Fermi-surface properties of alpha-phase alloys of copper with zinc

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We consider the Fermi-surface properties of the α-$Cu_{1-c}Zn_c$ system over the composition range $0 \leq c \leq 0.3$. Our calculations are based on the application of the self-consistent coherent potential approximation to the muffin-tin Hamiltonian. The predictions of the theory with respect to the radii k_{neck}, k_{100}, and k_{110}, and the size and shape of the alloy Fermi surface in several planes in the Brillouin zone are in good agreement with the available positron annihilation measurements and with the predictions of the rigid-band model. We discuss how the hitherto unmeasured disorder smearing of the alloy Fermi surface may be amenable to a direct experimental determination in concentrated alloys. The dilute impurity limit is considered in detail. The computed changes in areas for several orbits are in good accord with the corresponding results of de Haas–van Alphen experiments. The predicted Dingle temperatures, however, agree with measurements only to within a factor of 2. It is hoped that the present work will encourage further measurements, especially of the disorder smearing of the Fermi surface in concentrated alloys.

I. INTRODUCTION

Electronic spectra of the α-phase alloys of Cu with Zn have been the subject of many theoretical and experimental studies.[1,2] Most recently, the overall electronic structure of this system, on the basis of the average t-matrix approximation (ATA), was considered in Ref. 1. Since that time, however, new positron-annihilation,[3-7] differential reflectivity,[8,9] de Haas–van Alphen,[10-12] and photoemission studies[13] on α-$Cu_{1-c}Zn_c$ have appeared in the literature. Theoretical understanding of alloys has also advanced significantly within this period.[14-18] For example, the treatment of disorder on the basis of the self-consistent coherent potential approximation (CPA) has become possible.[14-15] Motivated by these developments, we have undertaken a comprehensive study of α-brasses within the framework of the muffin-tin Hamiltonian. The present paper focuses on the Fermi-surface properties; other aspects of the spectrum will be taken up elsewhere.

An outline of this article is as follows. Section II describes general aspects of the calculations. We emphasize that the present Cu and Zn potentials yield the overall spectra of Cu as well as α-brasses (in particular the position and width of the Cu and Zn $3d$ bands), in excellent agreement with the relevant experiments.[9-13] Section III presents and discusses the Fermi-surface properties. The predicted sizes and shapes of the CPA Fermi surfaces for a range of alloy compositions are in very good accord with the positron-annihilation measurements.[3-7] The isotropicity of the expansion of the alloy Fermi surface with increasing Zn content is examined. The CPA results are compared and contrasted with the corresponding rigid-band computations.

The half-width $|\Delta \vec{k}(E_F)|$ of the Fermi surface, owing to disorder smearing, is considered in detail. The quantity $|\Delta \vec{k}(E_F)|$ is a sensitive function of the direction in which the $\vec{k}$ point in question is scanned. We argue that $\Delta \vec{k}(E_F)$ should be amenable to determination in α-brasses by an appropriate choice of geometry in a two-dimensional positron-annihilation experiment with currently available resolution.

In the dilute impurity limit, the calculated values of $(1/c)(\Delta A/A)$ for the neck and belly orbits (here A denotes the orbit area) are in good accord with those obtained from recent de Haas–van Alphen experiments.[10,11] By contrast, the predicted Dingle temperatures (related to the smearing in energy of the states on the Fermi surface) are significantly lower than measured values.[10,11] We examine this discrepancy in some detail.

As is well known, various *ab initio* calculations of the properties of pure systems (particularly the transition and noble metals) differ in their predictions due to uncertainties in the crystal potential. Keeping this in mind, we have carried out a number of additional computations of the electronic structure of α-brasses, employing a variety of Cu and Zn muffin-tin potentials. On this basis, we find that the present Fermi-surface results are remarkably stable to such uncertainties inherent within the first-principles band theory of alloys.

