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Elastic constants of hexagonal transition metals: Theory

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The five different elastic constants of all the hexagonal $4d$ transition metals (Y, Zr, Tc, and Ru) and the $5d$ transition metals Re and Os have been calculated by means of first-principles electronic-structure calculations using the full-potential linear muffin-tin orbital method. The calculated data agree with the experimental values within $\sim 30\%$. We demonstrate, using experimental data, that the hexagonal transition metals obey the Cauchy relations much better than the cubic ones. This is due to the fact that the shape of the density of states for the hexagonal materials retains its form to a larger extent, for all types of shears, than it does for the cubic metals. We introduce normalized elastic constants $C'_{ij}=C_{ij}/B$, where B is the bulk modulus, which show a regular behavior for the hexagonal transition metals, in contrast to the cubic transition metals, where large irregularities are observed. These regular as well as irregular behaviors are well reproduced by the full-potential calculations.

I. INTRODUCTION

Recently the elastic constants for a number of cubic transition metals were calculated from first principles, and good agreement between theory and experiment was found.[1-4] For cubic materials, there are only three independent elastic constants; this makes a theoretical treatment considerably simpler than for a Bravais lattice with a lower symmetry. For a hexagonal lattice there are five independent elastic constants, usually referred to as C_{11}, C_{12}, C_{13}, C_{33}, and C_{55}.[5] A theoretical treatment of the elasticity of hexagonal systems is thus considerably more involved than for cubic materials. The task of calculating the elastic constants of hexagonal systems becomes even more difficult when realizing that the strains needed to calculate some of them give rise to a geometry with very low symmetry. Since it is a very strenuous task to calculate the total energy of a system with low symmetry, a first-principles calculation of the elastic constants of hexagonal materials is therefore a demanding problem. Possibly this is the reason why so far no theoretical work on elastic constants of hexagonal systems based on first-principle methods have been published.

Quite generally, a study of the elastic constants for materials is well motivated by, for example, the understanding one thereby gains about the chemical bonds and the cohesion of a material. It is of particular interest to examine the validity of simple and popular concepts such as central forces[5] in describing the elastic behavior of materials. In order to treat the elastic properties of hexagonal metals, we will in the present work not rely upon any assumptions about the nature of the interatomic forces. Rather, the total energy of the system is calculated from first principles. In the present investigation we have focused our attention to the elastic constants of a selected set of hexagonal transition metals, i.e., all hexagonal $4d$ metals as well as the $5d$ metals Re and Os. Previous work has shown that much of the chemical bonding in these materials can be understood quantitatively from simple models.[6] For instance, the Friedel model explains the parabolic trend of the equilibrium volume, bulk modulus, and the cohesive energy for the transition metals, including the presently studied hcp materials.[6] However, as mentioned, a study of the individual elastic constants of a material reveals much more information and a considerably more complex and detailed picture is required in order to explain the elastic behavior.

The rest of this paper is organized as follows. In Sec. II, we describe the underlying theory for the elasticity of hexagonal systems as well as the computational aspects of our study. In Sec. III, we present our results. In Sec. IV, we summarize our findings.

II. THEORY

The elastic constants C_{abcd} are defined by means of a Taylor expansion of the total energy for the system, $E(V,\alpha)$, with respect to a small strain α of the lattice (V is the volume). The letters a, b, c, and d refer to Cartesian components. In the present work we consider the hcp crystal structure, which is spanned by three vectors $(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)$, $(0, 1, 0)$, and $(0, 0, \frac{c}{a})$. The Bravais lattice vectors are normally written in a matrix form, i.e.,

$$\mathbf{R} = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{c}{a} \end{pmatrix}. \tag{1}$$

The distortion of the lattice is expressed by multiplying Eq. (1) with a symmetric ($\alpha_{xy} = \alpha_{yx}$) distortion matrix $\mathbf{e}$, which is written as,

$$\mathbf{e} = \begin{pmatrix} 1+\alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{yx} & 1+\alpha_{yy} & \alpha_{yz} \\ \alpha_{zx} & \alpha_{zy} & 1+\alpha_{zz} \end{pmatrix}. \tag{2}$$

The antisymmetric part of the matrix ($\alpha_{xy} = -\alpha_{yx}$) gives rise to pure rotations and can therefore be neglected. As mentioned above, we express the energy of the strained system by means of a Taylor expansion in the distortion parameters,

$$E(V,\alpha) = E(V_0,0) + V_0\left(\sum_{a,b} \tau_{ab}\alpha_{ab} + \sum_{a,b,c,d} \frac{1}{2} C_{abcd}\alpha_{ab}\alpha_{cd}\right). \tag{3}$$

