confirmation of the theory for the magnetic-field-induced surface quantum states.

Throughout the present work, we have aimed to illustrate how various physical parameters can be obtained from an analysis of the experimental data. Certain refinements in the calculation (as well as in the experiments) will be necessary to eventually produce a point-by-point fit of experiment and calculations. In view of remaining discrepancies, it would only be fair to emphasize that the present work is meant as an "in principle" demonstration of what one can learn. The assignment of the oscillatory signal, as due to a ridge along the Fermi surface of indium, must be considered as tentative until more exhaustive studies have been completed.

ACKNOWLEDGMENTS

We wish to thank J. D. Jensen for supplying the experimental data on the indium (111) plane that has been analyzed in this work, and acknowledge the support of the Naval Ordnance Laboratory in carrying out some of the experimental work. We thank the Computer Science Center of the University of Maryland for making available time for the numerical calculations.

PHYSICAL REVIEW VOLUME 174, NUMBER 3 15 OCTOBER 1968

Angular Forces in the Lattice Dynamics of Face-Centered Cubic Metals. II

Y. P. VARSHNI AND P. S. YUEN
Department of Physics, University of Ottawa, Ottawa 2, Canada
(Received 11 June 1968)

The lattice dynamics of the fcc lattice has been investigated with a model in which interatomic forces include, in addition to central forces, angular forces of the type suggested by de Launay. The model has been applied to copper, and results have been compared with a model investigated previously which had angular forces of the type employed by Clark, Gazis, and Wallis.

INTRODUCTION

RECENTLY, the authors[1] have investigated the lattice dynamics of fcc metals using a model in which, in addition to central forces, angular forces of the type employed by Clark, Gazis, and Wallis[2] (CGW) were included. The CGW model was applied to copper. The angular forces in this model arise from the resistance to deformation of certain angles formed by three lattice points. The change in the potential energy due to a change $\delta\theta$ in the angle θ is given by $\frac{1}{2}\kappa(\delta\theta)^2$, where κ is the angular-force constant.

de Launay[3] has considered another type of angular force which depends on the angle that the line joining the moving atoms makes with the equilibrium position of the line. The mechanical analogy is a rod connecting the particles, the rod being fastened at its ends to the equilibrium position by springs perpendicular to the rod. Hendricks, Riser, and Clark[4] have used a model that has central forces up to second neighbors and angular forces up to first neighbors to calculate the vibrational spectra and specific heats of lithium and vanadium (bcc lattice). In the present paper, we investigate a model for the fcc lattice that has central and angular forces (de Launay type) up to and including second neighbors and apply this model to copper. This model will be called the DAF (de Launay angular-force) model.[5]

DAF MODEL

We consider a monoatomic fcc lattice and represent the central-force constants for the first and second neighbors by α_1 and α_2 and the angular-force constants by σ_1 and σ_2.

As shown by de Launay,[2] the displacement that is effective for the angular-force constant σ due to displacements $\mathbf{s}_m$ and $\mathbf{s}_n$ of the particle m and particle n, respectively, is given by $\boldsymbol{\varepsilon}_{mn}\times(\mathbf{s}_n-\mathbf{s}_m)$, where $\boldsymbol{\varepsilon}_{mn}$ is the unit vector from the particle m to the particle n. Thus the change in potential energy due to $\mathbf{s}_m$ and $\mathbf{s}_n$ is

$$V_\sigma=\tfrac{1}{2}\sigma[\boldsymbol{\varepsilon}_{mn}\times(\mathbf{s}_n-\mathbf{s}_m)]^2. \quad (1)$$

Using standard methods, the secular equation for the determination of the angular frequencies ω may be derived. We merely quote here the result:

$$|D(\mathbf{q})-\omega^2MI|=0, \quad (2)$$

where M is the mass of a particle and I is the 3×3 unit matrix. The elements of the dynamical matrix $D(q)$ are as follows:

$$D_{xx}=4\alpha_1+8\sigma_1-2(\alpha_1+\sigma_1)C_1(C_2+C_3)-4\sigma_1C_2C_3+4\alpha_2S_1^2+4\sigma_2(S_2^2+S_3^2), \quad (3)$$

[1] P. S. Yuen and Y. P. Varshni, Phys. Rev. **164**, 895 (1967).
[2] B. C. Clark, D. C. Gazis, and R. F. Wallis, Phys. Rev. **134**, A1486 (1964).
[3] J. de Launay, Solid State Phys. **2**, 220 (1956).
[4] J. B. Hendricks, H. N. Riser, and C. B. Clark, Phys. Rev. **130**, 1377 (1963).
[5] Not to be confused with the better known de Launay electron-gas model.