II. GENERAL ASPECTS OF THE CALCULATIONS

The necessary muffin-tin potentials were generated by employing the overlapping charge densities Mattheiss prescription.[19,20] Our Cu potential is essentially the same as that used by

O'Sullivan *et al.*,[22] and yields the Fermi surface and principal energy gaps of Cu in excellent agreement with experiment.[22,23]

The lattice constant of $Cu_{1-c}Zn_c$ alloys increases linearly with Zn content (the increase amounts to 2% for 30-at. % Zn).[24] The inclusion of this effect requires the construction of muffin-tin potentials for the constituent atoms on a concentration-dependent lattice.[25] However, it is more convenient to carry out the computations for a fixed value of the lattice constant and apply a correction for the effect of expansion. These corrections (varying linearly with Zn content) were obtained by comparing the Fermi surface of $Cu_{0.7}Zn_{0.3}$ on the basis of observed (i.e., 2% expanded) and unexpanded (i.e., that of Cu) lattice.[26]

In briefly commenting on the aspects of electronic structure of α-brasses, other than the Fermi-surface properties, we note that the computed composition dependence of the edge in ϵ_2 spectrum (monitored by the energy of transitions from the top of the Cu $3d$ bands to the alloy Fermi energy) is in excellent agreement with the recent differential reflectivity experiments of Hummel and collaborators.[8,9] Therefore, in contrast to Ref. 1, no semiempirical adjustments of the alloy potential (in order to obtain the correct behavior of the edge) were necessary.[27] In the present calculations, the Zn $3d$ resonance appears 10.1 eV below the Fermi energy with a width of 1.0 eV. Furthermore, the position and width of the Cu $3d$ bands is found to be essentially independent of the alloy composition. These theoretical predictions are also in good accord with the photoemission measurements of Norris and Williams.[13]

The basic formalism for treating the muffin-tin Hamiltonian, employed in this article, has been discussed in the literature, and would therefore not be considered.[14-18] Nonetheless, two points concerning the implementation of the muffin-tin CPA that arose during the course of this work are noteworthy.

(i) The conventional iteration schemes for solving the CPA equation were generally found to converge slowly and often fail in the negative-energy regime (particularly in the Zn d bands). This necessitated the development of appropriate techniques for solving the self-consistency condition in such cases.

(ii) The CPA Fermi energy is obtainable directly without requiring the density-of-states function at all energies.[14,15] To use this property of the CPA, however, spurious jumps in the integrated density of states associated with the zeros of the constituent-atom phase shifts must be subtracted. This required a particular care in the regime of low impurity concentrations.

III. FERMI-SURFACE PROPERTIES

Figure 1 shows the CPA and rigid-band[28] predictions for the neck and belly radii against available positron-annihilation determinations of these quantities. The upper pairs of curves in these figures were obtained by assuming the alloy to possess the same lattice constant as pure Cu. The lower pairs of curves include the effects of lattice expansion and are to be compared with the experimental points. Of the various neck measurements, the data of Morinaga[29] and Williams *et al.*[30] [cf. Fig. 1(a)] employ the "rotating-specimen" method and may involve systematic errors.[31] The measurement of Becker *et al.*[32] for 15-at. % Zn is probably an upper limit and has a rather large error bar ($\simeq 0.55$ mrad, not shown). The remaining long-slit data of Triftshäuser and Stewart[33] and the recent two-dimensional multidetector measurements of Berko and collaborators[3-6] are in very good agreement with the theoretical curves. The data on k_{100} and k_{110}, although relatively scant, are also in good accord with the theory [see Fig. 1(b)]. It is noteworthy that the differences between the theory and experiment for the k_{110} radius are at the limits of the reported error bars on the experimental values. A more accurate determination of k_{110} might prove it to be particularly interesting. Finally, Fig. 2 compares the absolute magnitudes of theoretically predicted Fermi-surface dimensions in three symmetry planes for Cu and $Cu_{0.7}Zn_{0.3}$ with the recent two-dimensional positron-annihilation measurements.[6] The level of agreement between the theory and experiment is once again seen to be very good. The various calculated radii are summarized in Table I.