The volume of the unstrained system is denoted V_0 and $E(V_0,0)$ is the corresponding total energy. In the equation above, we have introduced the parameter τ_{ab}, which is an element in the stress tensor, and C_{abcd}, which is an adiabatic elastic constant.[5] The Taylor series in Eq. (3) is truncated after the third term and here we merely note that there are of course higher-order terms, of which the first involves the third-order elastic constants. Since the matrix in Eq. (2) is symmetric, it contains only six different parameters. It is often convenient to change to the Voigt notation in order to reduce the number of indices. The Voigt notation replaces xx by 1, yy by 2, zz by 3, xy (and yx) by 6, xz (and zx) by 5, and finally yz (and zy) by 4. In this notation the elastic constant is written as C_{ij} where the new indices i and j will run over 1, 2, 3, 4, 5, and 6. It follows that we have a double sum instead of a quadruple sum in Eq. (3). When introducing the Voigt notation, one has to remember that the α's are symmetric, $\alpha_{ab} = \alpha_{ba}$, and if $a \neq b$ both α_{ab} and α_{ba} are labeled with the same Voigt index. To account for this, we introduce the factor ξ_i, which takes the value 1 if the Voigt index is 1, 2, or 3 and the value 2 if the Voigt number is 4, 5, or 6. The Taylor expansion of the total energy can now be written,

$$E(V,\alpha) = E(V_0,0) + V_0\left(\sum_{i} \tau_i\alpha_i\xi_i + \frac{1}{2}\sum_{i,j} C_{ij}\alpha_i\xi_i\alpha_j\xi_j\right). \tag{4}$$

In the present work we use a first-principles theory to calculate $E(V,\alpha)$ for various strains of the system and use the equation above to evaluate the elastic constants, C_{ij}. As already mentioned, there are five independent elastic constants for a hexagonal material, called C_{11}, C_{12}, C_{13}, C_{33}, and C_{55}. Since we have five independent constants, we need five different strains to determine these. The five distortions used in the present investigation are described below. The first distortion is written as

$$\begin{pmatrix} 1+\alpha & 0 & 0 \\ 0 & 1+\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{5}$$

and it changes the size of the basal plane, while keeping the z axis constant. The symmetry of the strained lattice is therefore still hexagonal. The energy associated with this distortion can be obtained by putting the values of the strain matrix [Eq. (5)] into Eq. (4), and we obtain

$$E(V,\alpha) = E(V_0,0) + V_0[(\tau_1+\tau_2)\alpha + (C_{11}+C_{12})\alpha^2]. \tag{6}$$

The second distortion matrix is written as

$$\begin{pmatrix} 1+\alpha & 0 & 0 \\ 0 & 1-\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{7}$$

and this distortion increases the x axis and decreases the y axis, with an equal amount. The z axis is kept constant and the resulting symmetry of the strained object is monoclinic. The energy, using Eq. (7) in Eq. (4), is expressed as

$$E(V,\alpha) = E(V_0,0) + V_0[(\tau_1-\tau_2)\alpha + (C_{11}-C_{12})\alpha^2]. \tag{8}$$

From Eqs. (6) and (8) we extract $(C_{11}+C_{12})$ and $(C_{11}-C_{12})$ and can thus calculate C_{11} and C_{12}.

The third strain we have used is given by

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+\alpha \end{pmatrix}, \tag{9}$$

and it gives an expression for the energy in which only one elastic constant, C_{33}, enters. The strain in Eq. (9) involves stretching the z axis whereas the other axes are unchanged. Thus, this shear maintains the hexagonal symmetry of the lattice. The energy for this shear can be written as

$$E(V,\alpha) = E(V_0,0) + V_0\left(\tau_3\alpha + \frac{C_{33}}{2}\alpha^2\right). \tag{10}$$

The fourth elastic constant, C_{55}, is determined by means of a deformation of the lattice, which produces an object with low symmetry. The deformation is written as

$$\begin{pmatrix} 1 & 0 & \alpha \\ 0 & 1 & 0 \\ \alpha & 0 & 1 \end{pmatrix}, \tag{11}$$

and the resulting lattice has a triclinic symmetry. In this particular case we need to take into account the previously mentioned factor ξ_i=2, which according to Eq. (4) will give us a factor of 4 in front of the elastic constant. The energy can be written as

$$E(V,\alpha) = E(V_0,0) + V_0(\tau_5\alpha + 2C_{55}\alpha^2). \tag{12}$$

The strains in Eqs. (9) and (11) give directly the C_{33} and C_{55} elastic constants. We are left with one more elastic constant, C_{13}. This elastic constant can be calculated by observing that there is a useful relationship between certain elastic constants and the bulk modulus, B. Namely, the latter can be written as a linear combination of four elastic constants

$$B = \frac{2}{9}(C_{11} + C_{12} + 2C_{13} + C_{33}/2). \tag{13}$$

Equation (13) is obtained by inserting into Eq. (4) the following strain matrix (assuming that the c/a ratio is unchanged for a small lattice expansion)

$$\begin{pmatrix} 1+\alpha & 0 & 0 \\ 0 & 1+\alpha & 0 \\ 0 & 0 & 1+\alpha \end{pmatrix}. \tag{14}$$