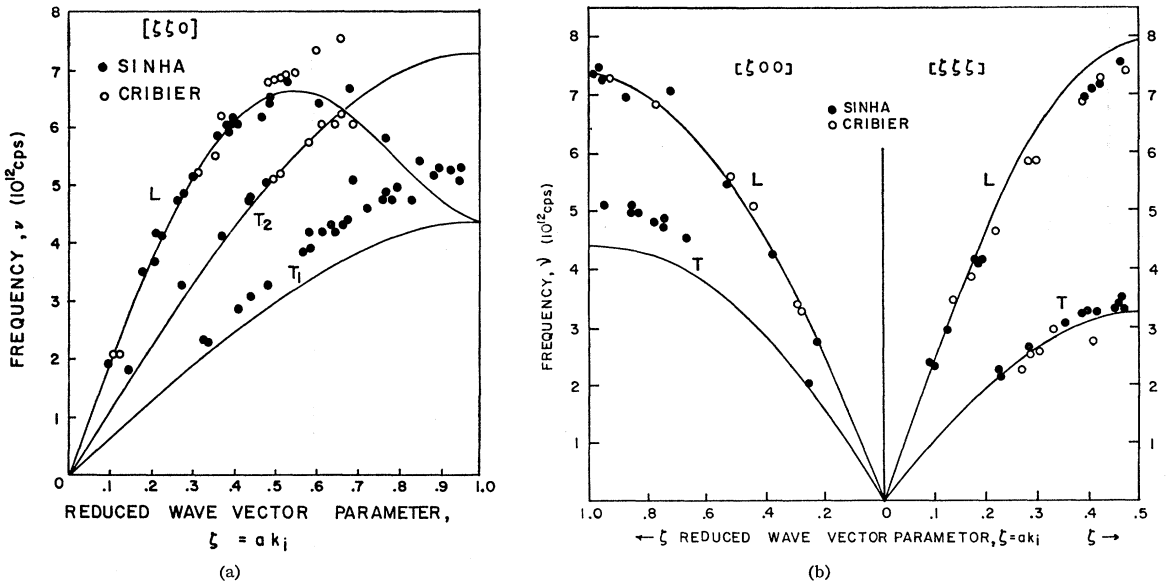

FIG. 1. Dispersion curves of copper at 300°K. The curves shown are theoretical ones obtained from the DAF model. Experimental points: ● (Ref. 6), ○ (Ref. 7).

and

$$D_{xy}=2(\alpha_1-\sigma_1)S_1S_2, \tag{4}$$

where

$$C_j=\cos\pi ak_j, \quad S_j=\sin\pi ak_j; \tag{5}$$

k_1, k_2, and k_3 are components of $\mathbf{k}$ in Cartesian coordinates, and a is the lattice constant.

As was the case in Ref. 1, we determine the four force constants in terms of the three elastic constants c_{11}, c_{12}, and c_{44} and the longitudinal-phonon frequency ν_b in the [100] direction at the Brillouin-zone boundary given by

$$\nu_b=(1/\pi)[(2/M)(\alpha_1+\sigma_1)]^{1/2}. \tag{6}$$

The resulting expressions are as follows:

$$\alpha_1=\tfrac{1}{4}a(c_{12}+c_{44})+\tfrac{1}{4}\pi^2\nu_b^2M, \tag{7}$$

$$\alpha_2=\tfrac{1}{4}ac_{11}-\tfrac{1}{4}\pi^2\nu_b^2M, \tag{8}$$

$$\sigma_1=-\tfrac{1}{4}a(c_{12}+c_{44})+\tfrac{1}{4}\pi^2\nu_b^2M, \tag{9}$$

and

$$\sigma_2=\tfrac{1}{8}a(c_{12}+3c_{44})-\tfrac{1}{4}\pi^2\nu_b^2M. \tag{10}$$

APPLICATION TO COPPER

With a view to comparing this model with the CGW model treated in Ref. 1, calculations were carried out for copper at two temperatures, 0 and 300°K. The experimental data used are the same as those given in Table I of Ref. 1. The force constants calculated from Eqs. (7)–(10) are shown in Table I. The dispersion curves were calculated from the 300°K data and are compared with the experimental data[6,7] in Figs. 1(a) and 1(b). Recently, Svensson, Brockhouse, and Rowe[8] have accurately measured the dispersion curves of copper; their results are close to those of Sinha.[6] The histogram for the vibrational frequency distribution $g(\nu)$ is shown in Fig. 2. The calculated effective calori-

TABLE I. Force constants for copper. All values are in the units of 10^3 dyn/cm.

Temp. (°K)	α_1	α_2	σ_1	σ_2
0	32.99	1.500	−4.248	2.304
300	31.66	1.344	−3.913	1.833

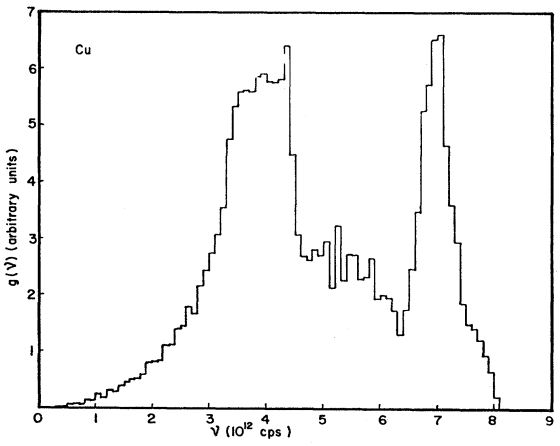

FIG. 2. Frequency-distribution histogram for copper at 0°K.

[6] S. K. Sinha, Phys. Rev. **143**, 422 (1966).
[7] D. Cribier, B. Jacrot, and D. Saint-James, in *Proceedings of the International Atomic Energy Agency Symposium on Inelastic Scattering of Neutrons in Solids and Liquids, Vienna, 1960* (International Atomic Energy Agency, Vienna, 1961), p. 549.
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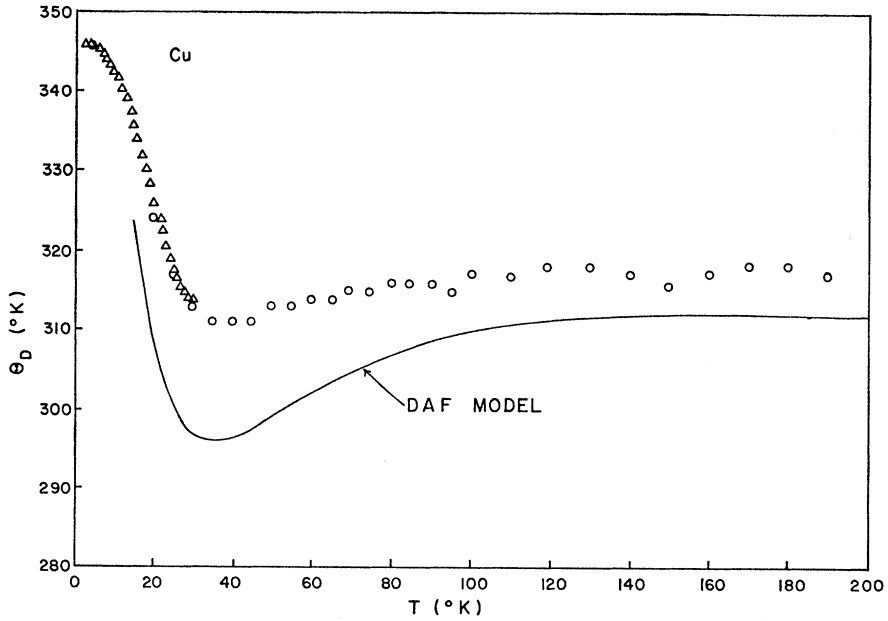