We turn now to the question of smearing of the alloy Fermi surface due to disorder scattering, which is represented by shading on the CPA curves in Figs. 1 and 2. Note that, in a perfect crystal, the spectral density function $A(\vec{k}, E)$ consists of δ-function peaks corresponding to real Bloch energy levels. In an alloy, the disorder causes these energy levels to become complex, and hence the peaks in the spectral function to assume finite widths. For a given real-crystal momentum $\vec{k}_F$ (on the Fermi surface) the half-widths at half maximum of $A(\vec{k}, E_F)$, as a function of energy E [denoted by $\Delta E(\vec{k}_F)$ here], have previously been related to the imaginary parts of the complex energy levels and also to the measured Dingle temperatures.[1] The diffuseness of the alloy Fermi surface, however, is to be characterized by the half-width $\Delta \vec{k}(E_F)$ of $A(\vec{k}, E_F)$ as a function of $|\vec{k}|$ along a given direction in the Brillouin zone. Although the two half-widths
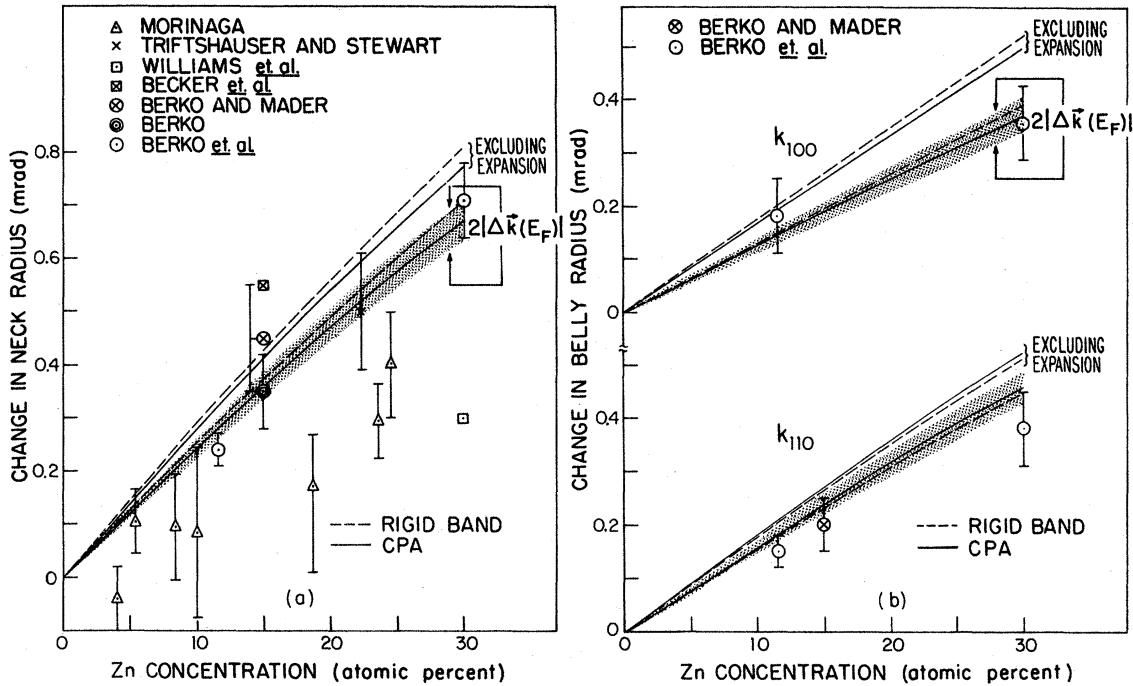
FIG. 1. Changes in (a) the [111] neck and (b) the [100] and [110] belly radii k_{100} and k_{110} of Cu in milliradians (1 mrad =0.137 a.u.) as a function of Zn concentration for the CPA (solid) and the rigid-band model (dashed) (Ref. 28). The upper pairs of curves exclude the effects of lattice expansion (see text). The vertical length of shading on the lower CPA curves gives the disorder smearing $2|\Delta\vec{k}(E_F)|$. For the neck orbit (a), $2|\Delta\vec{k}(E_F)|$ values correspond to a scan from the center of the neck orbit (i.e., the point L in the Brillouin zone) along a [110] direction on the hexagonal face. In (b), the $2|\Delta\vec{k}(E_F)|$ values are shown along the directions $\Gamma \rightarrow X$ (for k_{100}) and $\Gamma \rightarrow K$ (for k_{110}), respectively. The smearing for the CPA curves excluding lattice expansion (upper solid) is not shown. The various positron-annihilation measurements shown with the reported error bars are as follows: $\triangle$, Morinaga (Ref. 29), $\times$, Triftshäuser and Stewart (Ref. 33), $\square$, Williams et al. (Ref. 30), $\blacksquare$, Becker et al. (Ref. 32, estimated error bars of $\simeq \pm 0.55$ mrad are not shown), $\odot$, Berko and Mader (Ref. 3), $\bigodot$, Berko (Ref. 4), Berko et al. (Refs. 5 and 6).