We obtain the following expression for the energy,

$$E(V,\alpha) = E(V_0,0) + V_0\Bigg((\tau_1 + \tau_2 + \tau_3)\alpha + \frac{1}{2}(2C_{11} + 2C_{12} + 4C_{13} + C_{33})\alpha^2\Bigg). \tag{15}$$

The bulk modulus is defined by

$$B = V_0\frac{d^2E}{dV^2} = \frac{1}{9V_0}\frac{d^2E}{d\alpha^2}, \tag{16}$$

and Eq. (13) is obtained from Eqs. (15) and (16). In connection to the calculation of the bulk modulus, we note that in principal the c/a ratio will change as a function of volume dilatation. However, we have performed test calculations of the bulk modulus allowing for a modification of the c/a ratio and found that the effect is indeed very small.

Using the above mentioned strains, we have calculated the total energy self-consistently by means of a first-principles method and evaluated the elastic constants. This was done at the theoretical equilibrium volume (see below). The present calculations were performed in the same way as in our previous work;[1,2] however, we have not constrained the volume to be constant when distorting the lattice. We thus made use of a full-potential linear-muffin-tin-orbital method[7] in combination with the local density approximation. The density and potential were expanded in spherical harmonic functions inside muffin-tin spheres and in plane waves in the interstitial region. We also adopted a so-called "double basis"[7] of muffin-tin orbitals,[8,9] where two different tail functions (Hankel or Neuman functions) with different kinetic energy are attached to two different linear combinations of the radial solution to the Schrödinger equation ϕ_ν and its first energy derivative $\dot{\phi}_\nu$ evaluated at an energy E_ν. The Hamiltonian matrix was thus doubled in size compared to calculations with a single basis. The inclusion of a double basis was necessitated by the fact that a very good energy resolution is required and to achieve this a well converged wave function is needed.

In order to improve on the convergence in sampling the k space, we associated each eigenvalue with a small Gaussian function of width 20 mRy. Moreover, we performed specific tests of the convergence of the calculated results as a function of the number of k points. This will be specifically addressed below. The k-point sampling was done with the special point method.[10]

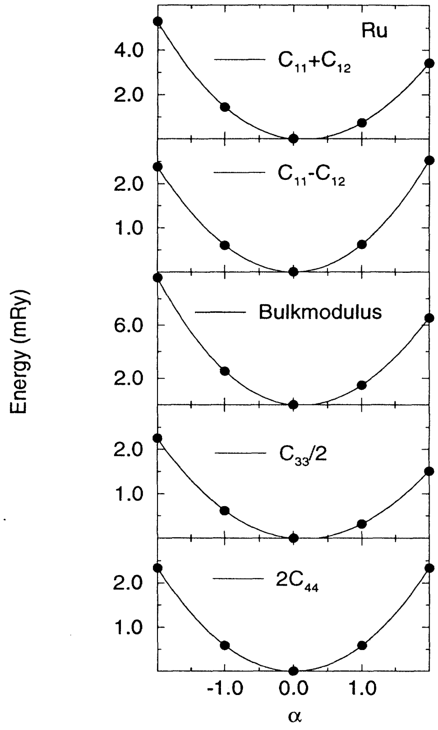

FIG. 1. Total energy of Ru as function of the lattice distortion parameter α, for the five different strains defined in the text. From the top panel to the bottom panel, the strains correspond to the distortions given in Eq. (5), Eq. (7), Eq. (14), Eq. (9), and Eq. (11), respectively.

In Fig. 1 we plot as an example the energy, $E(V,\alpha)$ versus strain, α, for the different types of strains for Ru. The total energy has been calculated for five different distortions $\alpha= -0.02$, -0.01, 0.00, 0.01, and 0.02, for everyone of the five different deformations of the lattice. By means of polynomial fits, we extract the zero-, first-, and second-order coefficients and from these we obtain $E(V_0,0)$, τ_i, and C_{ij} in Eq. (1). We note here that the polynomial fit to the points in Fig. 1 was truncated after the third-order term. The third-order component of the fit was always affecting the total energy with an amount which is less than an order of magnitude compared with the second-order (elastic constant) term.