FIG. 3. Calculated and experimental calorimetric Debye temperatures of copper. Experimental points: △ (Ref. 10), ● (Ref. 9).

metric (Θ_D) Debye temperatures are shown in Fig. 3, along with the experimental points due to Martin.[9,10]

DISCUSSION

The CGW model examined in Ref. 1 and the DAF model considered in this paper both have four parameters and a comparison would be appropriate. The results for the dispersion curves can be conveniently compared by writing down the expressions for the frequencies directly in terms of the elastic constants and ν_b. These are given below.

CGW Model

(i) [ζ00] direction:

$$\nu(L)=(1/2\pi)\{(1/M)[2\pi^2\nu_b^2M(1-C_1)+(ac_{11}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (11)$$

$$\nu(T)=(1/2\pi)\{(1/M)[(ac_{12}+ac_{44}-2\pi^2\nu_b^2M)\times(C_1-1)+(\tfrac{1}{2}ac_{12}+\tfrac{3}{2}ac_{44}-\pi^2\nu_b^2M)\times S_1^2]\}^{1/2}; \quad (12)$$

(ii) [ζζ0] direction:

$$\nu(L)=(1/2\pi)\{(1/M)[(ac_{12}+ac_{44}-2\pi^2\nu_b^2M)\times(C_1-1)+(ac_{11}+\tfrac{3}{2}ac_{12}+\tfrac{5}{2}ac_{44}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (13)$$

$$\nu(T_1)=(1/2\pi)\{(1/M)[(ac_{12}+ac_{44}-2\pi^2\nu_b^2M)\times(C_1-1)+(ac_{11}-\tfrac{1}{2}ac_{12}+\tfrac{1}{2}ac_{44}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (14)$$

and

$$\nu(T_2)=(1/2\pi)\{(1/M)[2\pi^2\nu_b^2M(1-C_1)+(2ac_{44}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}; \quad (15)$$

(iii) [ζζζ] direction:

$$\nu(L)=(1/2\pi)[(a/M)(c_{11}+2c_{12}+4c_{44})]^{1/2}S_1, \quad (16)$$

$$\nu(T)=(1/2\pi)[(a/M)(c_{11}-c_{12}+c_{44})]^{1/2}S_1. \quad (17)$$

DAF Model

(i) [ζ00] direction:

$$\nu(L)=(1/2\pi)\{(1/M)[2\pi^2\nu_b^2M(1-C_1)+(ac_{11}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (18)$$

$$\nu(T)=(1/2\pi)\{(1/M)[\pi^2\nu_b^2M(1-C_1)+(ac_{44}-\tfrac{1}{2}\pi^2\nu_b^2M)S_1^2]\}^{1/2}; \quad (19)$$

(ii) [ζζ0] direction:

$$\nu(L)=(1/2\pi)\{(1/M)[\pi^2\nu_b^2M(1-C_1)+(ac_{11}+ac_{12}+2ac_{44}-\tfrac{1}{2}\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (20)$$

$$\nu(T_1)=(1/2\pi)\{(1/\mathrm{M})[\pi^2\nu_b^2M(1-C_1)+(ac_{11}-ac_{12}-\tfrac{1}{2}\pi^2\nu_b^2M)S_1^2]\}^{1/2}, \quad (21)$$

and

$$\nu(T_2)=(1/2\pi)\{(1/M)[2\pi^2\nu_b^2M(1-C_1)+(2ac_{44}-\pi^2\nu_b^2M)S_1^2]\}^{1/2}; \quad (22)$$

(iii) [ζζζ] direction:

$$\nu(L)=(1/2\pi)[(a/M)(c_{11}+2c_{12}+4c_{44})]^{1/2}S_1, \quad (23)$$

$$\nu(T)=(1/2\pi)[(a/M)(c_{11}-c_{12}+c_{44})]^{1/2}S_1. \quad (24)$$

On comparing these two sets of equations, we note that the longitudinal dispersion curves in the [ζ00]

