Interpolation functions for Fermi surfaces in strained metals

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A straightforward method for finding expansion functions with the symmetry of a strained lattice is described. The method is applied to copper under hydrostatic and uniaxial strains. Changes in Fermi-surface cross-sectional areas are computed, based on a fit to energy shifts calculated by D. M. Gray and A. M. Gray [Phys. Rev. B **14**, 669 (1976)]. The results compare favorably with experimental values. The method is also used to find expansion functions for a crystal under an ultrasonic strain.

I. INTRODUCTION

When a metal is strained, the electron energy bands shift by an amount ΔE which depends on the tensor components of the strain $\underline{\epsilon}$ as well as the electron wave vector $\vec{k}$. For non-volume-conserving strains the Fermi energy will also change. As a result, the Fermi surface of the strained metal will differ slightly from that of the unstrained. Accurate prediction of the difference is a severe test of an energy-band calculation. Furthermore, ΔE is directly related to the deformation potential which determines the strength of the electron-phonon interaction in the metal.

Because of the reduction in symmetry for a strained crystal, Fermi energies are usually calculated only at points of relatively high symmetry. In order to make comparisons with experimental data, such as de Haas–van Alphen measurements of Fermi-surface cross-sectional areas, it is necessary to devise appropriate interpolation functions for the strained Fermi surface.

In this paper we outline a general method of obtaining functions with the proper symmetry for a strained lattice and apply it to face-centered-cubic crystals. We fit these functions to points calculated by Gray and Gray[1] (GG) for the basic static strains in copper, and compare computed area changes with those found experimentally. Finally, we show how the method also yields appropriate functions for acoustic strains and thus provides a convenient means of obtaining parametrized deformation-potential functions for calculations of the attenuation and velocity of ultrasonic waves.[2]

II. EXPANSION FUNCTIONS FOR A STRAINED LATTICE

We begin with a plane-wave expansion of $E(\vec{k})$, the electron energy in the unstrained lattice[3]:

$$E(\vec{k}) = \sum_{\vec{R}} C_{\vec{R}}\, e^{i\vec{k}\cdot\vec{R}}, \tag{1}$$

where $\vec{R}$ represents a crystal lattice vector. All of those vectors which are equivalent under a given symmetry operation are said to belong to a "star," and will have the same expansion coefficient $C_{\vec{R}}$.

It is convenient to rewrite Eq. (1) as

$$E(\vec{k}) = \sum_j C_j S_j(\vec{k}), \tag{2}$$

where $S_j(\vec{k})$ is the function belonging to the jth star of lattice vectors $\vec{R}$:

$$S_j(\vec{k}) = \sum_{\vec{R}\in j\text{th star}} e^{i\vec{k}\cdot\vec{R}}. \tag{3}$$

We will assume that $E(\vec{k})$ can be fitted by using the S_j for the first few nearest neighbors and finding the appropriate values of C_j.

In the strained lattice the stars are split (except in the hydrostatic case) into stars of lower symmetry which we designate as $S_j^i(\vec{k})$, where

$$S_j(\vec{k}) = \sum_i S_j^i(\vec{k}). \tag{4}$$

The five nearest-neighbor stars which result when a face-centered-cubic lattice is subjected to the various strains are listed in Table I.

The energy in the strained lattice may be expanded in terms of the stars of lower symmetry:

$$E'(\vec{k}) = \sum_{i,j} C_j^i S_j^i(\vec{k}). \tag{5}$$

The energy shift ΔE which results from straining the lattice is given by

$$\Delta E = E'(\vec{k}) - E(\vec{k}) = \sum_{i,j} C_j^i S_j^i - \sum_j C_j S_j. \tag{6}$$

If the magnitude of the strain ϵ is small, the coefficients C_j^i should differ little from the coefficients C_j for the high-symmetry star in the unstrained lattice. We make the expansion

$$C_j^i = C_j + \epsilon\left(\frac{\partial C_j}{\partial R_j^i}\frac{\partial R_j^i}{\partial \epsilon}\right)_{\epsilon=0} + O(\epsilon^2) \tag{7}$$

and neglect higher-order terms in ϵ.

TABLE I. Compatibility table indentifying lattice vectors $\vec{R}_j^i$ split from the same cubic star by each of the basic strains. P_{xyz} means permutations of all three components and P_{xy} permutations of the first two components of the vector which follows.