III. RESULTS

A. Convergence test of the number of k points

Before describing the main results of our study, let us first discuss in some detail one of the convergence tests that we have made for this type of calculation. It is important to ensure that the total energy is converged in terms of the expansion of the wave function, charge den-

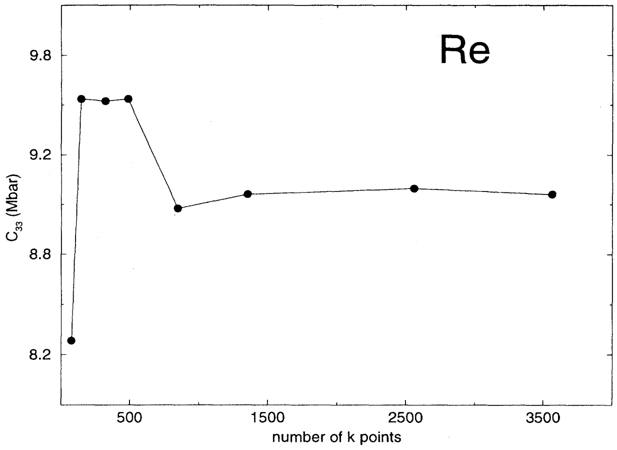

FIG. 2. The value of the calculated elastic constant C_{33} for Re as function of the number of k points in the full Brillouin zone.

sity, potential, and so on. One of the more crucial aspects of this is that one must have a good convergence in the sampling of the Brillouin zone. Therefore, we have as an explicit test of the k-space convergence computed the C_{33} elastic constant as a function of increasingly dense k-point sets. This was chosen to be done for Re. As can be seen in Fig. 2, the C_{33} elastic constant is converged for $\sim$ 847 k points in the full Brillouin zone. Therefore, for all the other materials and for all other types of shear, we choose to converge our total energy for 847 k points in the full zone (although the irreducible part of the Brillouin zone is of course different for different shears).

B. Calculated elastic constants

In Table I we list the calculated and experimental values of the equilibrium volume and the bulk modulus. The agreement between theory and experiment is comparable to previous studies[11] and the results in Table I are included for completeness. We have chosen to calculate the elastic constants at the theoretical equilibrium volumes listed in Table I. Notice that in agreement with earlier studies,[11] our calculations give a too low equilibrium volume for the earlier transition metals (with $\sim$ 5–10%) and that the error is decreasing as one traverses a series. For Os, we actually reach a situation where we overestimate the volume with a small amount, $\sim$ 2%. The bulk modulus is consistently overestimated in our calculations with 10–20%. These findings are in agreement with previous studies and these errors are quite common for theories based on the local density approximation.

In Table II we display the main result of this study, i.e., the elastic constants for the hexagonal 4d metals and for Re and Os. Unfortunately, we have not been able to find any experimental data for Os and Tc; therefore, in these two cases our calculations may serve as a prediction. When a comparison is possible we note from Table II that the agreement between theory and experiment sometimes is very good and sometimes somewhat less satisfactory. It is hard to distinguish general trends in the deviations from experiment; for certain materials a specific elastic constant is overestimated whereas for other materials the same elastic constant may be underestimated. However certain trends are distinguishable, for instance for the later transition metals (Ru and Re) the theoretical values are all larger than found experimentally and also for Y and Zr most of the theoretical data are larger than experiment. It is interesting to note that, for all elements the calculated C_{13} and C_{33} values are larger than the experimental data. Typically the deviations between theory and experiment range between −30 and +30%. The different elastic constants for the different materials vary between $\sim$ 0.1 Mbar to $\sim$ 8 Mbar, i.e., they differ by almost a factor of 100, and it is rewarding that our calculations reproduce this rather wide span of data quite well. The presently calculated elastic constants are of comparable quality, in terms of reproducing experiment, as the previously reported cubic elastic constants.[1–4] Hence the present work together with Refs. 1–4 gives a rather complete theoretical study of the elasticity of the 4d and 5d transition metals, and an overall rather satisfactory description of the experimental data is obtained.

C. Optimization of the axis ratio c/a

By use of Eq. (4), one can derive a criterion for when the energy is minimized with respect to the different shears, i.e., $\frac{dE}{d\alpha}=0$. A comparable analysis was also presented for a tetragonal system (MoSi$_2$) by Alouani *et al.*[12] This leads to the following equation:

$$0 = \tau_i + \sum_j \frac{1}{2} C_{ij} \alpha_j . \qquad (17)$$

TABLE I. Bulk properties for the 4d metals Y, Zr, Tc, and Ru; and the 5d metals Re and Os. Experimental data are taken from Ref. 14. Values in parentheses are estimates.