[9] D. L. Martin, Can. J. Phys. 38, 17 (1960).
[10] D. L. Martin, Phys. Rev. 141, 576 (1966).

direction, the transverse dispersion curves T_2 in the [$\zeta\zeta$0] direction, and the longitudinal and transverse dispersion curves in the [$\zeta\zeta\zeta$] direction are identical for the two angular-force models. Figure 1(a) and 1(b) of this paper and Figs. 3(a) and 3(b) of Ref. 1 show that for the remaining three branches the curves from the DAF model are in poorer agreement with the experimental data than those from the CGW model.

The frequency spectrum for the DAF model, while showing two peaks as in the case of CGW model, gives a somewhat greater weight to the low-frequency peak as compared with the spectrum obtained from the CGW model.

The theoretical curve for Θ_D lies below the experimental points over the whole temperature range. The curve shown in Fig. 3 was obtained from the 0°K frequency-spectrum histogram. If calculations are carried out in the quasiharmonic approximation, the theoretical curve is found to be lower than that shown in Fig. 3, i.e., the divergence from the experimental data is greater.

Further, note that the DAF model suffers from the defect of not being rotationally invariant. The CGW model, on the other hand, is rotationally invariant.[11]

In conclusion, we find that for copper the CGW model is better than the DAF model.

ACKNOWLEDGMENTS

The authors are grateful to Dr. J. A. Morrison for helpful discussions and to the National Research Council of Canada for financial support.

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PHYSICAL REVIEW VOLUME 174, NUMBER 3 15 OCTOBER 1968

Optimum Form of a Modified Heine-Abarenkov Model Potential for the Theory of Simple Metals*

ROBERT W. SHAW, JR.†
Division of Applied Physics, Stanford University, Stanford, California 94305
(Received 1 March 1968)

A modified form of the Heine-Abarenkov model potential is proposed. The core potential is replaced with a constant potential A_l only for those angular momenta for which there are core wave functions. Also, the model radius R_l is allowed to be different for each l and to depend on energy. It is shown that this potential can be optimized using a variational procedure. The optimum model parameters are obtained by choosing an R_l such that $A_l=-v(R_l)$. The optimized form of this modified model potential has several advantages. It provides a unique prescription for selecting model radii, and it eliminates the necessity of approximating the A_l for $l>2$. Also, the form factors tend to decay rather than oscillate at short wavelengths. The linear extrapolation of A_l versus E proposed by Animalu is shown to be valid for most simple metals. Optimum model potential parameters are obtained, and form factors and depletion holes are evaluated for a group of simple metals using the optimized model potential.

1. INTRODUCTION

THE Heine-Abarenkov (HA) model-potential theory[1–3] is, in a sense, a cross between the quantum-defect method[4] (QDM) and the pseudopotential method.[5] As in the pseudopotential method, the deep potential at each ion center is replaced with a shallow potential which is chosen so that the valence-electron wave functions have no nodes within the core. The actual value of the model potential, chosen for convenience to be a constant A_l for each value of angular momentum l, is determined in the spirit of QDM. One chooses a radius R_M outside the core and then adjusts A_l until the logarithmic derivative of the wave function inside R_M precisely matches the logarithmic derivative of the Coulomb wave function outside R_M. This matching is done only at the free-ion-term values, since only for these energies can we evaluate the external wave function without knowing the core potential (it is the Coulomb wave function that decays at infinity).

There are several features of this procedure that have never been adequately discussed. First, a single value of R_M is chosen for all l. This is not a necessary restriction but was made largely for simplicity. The choice of R_M for each element seems to have been somewhat arbitrary. Heine and Animalu[6] did notice that if they selected $A_l \cong Z/R_M$, the magnitude of the form-factor oscillations at short wavelength (large q) was reduced. Aside from this observation, no criterion has ever been given for the choice of model radius.

* Work supported by the Advanced Research Projects Agency through the Center for Materials Research at Stanford University.
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