0.03$ Mbar.

Elastic anomalies in metal superlattices have been manifested, e.g., in Young's modulus Y. The calculated Young's modulus will here be compared to the one obtained from continuum theory for laminates and to a hypothetical situation of a two-phase composite of Mo and V with randomly oriented phases. The latter will serve as a crude estimate of the effect of disorder at the interfaces. Young's modulus is given by $Y=9B\mu/(3B+\mu)$. For Mo_1/V_1, $\mu=C'$ gives Young's modulus for extension of the lattice in the growth direction. From the calculated values for Mo_1/V_1, it is obtained $Y=3.46\pm0.03$ Mbar, as can be seen in Table V. The corresponding values from continuum theory for laminates is calculated from Eqs. (8) and (10). For Mo_1/V_1, which has cubic symmetry, we have the restriction that the strain should be uniform, corresponding to $C'=C_{12}^{\rm eff}$, which is the value used to obtain Y from Eqs. (8) and (10). There is agreement between the calculated Y and Young's modulus from continuum theory of laminates. The Hashin-Shtrikman bounds (11)–(14) give a *softer* Y with ~30% primarily due to the smaller value of the representative shear modulus. A consequence of the present finding would be that the more anisotropic the materials are (i.e., the larger the difference between C' and C_{44}), the larger would be the elastic anomalies due to disordered interfaces. Recent experiments[48] seem to confirm the close connection between interface quality and elastic anomalies for metallic superlattices of small modulation wavelength.

IV. SUMMARY AND CONCLUSIONS

The FP-LMTO scheme has been employed in order to calculate all elastic moduli of Mo, V, and of the Mo_1/V_1 superlattice. In addition, the equilibrium volumes and bulk moduli of Mo_n/V_n superlattices, grown in the [001] direction, with $n=1,2,3$ are calculated. The aim has been to investigate the effective elastic moduli of the superlattice formation and the influence of the interfaces upon their values. Satisfactory agreement is achieved with respect to experimental results for the constituent metals, especially for the bulk moduli, within the uncertainties of the calculations and the procedure of extraction of the elastic moduli from total-

TABLE III. Elastic moduli in Mbar of Mo_1/V_1 in the CsCl structure, calculated in the present work are presented and compared to continuum theory predictions for laminated media, according to Eqs. (8). The notations $C_{126}^{\rm eff}$ and $C_{134}^{\rm eff}$ refer to effective moduli under the condition of uniform strain and uniform stress, respectively. The relevant ones for comparison with the calculations are the $C_{126}^{\rm eff}$.

Mo_1/V_1	B_0	C'	C_{11}	C_{12}	C_{44}
Present work	2.25±0.01	1.39±0.01	4.10±0.03	1.32±0.01	0.48±0.1
Continuum theory, $C_{126}^{\rm eff}$	2.23±0.03	1.35±0.04	4.06±0.05	1.36±0.04	0.66±0.03
Continuum theory, $C_{134}^{\rm eff}$		1.16±0.04	3.85±0.04	1.35±0.04	0.46±0.04

TABLE IV. Tabulated are bulk moduli, B_0 in Mbar, and equilibrium lattice constants, a_0 in a.u., of Mo_n/V_n superlattices. The continuum theory value is obtained from Eq. (10).

	B_0	a_0
Mo_1/V_1	2.25±0.01	5.615
Mo_2/V_2	2.26±0.02	5.63
Mo_3/V_3	2.24±0.04	5.64
Continuum elasticity	2.23±0.03	

energy differences. The agreement is best for Mo, not as good for V, which most probably is due to neglect of ferromagnetism. We find that continuum elasticity theory gives a surprisingly good account for the values of the effective elastic moduli in small-modulation Mo/V superlattices. This indicates that the energetics of the Mo/V interfaces do not have any dramatic influence on the overall elastic properties. The equilibrium lattice constant of the Mo_n/V_n lattices is found to depend on n, but this dependence did not show up in the bulk modulus, inferring that electronic BZ effects are not prominent for these materials for a modulation wavelength $\Lambda \leqslant 9$ Å. An estimate of the effects of disorder at the interfaces on Young's modulus, employing the Hashin-Shtrikman bounds for polycrystalline two-phase composites, gives that Young's modulus can soften with up to 30%. This suggests that the precise interfacial structure has important impact upon the measured elastic moduli. The still existing confusion about elastic, modulation-wavelength-dependent, anomalies in metal superlattices underlines the need for full-scale electronic structure calculations where *both* an accurate description of the electronic properties *and* structural relaxations in the materials, especially at the interfaces, are addressed. This may, however, not be feasible in the near future.