	Experiment		Theory	
Element	Bulk modulus (Mbar)	Volume (Å)	Bulk modulus (Mbar)	Volume (Å)
Y	0.366	33.12	0.438	30.51
Zr	0.833	23.28	1.032	22.19
Tc	(2.97)	14.30	3.486	13.89
Ru	3.208	13.49	3.688	13.24
Re	3.72	14.71	4.473	14.63
Os	(4.18)	13.99	4.761	14.25

TABLE II. Elastic constants (in Mbar) for the 4*d* metals Y, Zr, Tc, and Ru; and for the 5*d* metals Re and Os. Experimental data are taken from Ref. 15.

Element	C_{11}	C_{12}	C_{13}	C_{33}	C_{55}
Y theory	0.806	0.184	0.271	0.881	0.311
Y expt.	0.834	0.291	0.190	0.801	0.269
Zr theory	1.564	0.654	0.758	1.820	0.248
Zr expt.	1.554	0.672	0.646	1.725	0.363
Tc theory	6.117	2.187	2.075	6.450	1.966
Tc expt.					
Ru theory	7.010	1.962	1.874	7.745	2.400
Ru expt.	5.763	1.872	1.673	6.405	1.891
Re theory	8.373	2.933	2.168	8.946	2.225
Re expt.	6.344	2.66	2.02	7.011	1.691
Os theory	8.945	2.492	2.456	10.164	1.622
Os expt.					

Using this expression we have found the values of α_j, which minimizes the total energy. This method is of course less accurate than to calculate the c/a ratio by means of minimizing the total energy as a function of this ratio. However, once the τ_i's and C_{ij}'s have been calculated, it is an easy task to get a good estimate of the c/a ratio by means of Eq. (17). Thus, we have calculated theoretical values for the c/a ratio and we compare with experimental data in Table III. Note that the agreement is excellent, the difference between theory and experiment is never larger than $\sim$ 1%. To illustrate this, we plot in Fig. 3 the theoretical c/a ratio as a function of the experimental c/a ratio, for Y, Zr, Tc, Ru, Re, and Os. We observe that the worst agreement is found for Y, where the calculated c/a ratio is 1.1% larger than the experimental value. We also note that the theoretical values are sometimes larger and sometimes smaller than the experimental data.

D. Analysis of the results

Traditionally the elasticity of materials has very often been studied theoretically by means of models which assume that the interatomic forces have a certain shape and directionality. One of the more common approaches is to assume that the atoms are connected with springs and that the resulting forces are only in the direction of the nearest neighbors (central force model). In this section we analyze our results and compare the experimental elastic constants with what one expects from a simple central force model. As is obvious from Table II, the experimental as well as the theoretical elastic constants vary a lot between the different elements. In terms of central forces, this means that the values of the spring constants vary substantially through the two transition metal series. This conclusion is maybe not too surprising since from the behavior of the bulk modulus, the equilibrium volume, and the cohesive energy, one knows that this must be the case. However, a study

TABLE III. c/a ratio for the 4*d* metals Y, Zr, Tc, and Ru; and the 5*d* metals Re and Os. Experimental data are taken from Ref. 14.

Element	Experiment c/a	Theory c/a
Y	1.572	1.588
Zr	1.593	1.583
Tc	1.605	1.606
Ru	1.583	1.584
Re	1.615	1.628
Os	1.579	1.578

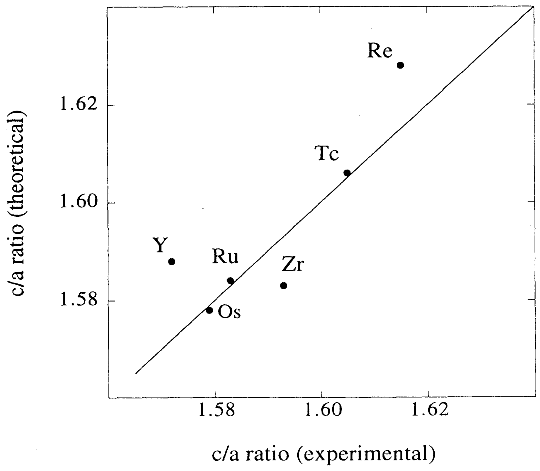

FIG. 3. The theoretical c/a ratio plotted as a function of the experimental c/a ratio for Y, Zr, Tc, Ru, Re, and Os.