	Hydrostatic strain			Tetragonal strain				Trigonal strain			
Cubic star	$\vec{R}_j^i/a_0$	No. of $\vec{R}_j^i$	$(\partial\vec{R}_j^i/\partial\epsilon)/a_0$	Star	$\vec{R}_j^i/a_0$	No. of $\vec{R}_j^i$	$(\partial\vec{R}_j^i/\partial\epsilon)/a_0$	Star	$\vec{R}_j^i/a_0$	No. of $\vec{R}_j^i$	$(\partial\vec{R}_j^i/\partial\epsilon)/a_0$
S_1	$P_{xyz}(\pm\frac{1}{2},\pm\frac{1}{2},0)$	12	$\frac{1}{2}\sqrt{2}$	S_1^1	$P_{xy}(\pm\frac{1}{2},\pm\frac{1}{2},0)$	4	$-\frac{1}{2}(1/\sqrt{2})$	S_1^1	$\pm P_{xyz}(\frac{1}{2},\frac{1}{2},0)$	6	$1/\sqrt{2}$
				S_1^2	$P_{xy}(\pm\frac{1}{2},0,\pm\frac{1}{2})$	8	$\frac{1}{4}(1/\sqrt{2})$	S_1^2	$\pm P_{xyz}(-\frac{1}{2},\frac{1}{2},0)$	6	$-1/\sqrt{2}$
S_2	$P_{xyz}(\pm1,0,0)$	6	1	S_2^1	$P_{xy}(\pm1,0,0)$	4	$-\frac{1}{2}$	S_2^1	$\pm P_{xyz}(1,0,0)$	6	0
				S_2^2	$P_{xy}(0,0,\pm1)$	2	1				
S_3	$P_{xyz}(\pm\frac{1}{2},\pm\frac{1}{2},\pm1)$	24	$\sqrt{3/2}$	S_3^1	$P_{xy}(\pm\frac{1}{2},\pm1,\pm\frac{1}{2})$	16	$-\frac{3}{4}(1/\sqrt{6})$	S_3^1	$\pm P_{xyz}(\frac{1}{2},\frac{1}{2},1)$	6	$5/\sqrt{6}$
				S_3^2	$P_{xy}(\pm\frac{1}{2},\pm\frac{1}{2},\pm1)$	8	$\frac{3}{2}(1/\sqrt{6})$	S_3^2	$\pm P_{xyz}(\frac{1}{2},\frac{1}{2},-1)$	6	$-3/\sqrt{6}$
								S_3^3	$\pm P_{xyz}(-\frac{1}{2},\frac{1}{2},1)$	12	$-1/\sqrt{6}$
S_4	$P_{xyz}(\pm1,\pm1,0)$	12	$\sqrt{2}$	S_4^1	$P_{xy}(\pm1,\pm1,0)$	4	$-1/\sqrt{2}$	S_4^1	$\pm P_{xyz}(1,1,0)$	6	$\sqrt{2}$
				S_4^2	$P_{xy}(\pm1,0,\pm1)$	8	$\frac{1}{2}(1/\sqrt{2})$	S_4^2	$\pm P_{xyz}(1,-1,0)$	6	$-\sqrt{2}$
S_5	$P_{xyz}(\pm\frac{3}{2},\pm\frac{1}{2},0)$	24	$\sqrt{5/2}$	S_5^1	$P_{xy}(\pm\frac{1}{2},\pm\frac{3}{2},0)$	8	$-\frac{5}{4}\sqrt{2/5}$	S_5^1	$\pm P_{xyz}(\frac{1}{2},\frac{3}{2},0)$	12	$\frac{3}{2}\sqrt{2/5}$
				S_5^2	$P_{xy}(\pm\frac{3}{2},0,\pm\frac{1}{2})$	8	$-\frac{7}{8}\sqrt{2/5}$	S_5^2	$\pm P_{xyz}(\frac{1}{2},-\frac{3}{2},0)$	12	$-\frac{3}{2}\sqrt{2/5}$
				S_5^3	$P_{xy}(\pm\frac{1}{2},0,\pm\frac{3}{2})$	8	$\frac{17}{8}\sqrt{2/5}$				

Substitution of the zero- and first-order terms of the expansion into Eq. (6) yields

$$\Delta E/\epsilon \equiv \sum_j B_j f_j(\vec{k}) , \tag{8}$$

where the

$$f_j(\vec{k}) = \sum_i (\partial R_j^i/\partial\epsilon)_{\epsilon=0} S_j^i \tag{9}$$

are fitting functions with the symmetry of the strained lattice. We assume that the $\partial C_j^i/\partial R_j^i$ are independent of i at $\epsilon = 0$ and replace them by fitting coefficients B_j. The derivatives of R_j^i with strain can, of course, be evaluated explicitly for each strain.