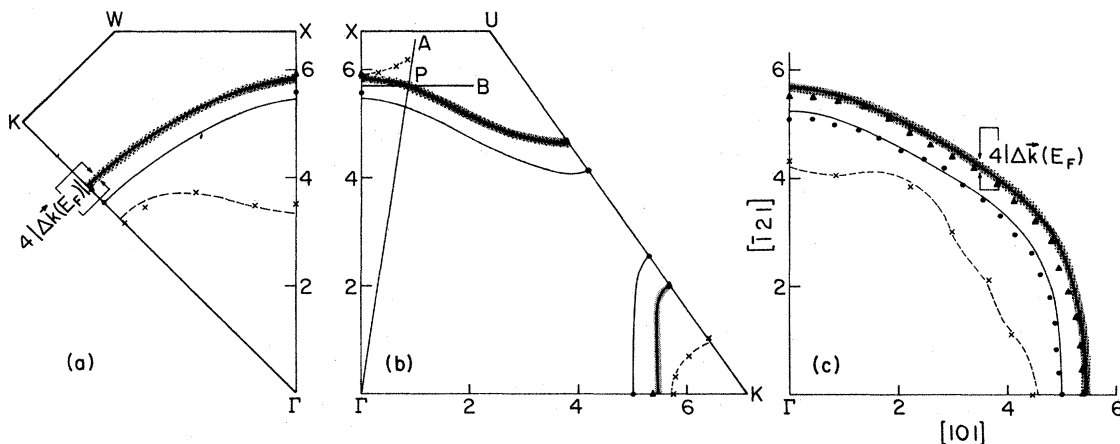
FIG. 2. Intersections of the Fermi surface of Cu (unshaded solid) and $Cu_{0.7}Zn_{0.3}$ (shaded solid) in three different planes in the Brillouin zone. For CPA curves, the length of the shading intersecting any line drawn in the plane of the figure gives 4 times the apparent half-width of the Fermi surface $|\Delta\vec{k}(E_F)|$ along this direction. Experimental data for Cu (filled circles) and $Cu_{0.7}Zn_{0.3}$ (filled triangles) is from Ref. 6. In (b), A and B denote two different lines going through the point P (with $P_x =5.7$ mrad) on the alloy Fermi surface (discussed in the text). The dashed curves give the ratio $|\delta k /k|$ in arbitrary units of the change δk in the radius k of a given orbit along various directions for 30-at.% Zn, where $|\vec{k}|$ is measured from the point Γ in (a) and (c), and from the points X and K in (b). The crosses give the corresponding rigid-band values of $|\delta k /k|$.

TABLE I. Fermi-surface radii k_{neck}, k_{100}, and k_{110} and the corresponding disorder smearings [see caption to Fig. 1 for the definition of $|\Delta\vec{k}(E_F)|$] for the CPA. The rigid-band (RB) results are also listed. All values are given in units of milliradians. [This table gives numerical values corresponding to the lower pairs of curves in Figs. 1(a) and 1(b)].