of the bulk modulus, equilibrium volume, and cohesive energy gives little information about the validity of concepts such as central forces. Instead, an investigation of the elastic constants gives considerably more information about interatomic interactions. In this connection we observe that Cauchy derived a number of relationships, which hold if the atoms are interacting with central forces only.[5] For hexagonal materials, he showed that for central forces the following relations hold; $C_{13}{=}C_{55}$ and $C_{12}{=}C_{66}{=}\frac{1}{2}(C_{11}-C_{12})$. For cubic materials Cauchy showed that $C_{12}{=}C_{44}$, if the atoms are interacting with central forces. From Table II we observe that these relations are fairly well fulfilled for the hexagonal transition metals. The Cauchy relation is better satisfied for the hexagonal transition metals than it is for the cubic (fcc and bcc) ones.[1-4] In cubic materials one sometimes finds a C_{44}, which is four times smaller than C_{12}.[1-4] In Figs. 4(a) and 4(b), we show the Cauchy ratio (using the experimental values), for the various hexagonal [in Fig. 4(a), C_{12}/C_{66} and C_{13}/C_{55}] and cubic [in Fig. 4(b), C_{12}/C_{44}] elements. In Figs. 4(a) and 4(b), we have listed the elements according to the so-called standard order of arrangement of the elements.[13] Notice from Fig. 4(a) that the Cauchy ratio is close to one for most of the hexagonal transition metals, with some exceptions—for Co, Ti, and Zr it is closer to two. The overall deviations from one much smaller than what one finds for certain cubic materials where the Cauchy ratio quite often is 3 or 4 [see Fig. 4(b)].

In order to investigate this in more detail, we have introduced a normalized elastic constant, C'_{ij}, by dividing a specific elastic constant with the bulk modulus, i.e., $C'_{ij} = C_{ij}/B$. By introducing this quantity it becomes easier to study trends, since by dividing by the bulk modulus one is normalizing the interatomic forces with an average restoring force of the system. In Figs. 5(a) and 5(b), we show the experimental values of C'_{ij} for all hexagonal transition metals, including the hexagonal rare-earth metal Gd. In these figures we also include our presently calculated values. Note that the C'_{11} and C'_{33} renormalized constants are scattered around 1.8 for all transition metals, both experimentally and theoretically. In a similar fashion, the normalized C'_{12}, C'_{13}, and C'_{55} constants are grouped around 0.6. It is interesting to note that for an isotropic medium the following relations are valid; $C_{11}{=}C_{13}$, $C_{12}{=}C_{13}{=}C_{55}$. In this case the Cauchy relation, $C_{12}{=}(C_{11}-C_{12})/2$, is valid and we calculate the primed elastic constants to be, $C'_{11}{=}1.8$ and $C'_{12}{=}0.6$. Figures 5(a) and 5(b) thus suggest that the hexagonal transition metals are quite isotropic. Among the transition metals this is a property that is quite exclusive for the hexagonal metals, since for the fcc and bcc transition metals this is not the case. We observe again, now based on Figs. 5(a) and 5(b), that the Cauchy relation is fairly well satisfied for most of the hexagonal transition metals.

In order to analyze the results in Figs. 5(a) and 5(b) in more detail, we show in Fig. 6 the canonical d density of states (DOS) for an hcp system. The d DOS is plotted for the different strains used in the calculations of the elastic constants described above [Eqs. (2)–(6)]. The canonical d DOS is intimately connected to the linear muffin-tin orbital band-structure method, especially in the atomic sphere approximation (LMTO-ASA).[8,9] The canonical d bands are the eigenvalues of the d part of the structure constant matrix, which represents the multipole expansion of the basis (envelope) functions centered around sites $\mathbf{R} \neq \mathbf{0}$ in terms of basis functions centered around $\mathbf{R} = \mathbf{0}$. As a result of the theories behind the LMTO-ASA method the structure constants are energy and volume independent and the eigenvalues of a specific l subblock are therefore labeled canonical. Notice in Fig. 6 that the d DOS maintains its general shape for all