III. FUNCTIONS FOR A STRAINED FACE-CENTERED-CUBIC LATTICE

The strain dependence of the R_j^i may be found by first writing them as linear combinations of basis vectors $\vec{a}_i$ which depend explicitly on the strain:

$$\vec{R}_j^i = l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3 . \tag{10}$$

In what follows, we assume a cubic lattice with lattice constant a_0. For hydrostatic strain $a_i = (1+\epsilon)a_0$; for tetragonal strain along $\vec{a}_3$, $a_1 = a_2 = (1-\epsilon/2)a_0$, $a_3 = (1+\epsilon)a_0$; for trigonal strain $\vec{a}_1 = [\hat{x} + \epsilon(\hat{y}+\hat{z})]a_0$, $\vec{a}_2 = [\hat{y} + \epsilon(\hat{z}+\hat{x})]a_0$, and $\vec{a}_3 = [\hat{z} + \epsilon(\hat{x}+\hat{y})]a_0$. Substitution of these relations into Eq. (10) yields

$$(1/a_0)(\partial R_j^i/\partial\epsilon)_{\epsilon=0} = \begin{cases} (l^2+m^2+n^2)^{1/2} , \\ [n^2 - \tfrac{1}{2}(l^2+m^2)] \\ \times (l^2+m^2+n^2)^{-1/2} , \\ 2(lm+mn+nl) \\ \times (l^2+m^2+n^2)^{-1/2} , \end{cases} \tag{11}$$

for hydrostatic, tetragonal, and trigonal strain, respectively. Strain derivatives for the first five stars of the face-centered-cubic lattice are given in Table I.

In order to illustrate the method, we solve for f_1 for a face-centered-cubic crystal subjected to a tetragonal strain. From Table I we find

$$S_1^1(\text{tet}) = \exp[i(\tfrac{1}{2}k_x + \tfrac{1}{2}k_y)a_0] + \exp[i(\tfrac{1}{2}k_x - \tfrac{1}{2}k_y)a_0] + \text{c.c.}$$
$$= 2[\cos(\tfrac{1}{2}k_x + \tfrac{1}{2}k_y)a_0 + \cos(\tfrac{1}{2}k_x - \tfrac{1}{2}k_y)a_0] . \tag{12}$$

Similarly,

$$S_1^2(\text{tet}) = 2[\cos(\tfrac{1}{2}k_x + \tfrac{1}{2}k_z)a_0 + \cos(\tfrac{1}{2}k_x - \tfrac{1}{2}k_z)a_0$$
$$+ \cos(\tfrac{1}{2}k_y + \tfrac{1}{2}k_z)a_0 + \cos(\tfrac{1}{2}k_y - \tfrac{1}{2}k_z)a_0] . \tag{13}$$

Using the values of $\partial R_j^i/\partial\epsilon$ from Table I, we have

$$f_1(\text{tet}) = -\tfrac{1}{2}(1/\sqrt{2})S_1^1(\text{tet}) + \tfrac{1}{4}(1/\sqrt{2})S_1^2(\text{tet}) . \tag{14}$$

(The factor a_0^{-1} has been omitted, since it is common to all terms in the expression.) We substitute into this expression Eqs. (12) and (13) and obtain, after some reduction,

$$f_1(\text{tet}) = -(1/\sqrt{2})\{2\cos(\tfrac{1}{2}k_x a_0)\cos(\tfrac{1}{2}k_y a_0)$$
$$-\cos(\tfrac{1}{2}k_z a_0)[\cos(\tfrac{1}{2}k_x a_0)$$
$$+ \cos(\tfrac{1}{2}k_y a_0)]\} . \tag{15}$$

Functions derived in this fashion are given in Table II for $j = 1-5$.