TABLE V. Shown are results for Young's modulus (in Mbar) obtained from bulk and shear moduli of Mo_1/V_1. The calculated value is compared to continuum theory results for laminates and to Hashin-Shtrikman bounds of the equally composed Mo/V two-phase random composite. The laminate value is obtained from Eqs. (8) and (10) with C' given by $\frac{1}{2}(C_{11}^{\rm eff}-C_{12}^{\rm eff})$. The Hashin-Shtrikman bounds are obtained from Eqs. (11)–(14).

Mo_1/V_1	B_0	μ	Y
This work	2.25±0.03	1.39±0.01	3.46±0.03
Laminate	2.23±0.03	1.36±0.04	3.39±0.09
Hashin-Shtrikman bounds	2.07	0.89–0.93	2.34–2.43

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[1] W. C. Yang, T. Tsakalakos, and J. E. Hilliard, J. Appl. Phys. **48**, 876 (1977).
[2] L. R. Testardi, R. H. Willens, J. T. Krause, D. B. McWhan, and S. Nakahara, J. Appl. Phys. **52**, 510 (1981).
[3] T. Tsakalakos and J. E. Hilliard, J. Appl. Phys. **54**, 734 (1983).
[4] G. E. Hénein and J. E. Hilliard, J. Appl. Phys. **54**, 728 (1983).
[5] B. M. Davis, D. N. Seidman, A. Moreau, J. B. Ketterson, J. Mattson, and M. Grimsditch, Phys. Rev. B **43**, 9304 (1991).
[6] A. Kueny, M. Grimsditch, K. Miyano, I. Banerjee, C. M. Falco, and I. K. Schuller, Phys. Rev. Lett. **48**, 166 (1982).
[7] M. R. Khan, C. S. L. Chun, G. P. Felcher, M. Grimsditch, A. Kueny, C. M. Falco, and I. K. Schuller, Phys. Rev. B **27**, 7186 (1983).
[8] R. Danner, R. P. Huebener, C. S. L. Chun, M. Grimsditch, and I. K. Schuller, Phys. Rev. B **33**, 3696 (1986).
[9] J. R. Dutcher, S. Lee, J. Kim, G. I. Stegman, and C. M. Falco, Phys. Rev. Lett. **65**, 1231 (1990).
[10] A. Fartash, E. E. Fullerton, I. K. Schuller, S. E. Bobbin, J. W. Wagner, R. C. Cammarata, S. Kumar, and M. Grimsditch, Phys. Rev. B **44**, 13 760 (1991).
[11] A. F. Jankowski and T. Tsakalakos, J. Phys. F **15**, 1279 (1985); A. F. Jankowski, *ibid.* **18**, 413 (1988).
[12] G. E. Hénein, Ph.D. thesis, Northwestern University, 1979; W. E. Pickett, J. Phys. F **12**, 2195 (1982).
[13] J. Mei and G. W. Fernando, Phys. Rev. Lett. **66**, 1882 (1991).
[14] D. Wolf and J. F. Lutsko, Phys. Rev. Lett. **60**, 1170 (1988).
[15] J. Chang and M. J. Stott, Phys. Rev. B **46**, 10 423 (1992); J. Chang and M. J. Stott, Phys. Rev. B **47**, 15 976 (1993).
[16] C. Arcangeli, F. Nizzoli, and A. I. Liechtenstein, Phys. Rev. B **51**, 4497 (1995).
[17] A. Banerjea and J. Smith, Phys. Rev. B **35**, 5413 (1987).
[18] B. Dodson, Phys. Rev. B **37**, 727 (1988).
[19] C. M. Gilmore and V. Provenanzo, Phys. Rev. B **42**, 6899 (1990).
[20] R. S. Jones, J. A. Slotwinski, and J. W. Mintmire, Phys. Rev. B **45**, 13 624 (1992).
[21] M. J. Mehl, J. E. Osburn, D. A. Papaconstantopoulos, and B. M. Klein, Phys. Rev. B **41**, 10 311 (1990).
[22] M. Alouani, R. C. Albers, and M. Methfessel, Phys. Rev. B **43**, 6500 (1991).
[23] J. M. Wills, O. Eriksson, P. Söderlind, and A. M. Boring, Phys. Rev. Lett. **68**, 2802 (1992); P. Söderlind, R. Ahuja, O. Eriksson, J. M. Wills, and B. Johansson, Phys. Rev. B **50**, 5918 (1994).
[24] M. J. Mehl, Phys. Rev. B **47**, 2493 (1993).
[25] M. Methfessel, Phys. Rev. B **38**, 1537 (1988).
[26] J. Birch, M. Severin, U. Wahlström, Y. Yamamoto, G. Radnoczi, R. Riklund, J.-E. Sundgren, and L. R. Wallenberg, Phys. Rev. B **41**, 10 398 (1990).
[27] J. Birch, J.-E. Sundgren, and P. F. Fewster, J. Appl. Phys. **78**, 6562 (1995).
[28] B. Hjörvarsson (private communication).
[29] B. Hjörvarsson, S. Ólafsson, F. Stillesjö, E. Karlsson, J. Birch, and J.-E. Sundgren, Z. Phys. Chem. **181**, 343 (1993).
[30] U. Von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
[31] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon Press, London, 1959).
[32] S. Tang, K. Zhang, and X. Xi, J. Phys. C **21**, L777 (1988).