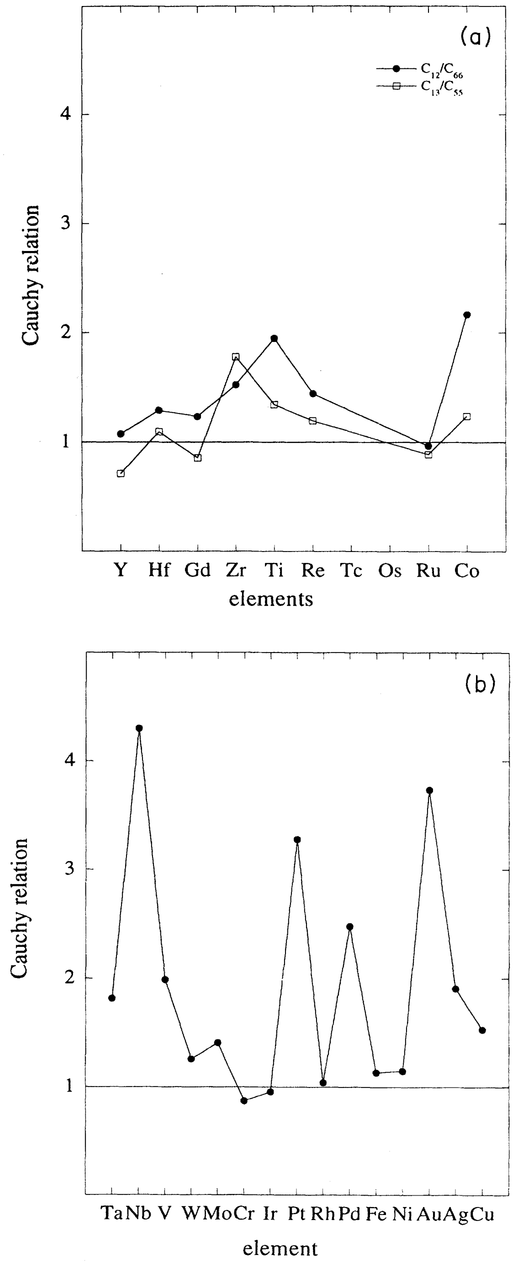

FIG. 4. Illustration of the Cauchy relations for the hexagonal transition metals (a) and for the cubic transition metals (b), using experimental data for the elastic constants.

types of distortions. This is quite different from the analysis of canonical fcc and bcc bands discussed in Refs. 1 and 2, where one observes a larger change in the DOS, when distorting the lattice. As a result, we expect that all the different types of shears (corresponding to certain combinations of elastic constants) will give rather similar changes in the total energy (in agreement with the total energy results given in Fig. 1). This is again in contrast to the cubic materials, which display a strong anisotropy in this respect.[1,2] In Fig. 7, we show for Ru the self-consistently calculated DOS for the strains described in Eqs. (2)–(6). Note that the shears correspond-

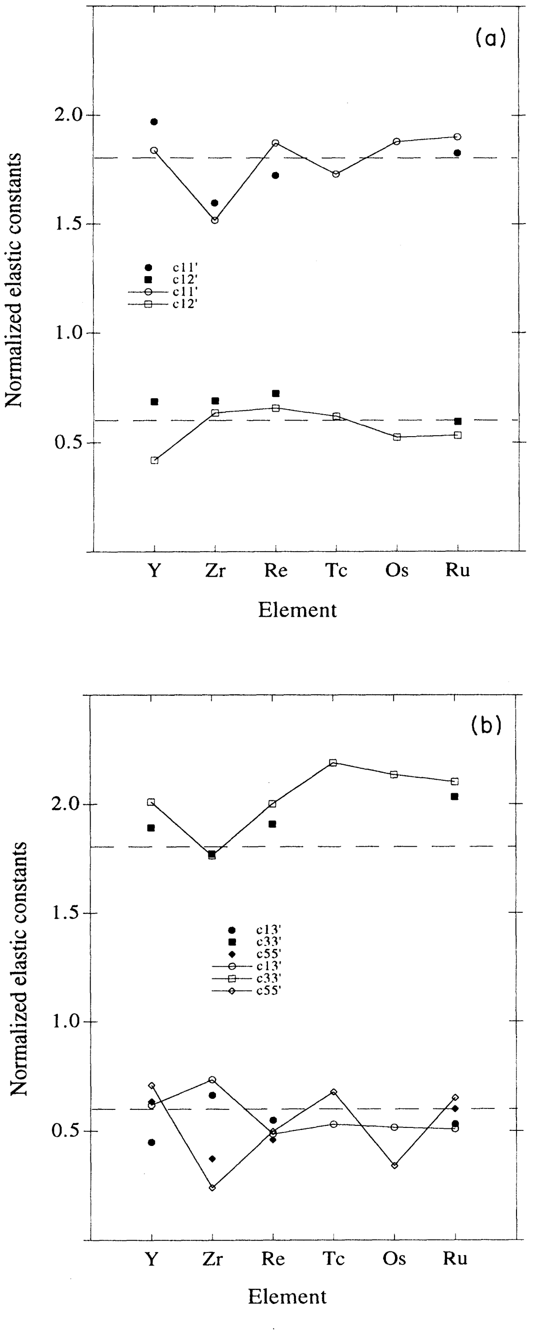

FIG. 5. Normalized elastic constants (see text), $C'_{ij}=C_{ij}/B$, for selected hexagonal transition metals. Closed symbols represent experimental data and open symbols represent theoretical data. C'_{11} and C'_{12} are presented in (a) and C'_{13}, C'_{33}, and C'_{55} are shown in (b). The dashed lines correspond to the values appropriate for an isotropic medium.