IV. APPLICATION TO COPPER

To illustrate the use of this expansion technique, we will apply it to copper. Davis, Faulkner, and Joy[4] (DFJ) calculated the energy bands in copper under small hydrostatic strains using the Koringa-Kohn-Rostoker method. From the strained and unstrained bands they found the change in Fermi-surface cross-sectional area for several extremal orbits. GG used a perturbation technique in conjunction with the modified plane-wave method to find electron energy shifts at four relatively high-symmetry points on the copper Fermi surface.

We fit our expansion functions to the results of GG because they are given for three basic strains (hydrostatic, tetragonal, and trigonal) and can easily be used to demonstrate the use of our method. Since only four points are available, we chose to fit the first three nonzero f_j to them by a least-squares method. The resulting values of B_j are given in Table II.

We can test the validity of the fitted functions by using them to compute changes in extremal cross-sectional areas to be compared with those measured with the de Haas–van Alphen effect. The change in Fermi wave vector $\vec{k}_F$ can be found from $\Delta E(\vec{k}_F)$ for a given strain $\underline{\epsilon}$ using a relation based on Eq. (8) of GG:

$$\Delta\vec{k}_F = -\hat{v}(\Delta E - \Delta E_F)/|\partial E/\partial\vec{k}| - \underline{\epsilon}\cdot\vec{k}_F , \tag{16}$$

where $\hat{v}$ is a unit vector along $\partial E/\partial\vec{k}$ which, along with $\vec{k}_F$, is computed by using the coefficients in Table I of Bosacchi and Franzosi[5] to evaluate Eq. (29) of Bosacchi, Ketterson, and Windmiller.[6] Area changes are then calculated from $\Delta\vec{k}_F$ values around extremal orbits.

In order to compare the calculated values with experimental results for hydrostatic strains, the volume compressibility of copper was used, as in GG, to convert strains to pressures. Our results are given in Table III along with the experimental results of Templeton[7] and the calculations of GG and DFJ.

For uniaxial tensions, linear combinations of

TABLE II. Interpolation functions f_j for a face-centered-cubic lattice and coefficients B_j fitted to values calculated by Gray and Gray (see Ref. 1) for copper. The summation $\sum$ implies a permutation of the crystal coordinates $\hat{k}_1$, $\hat{k}_2$, $\hat{k}_3$. Here, $C(\frac{1}{2}x) \equiv \cos(\frac{1}{2}k_x a_0)$, $S(y) \equiv \sin(k_y a_0)$, etc.

Strain	j	B_j (Ry)	f_j
Hydrostatic	1	0.139	$2\sqrt{2}\sum C(\frac{1}{2}x)C(\frac{1}{2}y)$
	2	−0.101	$2\sum C(x)$
	3	−0.097	$8\sqrt{3/2}\sum C(x)C(\frac{1}{2}y)C(\frac{1}{2}z)$
	4		$4\sqrt{2}\sum C(x)C(y)$
	5		$4\sqrt{5/2}\sum C(3x/2)[C(\frac{1}{2}y)+C(\frac{1}{2}z)]$
Tetragonal	1	0.387	$(1/\sqrt{2})\{C(\frac{1}{2}z)[C(\frac{1}{2}x)+C(\frac{1}{2}y)]-2C(\frac{1}{2}x)C(\frac{1}{2}y)\}$
	2	0.110	$2C(z)-C(x)-C(y)$
	3	0.025	$\sqrt{6}\{2C(z)C(\frac{1}{2}x)C(\frac{1}{2}y)-C(\frac{1}{2}z)[C(\frac{1}{2}x)C(y)+C(\frac{1}{2}y)C(x)]\}$
	4		$\sqrt{2}\{C(z)[C(x)+C(y)]-2C(x)C(y)\}$
	5		$\frac{1}{2}\sqrt{2/5}\{17C(3z/2)[C(\frac{1}{2}x)+C(\frac{1}{2}y)]-7C(\frac{1}{2}z)[C(3x/2)+C(3y/2)]-10[C(\frac{1}{2}x)C(3y/2)+C(\frac{1}{2}y)C(3x/2)]\}$
Trigonal	1	0.262	$-2\sqrt{2}\sum S(\frac{1}{2}x)S(\frac{1}{2}y)$
	2		0
	3	0.040	$-(8/\sqrt{6})\{2\sum S(z)[S(\frac{1}{2}x)C(\frac{1}{2}y)+C(\frac{1}{2}x)S(\frac{1}{2}y)]+\sum C(z)S(\frac{1}{2}x)S(\frac{1}{2}y)\}$
	4	0.120	$-4\sqrt{2}\sum S(x)S(y)$
	5		$-6\sqrt{2/5}[\sum S(\frac{1}{2}x)S(3y/2)+\sum S(3x/2)S(\frac{1}{2}y)]$