Zn conc. (at.%)	k_{neck}		k_{100}		k_{110}		$\|\Delta\vec{k}(E_F)\|$ (Disorder half-width)		
	CPA	RB	CPA	RB	CPA	RB	k_{neck}	k_{100}	k_{110}
0	0.967	0.967	5.471	5.471	5.003	5.003	0.0	0.0	0.0
3	1.040	1.041	5.507	5.505	5.049	5.049	0.007	0.006	0.005
10	1.212	1.220	5.594	5.594	5.163	5.163	0.020	0.015	0.016
20	1.438	1.457	5.720	5.724	5.320	5.314	0.036	0.029	0.028
30	1.639	1.676	5.834	5.861	5.460	5.453	0.040	0.032	0.031

$\Delta E(\vec{k}_F)$ and $|\Delta\vec{k}(E_F)|$ possess the same physical origin, i.e., the disorder in the alloy, they differ in substantial ways. $|\Delta\vec{k}(E_F)|$ is approximately equal to $\Delta E(\vec{k}_F)|\partial E/\partial k|^{-1}$, and can, therefore, be much larger in magnitude than $\Delta E(\vec{k}_F)$ in the vicinity of flat bands. Furthermore, the width $|\Delta\vec{k}(E_F)|$ depends strongly on the direction in which a given $\vec{k}$ point on the Fermi surface is scanned. As an illustration, consider the point P in Fig. 2(b), corresponding to $P_x = 5.7$ mrad. The width of this point along the horizontal direction (i.e., the length of shading intersecting line B) is nearly 3–4 times greater than the width along line A. [This effect is seen in Fig. 2(b) to become more pronounced as one approaches higher values of the momentum component P_x on the alloy Fermi surface.] Therefore, a two-dimensional positron-annihilation experiment with $P_x = 5.7$ mrad and integration along the direction perpendicular to the plane of Fig. 2(b) should be able to measure this half-width with the currently available resolutions on the order of 0.07 mrad. With the preceding remarks in mind, it is not hard to pick directions suitable for this sort of "geometrical magnification" of the width of other features of the alloy Fermi surface (particularly the necks).[34] We emphasize that, in view of Figs. 1 and 2, the "intrinsic" width (which may be defined as the width normal to the surface) is rather isotropic. Therefore, the measurement of $|\Delta\vec{k}(E_F)|$ at relatively few points should lead to a good overall description of the smearing of the entire alloy Fermi surface.

As has been noted elsewhere,[1,7] Figs. 1 and 2 also show that the current positron-annihilation data is in good overall agreement with the rigid-band predictions. The reason for the close similarity between the CPA and rigid-band curves is that the volume enclosed by the CPA Fermi surface in $Cu_{1-c}Zn_c$ would accommodate $(1+c)$ electrons (within numerical accuracy) as is the case for the rigid-band model.[35] In fact, so long as

this volume constraint is satisfied, many widely different models can lead to essentially similar Fermi surfaces.[36] This does not mean that the underlying spectrum is correct in each case. For example, the rigid-band description of $Cu_{1-c}Zn_c$ suffers from very serious deficiencies; the disorder scattering is zero and, in addition, only one d resonance is obtained whose energy location drops rapidly with increasing Zn content.[1]

To consider the isotropicity of expansion of the Fermi surface with increasing Zn content, the quantities $(\delta k/k)$ (with δk representing the change, in a given direction of the radius k of a specific orbit from its center for 30-at. % Zn) are also plotted in Fig. 2. The deviations of the dashed curves in this figure from a circular shape are relatively small and represent the extent to which the expansion is anisotropic. Much of this anisotropy, however, appears to be inherent to the band structure of Cu, rather than being the effect of disorder, since this anisotropy is also present in the rigid-band model (shown by crosses).

In any first-principles calculation, the predictions of the theory depend upon the particular choice of muffin-tin potentials for the constituent atoms.[1] To ascertain the magnitude of such uncertainties, inherent to the present framework, we have carried out a number of additional computations (CPA and ATA) of the alloy Fermi surface, on the basis of Cu and Zn potentials which differ[39] from those used to obtain the results reported in this article. The uncertainty in incorporating the lattice-expansion effects was estimated by considering several different computations of the Fermi surface of Cu as a function of a varying lattice constant.[26,40] Finally, the CPA and the corresponding ATA predictions were compared[41] to determine the extent to which the Fermi surface of the CuZn alloys is influenced by self-consistency in the treatment of disorder.