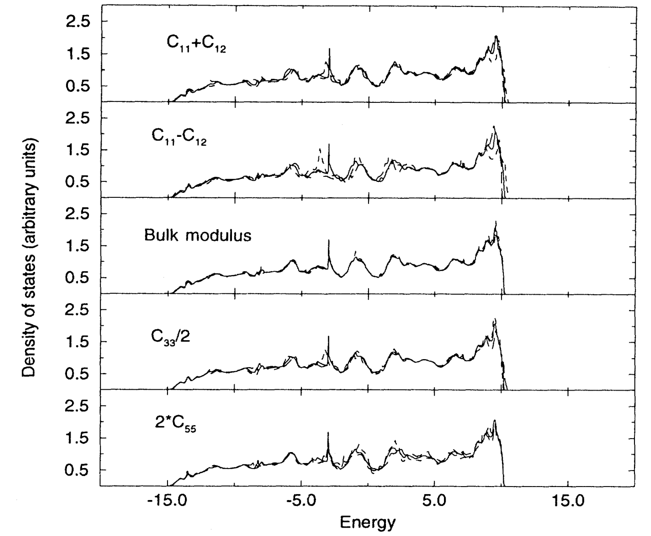

FIG. 6. The canonical density of states for various strains. Full drawn line corresponds to an undistorted lattice, dotted line corresponds to a −2% distortion, and dashed line corresponds to a +2% distortion. From the top panel to the bottom panel, the strains correspond to the distortion given in Eq. (5), Eq. (7), Eq. (14), Eq. (9), and Eq. (11), respectively.

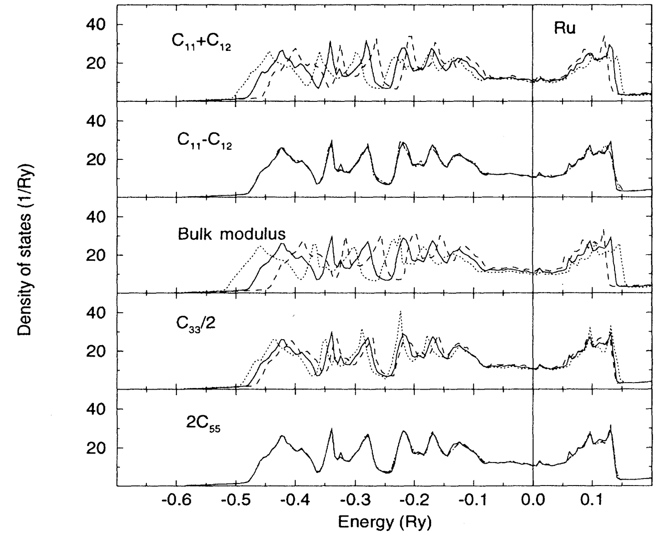

FIG. 7. The density of states for Ru for various strains. Full drawn line corresponds to an undistorted lattice, dotted line corresponds to a −2% distortion, and dashed line corresponds to a +2% distortion. From the top panel to the bottom panel, the strains correspond to the distortion given in Eq. (5), Eq. (7), Eq. (14), Eq. (9), and Eq. (11), respectively. The energy is in Rydberg and the Fermi level E_F is at zero energy.

ing to $C_{11} + C_{12}$, the bulk modulus, and $C_{33}/2$ are not volume conserving whereas the shears corresponding to $C_{11} - C_{12}$ and C_{55} are almost volume conserving. As a consequence, the bandwidth is almost unchanged in the latter two cases whereas for the other shears it is not. However, in agreement with Fig. 6, the general shape of the DOS is not modified very much by the different shears.

IV. CONCLUSIONS

To summerize, we have calculated the (five) elastic constants for all 4*d* and selected 5*d* (Re and Os) hexagonal transition metals. The agreement between theory and experiment is relatively good, of the same accuracy as in our previous study of the cubic transition metals.[1,2] Hence, this work together with the studies in Refs. 1 and 2, give a rather complete theoretical picture of the elastic constants of the transition metals. We have shown that the hexagonal metals satisfy the Cauchy relation much better than their cubic counterparts. Hence, one can expect to describe the elasticity (and possibly lattice dynamics) reasonably well by means of central forces in the hexagonal transition metals. This is shown to be connected to the relative lack of change in the DOS when the lattice is distorted, and we have used both self-consistent as well as canonical bands to demonstrate this. We have also introduced a new quantity, the normalized elastic constant, by dividing a particular elastic constant with the bulk modulus, ($C'_{ij} = C_{ij}/B$). The resulting normalized elastic constants are remarkably constant for the various elements, with the C'_{11} and C'_{13} constants having values close to 1.9 and the C'_{12}, C'_{13}, and C'_{55} constants grouping around 0.6, i.e., values appropriate for an isotropic medium. The c/a ratios have also been calculated for the hexagonal metals and the deviation from experiment is found to never exceed $\sim 1\%$.

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