TABLE III. Dependence of Fermi-surface extremal cross-sectional areas in copper on hydrostatic strain. $(\Delta A/A)/\Delta P$ is given in units of 10^{-7} bar^{-1}.

Orbit	Present work	GG[a]	DFJ[b]	Templeton[c](Expt.)
[100] belly	4.66	4.28	4.62	4.42±0.03
[111] neck	16.0	12.6	15.3	19.8 ±0.5
[111] belly	4.11		4.36	4.21±0.03
[110] dog bone	3.79		4.04	4.04±0.02
[100] rosette	2.83			4.42±0.03

[a] Reference 1.
[b] Reference 4.
[c] Reference 7.

hydrostatic and tetragonal or trigonal strains are used, as in GG. Tables IV and V present calculated and experimental results for uniaxial tension along [001] and [111], respectively. Here the experimental values are those of Shoenberg and Watts[8] and the calculated values are those of GG and Davis.[9] In most cases, area changes obtained from our three-term fitting function agree with experiment almost as well as the more detailed calculations of DFJ and Davis.

V. EXPANSION FUNCTIONS FOR ULTRASONIC STRAINS

In order to compute the effect of conduction electrons on the attenuation and dispersion of ultrasonic waves, one must know the deformation potential. As shown elsewhere,[2] the deformation potential is simply related to $\Delta E(\vec{k}_F)$.

One can construct any ultrasonic strain from a linear combination of hydrostatic, tetragonal, and trigonal strains; thus a linear combination of ΔE's for these strains should give the deformation potential. However, for model or parametrized calculations it is more convenient to expand ΔE in basis functions which are natural to the ultrasonic strain.

An ultrasonic strain $\underline{\epsilon}$ can be expressed in terms of the propagation vector $\vec{q}$, the particle velocity $\vec{u}$, and the frequency ω as

$$\epsilon_{ij} = -\frac{1}{2\omega}(q_i u_j + u_i q_j), \tag{17}$$

or, equivalently, as

$$\epsilon_{ij} = (e/2)(\hat{q}\hat{u} + \hat{u}\hat{q}), \tag{18}$$

where e is the strain amplitude and $\hat{q}$ and $\hat{u}$ are unit vectors.

We now follow the same procedure as in Sec. III to find the expansion functions with the symmetry of the ultrasonic strain. The strain derivatives can be computed from

$$\left.\frac{\partial|\vec{R}'|}{\partial e}\right|_{e=0} = \frac{1}{|\vec{R}|}\vec{R}\cdot\underline{\epsilon}\cdot\vec{R}. \tag{19}$$

This method has been used[2] to obtain expansion functions for shear waves propagating along [111] in copper. The two modes used in the experiment had $\vec{u} \| [11\bar{2}]$ for $\underline{\epsilon}_1$ and $\vec{u} \| [1\bar{1}0]$ for $\underline{\epsilon}_2$. For simplicity we carry out the calculations in a reference

TABLE IV. Dependence of Fermi-surface extremal cross-sectional areas in copper on unaxial tension along [001] $[d(\ln A)/d(\ln A_s)$, where A_s is the diametral area of a free-electron sphere whose volume remains exactly half that of the Brillouin zone].

Orbit	Present work	GG[a]	Davis[b]	SW[c] (expt.)
[100] belly	−0.52	0.5	−0.3	
[001] belly	3.94	2.7	3.6	2.4±0.5
[111] neck	−0.99	2.9	5.1	
[111] belly	0.97		−0.6	
[110] dog bone	21.1		18	
[100] rosette	1.72		2.0	
[011] dog bone	−8.88		−7.8	
[001] rosette	−2.40		−3.0	−2.1±0.8

[a] Reference 1.
[b] Reference 9.
[c] Reference 8.