[33] A. R. Mackintosh and O. K. Andersen, in *Electrons at the Fermi Surface*, edited by M. Springford (Cambridge University, Cambridge, England, 1979).
[34] M. Dacorogna, J. Ashkenazi, and M. Peter, Phys. Rev. B **26**, 1527 (1982).
[35] N. E. Christensen, Solid State Commun. **49**, 701 (1984).
[36] R. Hill, J. Mech. Phys. Solids **11**, 357 (1963).
[37] F. Birch, J. Geophys. Res. **83**, 1257 (1978).
[38] M. Grimsditch, Phys. Rev. B **31**, 6818 (1985).
[39] M. Grimsditch and F. Nizzoli, Phys. Rev. B **33**, 5891 (1986).
[40] J. O. Kim, J. D. Achenbach, M. Shinn, and S. Barnett, J. Mater. Res. **7**, 2248 (1992).
[41] Z. Hashin and S. Shtrikman, J. Mech. Phys. Solids **11**, 127 (1963); L. J. Walpole, J. Mech. Phys. Solids **14**, 151 (1966).
[42] N. Laws, in *Physics of Modern Materials* (International Atomic Energy Agency, Vienna, 1980), p. 465.
[43] V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, New York, 1978).
[44] N. Takeuchi, C. T. Chan, and K. M. Ho, Phys. Rev. B **40**, 1565 (1989).
[45] K. W. Katahara, M. H. Manghnani, and E. S. Fisher, J. Phys. F **9**, 773 (1979).
[46] A. T. Paxton, M. Methfessel, and H. M. Polatoglou, Phys. Rev. B **41**, 8127 (1990).
[47] S. Papadia, K. Karlsson, P. O. Nilsson, and T. Jarlborg, Phys. Rev. B **45**, 1857 (1992).
[48] G. Carlotti, A. Montone, C. Petrillo, and M. V. Antisari, J. Phys. Condens. Matter **5**, 4611 (1993); G. Carlotti, G. Socino, A. Hu, H. Xia, and S. S. Jiang, J. Appl. Phys. **75**, 3081 (1994); J. O. Kim, J. D. Achenbach, M. Shinn, and S. A. Barnett, J. Eng. Mat. Tech. **117**, 395 (1995).
[49] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston International Editions, Philadelphia, 1976).