TABLE V. Dependence of Fermi-surface extremal cross-sectional areas in copper on uniaxial tension along [111] $[d(\ln A)/d(\ln A_s)]$.

Orbit	Present work	GG[a]	Davis[b]	SW[c] (expt.)
[001] belly	0.98	1.0	−1.2	
[111] neck	−50	−32	−28	−44±10
$[1\bar{1}1]$ neck	14.4	14	19	
[111] belly	−1.36		1.0	0.6±0.2
$[1\bar{1}1]$ belly	1.72		−0.1	
[100] rosette	0.23		7.7	

[a] Reference 1.
[b] Reference 9.
[c] Reference 8.

TABLE VI. S^i split from cubic stars S_j by two different strains: $\underline{\epsilon}_1$ is for a shear wave with $\vec{q}\,||\,[111]$, $\vec{u}\,||\,[11\bar{2}]$; $\underline{\epsilon}_2$ is for $\vec{q}\,||\,[111]$, $\vec{u}\,||\,[1\bar{1}0]$. Experimental coordinates are defined so that $\vec{q}\,||\,[100]$, $\vec{u}\,||\,[001]$ for $\underline{\epsilon}_1$, and $\vec{u}\,||\,[010]$ for $\underline{\epsilon}_2$. Direction cosines have been supressed so that $(1/\sqrt{3},\ 1/\sqrt{2},\ 1/\sqrt{6})$ is represented by $(1,1,1)$.

Cubic Star	Star	$\underline{\epsilon}_1$ $\vec{R}_j^i/a_0$ Crystal coord.	$\underline{\epsilon}_1$ $\vec{R}_j^i/a_0$ Expt. coord.	No. of $\vec{R}_j^i$	$(\partial\vec{R}_j^i/\partial e)/a_0$	Star	$\underline{\epsilon}_2$ $\vec{R}_j^i/a_0$ Crystal coord.	$\underline{\epsilon}_2$ $\vec{R}_j^i/a_0$ Expt. coord.	No. of. $\vec{R}_j^i$	$(\partial\vec{R}_j^i/\partial e)/a_0$
S_1	S_1^1	$\pm(\frac{1}{2},\frac{1}{2},0)$	$\pm(1,0,1)$	2	$\frac{1}{3}$	S_1^1	$\pm(\frac{1}{2},0,\frac{1}{2})$	$\pm(1,\frac{1}{2},-\frac{1}{2})$	2	$\frac{1}{2}(1/\sqrt{3})$
	S_1^2	$\pm P_{xy}(\frac{1}{2},0,\frac{1}{2})$	$\pm(1,\pm\frac{1}{2},-\frac{1}{2})$	4	$-\frac{1}{6}$	S_1^2	$\pm(0,\frac{1}{2},\frac{1}{2})$	$\pm(1,-\frac{1}{2},-\frac{1}{2})$	2	$-\frac{1}{2}(1/\sqrt{3})$
	S_1^3	$\pm P_{xy}(-\frac{1}{2},\frac{1}{2},0)$		6	0	S_1^3	$\pm P_{xyz}(\frac{1}{2},-\frac{1}{2},0)$ $\pm(\frac{1}{2},\frac{1}{2},0)$		8	0
S_2	S_2^1	$\pm P_{xy}(1,0,0)$	$\pm(1,\pm1,1)$	4	$\frac{1}{3}(1/\sqrt{2})$	S_2^1	$\pm(1,0,0)$	$\pm(1,1,1)$	2	$1/\sqrt{6}$
	S_2^2	$\pm(0,0,1)$	$\pm(1,0,-2)$	2	$-\frac{2}{3}(1/\sqrt{2})$	S_2^2	$\pm(0,1,0)$	$\pm(1,-1,1)$	2	$-1/\sqrt{6}$
						S_2^3	$\pm(0,0,1)$		2	0
S_3	S_3^1	$\pm P_{xy}(1,\frac{1}{2},\frac{1}{2})$	$\pm(2,\pm\frac{1}{2},\frac{1}{2})$	4	$\frac{1}{3}(1/\sqrt{3})$	S_3^1	$\pm(1,\frac{1}{2},\frac{1}{2})$	$\pm(2,\frac{1}{2},\frac{1}{2})$	4	$\frac{1}{3}$
	S_3^2	$\pm P_{xy}(1,-\frac{1}{2},\frac{1}{2})$	$\pm(1,\pm\frac{3}{2},-\frac{1}{2})$	4	$-\frac{1}{6}(1/\sqrt{3})$		$\pm(1,-\frac{1}{2},\frac{1}{2})$	$\pm(1,1,-2)$		
	S_3^3	$\pm(\frac{1}{2},\frac{1}{2},1)$	$\pm(2,0,-1)$	6	$-\frac{2}{3}(1/\sqrt{3})$	S_3^2	$\pm(\frac{1}{2},1,\frac{1}{2})$	$\pm(2,-\frac{1}{2},\frac{1}{2})$	4	$-\frac{1}{3}$
		$\pm P_{xy}(\frac{1}{2},-\frac{1}{2},1)$	$\pm(1,\pm1,-2)$				$\pm(-\frac{1}{2},\frac{1}{2},1)$	$\pm(1,-1,-2)$		
	S_3^4	$\pm P_{xy}(1,\frac{1}{2},-\frac{1}{2})$	$\pm(1,\pm\frac{1}{2},\frac{5}{2})$	4	$\frac{5}{6}(1/\sqrt{3})$	S_3^3	$\pm(1,-\frac{1}{2},\frac{1}{2})$	$\pm(1,\frac{3}{2},-\frac{1}{2})$	2	$\frac{1}{2}$
	S_3^5	$\pm P_{xyz}(-1,\frac{1}{2},\frac{1}{2})$		6	0	S_3^4	$\pm(-\frac{1}{2},1,\frac{1}{2})$	$\pm(1,-\frac{3}{2},-\frac{1}{2})$	2	$-\frac{1}{2}$
						S_3^5	$\pm(1,\frac{1}{2},-\frac{1}{2})$	$\pm(1,\frac{1}{2},\frac{5}{2})$	2	$\frac{1}{6}$
						S_3^6	$\pm(\frac{1}{2},1,-\frac{1}{2})$	$\pm(1,-\frac{1}{2},\frac{5}{2})$	2	$-\frac{1}{6}$
						S_3^7	$\pm P_{xyz}(-1,\frac{1}{2},\frac{1}{2})$ $\pm(\frac{1}{2},\frac{1}{2},1)$		8	0
S_4	S_4^1	$\pm(1,1,0)$	$\pm(2,0,2)$	2	$\frac{2}{3}$	S_4^1	$\pm(1,0,1)$	$\pm(2,1,-1)$	2	$1/\sqrt{3}$
	S_4^2	$\pm P_{xy}(1,0,1)$	$\pm(2,\pm1,-1)$	4	$-\frac{1}{3}$	S_4^2	$\pm(0,1,1)$	$\pm(2,-1,-1)$	2	$-1/\sqrt{3}$
	S_4^3	$\pm P_{xyz}(1,-1,0)$		6	0	S_4^3	$\pm P_{xyz}(1,-1,0)$ $\pm(1,1,0)$		8	0

TABLE VII. Interpolation functions f_j for a face-centered cubic lattice and coefficients B_j fitted to ultrasonic-attenuation measurements in copper (Ref. 2). The strains are those described in Table VI. The notation for crystal coordinates is the same as that given in Table II. For experimental coordinates $X \equiv k_1 a_0/\sqrt{3}$, $Y \equiv k_2 a_0/\sqrt{2}$, $Z \equiv k_3 a_0/\sqrt{6}$, where $\vec{k}_1 \| [100]$, $\vec{k}_2 \| [010]$, and $\vec{k}_3 \| [001]$ in the experiment reference frame.

	j	B_j	f_j (crystal coord.)	f_j (expt. coord.)
ϵ_1	1	0.300	$\frac{1}{3}[2C(\frac{1}{2}x+\frac{1}{2}y)-C(\frac{1}{2}x+\frac{1}{2}z)-C(\frac{1}{2}y+\frac{1}{2}z)]$	$\frac{2}{3}[C(X+Z)-C(X-\frac{1}{2}Z)C(\frac{1}{2}Y)]$
($\vec{q} \| [111]$,	2	0.266	$(\sqrt{2}/3)[C(x)+C(y)-2C(z)]$	$(2\sqrt{2}/3)[C(X+Z)C(Y)-C(X-2Z)]$
$\vec{u} \| [11\bar{2}]$)	3	0.099	$\frac{1}{3}[2C(x+\frac{1}{2}y+\frac{1}{2}z)+2C(\frac{1}{2}x+y+\frac{1}{2}z)-C(\frac{1}{2}x-y-\frac{1}{2}z)$ $-C(x-\frac{1}{2}y+\frac{1}{2}z)-4C(\frac{1}{2}x-\frac{1}{2}y+z)-4C(\frac{1}{2}x-\frac{1}{2}y-z)$ $-4C(\frac{1}{2}x+\frac{1}{2}y+z)+5C(\frac{1}{2}x+y-\frac{1}{2}z)+5C(x+\frac{1}{2}y-\frac{1}{2}z)]/\sqrt{3}$	$\frac{2}{3}\{[2C(2X+Z)+5C(X+5Z/2)]C(\frac{1}{2}Y)-2C(2X-Z)$ $-4C(X-2Z)C(Y)-2C(X-\frac{1}{2}Z)C(3Y/2)\}/\sqrt{3}$
	4	0.155	$\frac{2}{3}[2C(x+y)-C(x+z)-C(y+z)]$	$(4/3)[C(2X+2Z)-C(2X-Z)C(Y)]$
ϵ_2	1	0.171	$[C(\frac{1}{2}x+\frac{1}{2}z)-C(\frac{1}{2}y+\frac{1}{2}z)]/\sqrt{3}$	$-(2/\sqrt{3})S(X-\frac{1}{2}Z)S(\frac{1}{2}Y)$
($\vec{q} \| [111]$,	2	0.247	$(\sqrt{2}/\sqrt{3})[C(x)-C(y)]$	$-(2\sqrt{2}/\sqrt{3})S(X+Z)S(Y)$
$\vec{u} \| [1\bar{1}0]$)	3	−0.016	$\frac{1}{3}[C(x+\frac{1}{2}y-\frac{1}{2}z)-C(\frac{1}{2}x+y-\frac{1}{2}z)+2C(\frac{1}{2}x-\frac{1}{2}y+z)$ $-2C(\frac{1}{2}x-\frac{1}{2}y-z)+2C(x+\frac{1}{2}y+\frac{1}{2}z)-2C(\frac{1}{2}x+y+\frac{1}{2}z)$ $+3C(x-\frac{1}{2}y+\frac{1}{2}z)-3C(\frac{1}{2}x-y-\frac{1}{2}z)]$	$-\frac{2}{3}\{[2S(2X+\frac{1}{2}Z)+S(X+5Z/2)]S(\frac{1}{2}Y)$ $+2S(X-2Z)S(Y)+3S(X-\frac{1}{2}Z)S(3Y/2)\}$
	4	0.038	$(2/\sqrt{3})[C(x+z)-C(y+z)]$	$-(2/\sqrt{3})S(2X-Z)S(Y)$

frame related to the geometry of the experiment. We take $\vec{q} \| [100]$, $\vec{u} \| [1\bar{1}0]$ for $\underline{\epsilon}_1$, and $\vec{u} \| [010]$ for $\underline{\epsilon}_2$; i.e.,

$$\underline{\epsilon}_1 = \frac{e}{2}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \underline{\epsilon}_2 = \frac{e}{2}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{20}$$

in the experiment reference frame. Vectors can be transformed from the crystal to the experiment frame using

$$\vec{R}_{expt} = \underline{A} \cdot \vec{R}_{crystal}, \tag{21}$$

where

$$\underline{A} = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{bmatrix}. \tag{22}$$

The stars which are split from the cubic stars are shown in Table VI for the two strains, along with values calculated for the strain derivatives of the lattice vectors. These are used to construct the expansion functions f_j shown in Table VII along with the coefficients obtained by fitting to ultrasonic attenuation measurements.[2]

VI. SUMMARY AND CONCLUSIONS

A straightforward method for deriving expansion functions with the symmetry of a strained lattice has been developed. Fermi-surface cross-sectional area changes, computed with expansion functions fitted to calculated energy shifts, are in good agreement with de Haas–van Alphen experiments.

Expansion functions with symmetries appropriate to ultrasonic waves are convenient for parametrized calculations of attenuation and can be used, in conjunction with experiments, to obtain values of the deformation potential over the Fermi surfaces of metals.

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