The calculations referred to in the preceding paragraph show that our predictions concerning

the Fermi surface of CuZn alloys are remarkably stable to a variety of changes in the constituent potentials and also to the degree of self-consistency achieved in treating disorder. We emphasize that, within the present single-site framework, various physical effects (such as lattice expansion, transfer of charge between atomic species, etc.) must eventually induce changes in the atomic potentials in order to be manifest in the electronic spectrum. On this basis, we estimate the margin of variability in the CPA neck and belly radii given in Fig. 1 to be ±0.07 mrad for 30-at.% Zn. (Note that since changes in radii, with respect to Cu, are plotted in Fig. 1, this uncertainty will decrease linearly to zero for vanishing Zn concentration.) The corresponding variability in the disorder smearing of the Fermi surface is estimated to be ±30% of the values given in Table I and shown in Fig. 1. It is quite unlikely that, within the single-site framework, deviations from the present predictions concerning the Fermi surface well beyond the ranges indicated above can be explained in a manner consistent with the optical reflectivity and photoemission experiments on α-brasses. The relative lack of sensitivity of the Fermi surface of this system also implies that measurements with resolutions on the order of 0.01 mrad will be necessary to discriminate meaningfully between different theoretical computations.

Turning to the low-impurity-concentration regime, Table II shows that the predicted CPA changes in the areas of neck and belly orbits are in excellent accord with the corresponding experimental values.[10] The agreement between the CPA and the rigid-band computations of $(1/c)(\Delta A/A)$ is to be anticipated in view of the closeness of the two approximations seen in Fig. 1. The corrections due to lattice expansion listed in column 4 are in good agreement with the pressure measurements on various orbits in Cu.[44]

In contrast to the size of the alloy Fermi surface (determined by the real parts of complex energy levels), the computed Dingle temperatures (related to the imaginary parts of complex levels) are seen from Table II to be substantially lower than the experimental values.[45] The scattering of electrons due to lattice defects and strain fields around impurities,[47,48] neglected in the present theory, would account for a part of this discrepancy. The neglected electron-phonon renormalization effects,[46,49] on the other hand, would *decrease* the theoretical x values by approximately 10%, thereby worsening this discrepancy. In this connection, values of m^*x are also listed in Table II, since this quantity is expected to be independent of such electron-phonon effects.[46]

Figure 3 shows what may be called local Dingle temperatures[45] at various points on the Fermi surface of Cu. It is evident that the disorder scattering is the weakest for the neck electrons. This is reflected in the CPA values (see Table II) of the $x_N/x_B < 1$. The predicted anisotropy of scattering, however, is not in accord with experiment, which yields $x_N/x_B \gtrsim 1$. Our conclusion on the basis of calculations employing a variety of Cu and Zn atomic potentials is that the discrepancies between theory and experiment with regard to Dingle temperatures seen in Table II are at the upper limit of what can possibly be explained as uncertainties inherent within the present framework.[50]

The fact that the present CPA Fermi-surface radii in CuZn are in good agreement with the rigid-band (RB) model should not be taken to imply that this model can be generally relied upon to predict the Fermi-surface geometry in transition and noble-metal alloys. For example, large deviations from the RB behavior are found in CuNi (Ref. 52), CuGe (Ref. 53), and PdH$_x$ (Ref. 54) alloys. The growing evidence is that the simple RB model would generally predict poorly the over-

TABLE II. Changes $(1/c)$ $(\Delta A/A)$ in orbital areas A, in the dilute limit, for three Fermi-surface orbits on the basis of CPA and the rigid-band (RB) model. The corresponding orbital Dingle temperatures x and the quantities m^*x (here m^* denotes the cyclotron mass in units of bare electronic mass) are also listed, together with the results of de Haas–van Alphen measurements of Templeton and Vasek (Ref. 10). The lattice-expansion corrections (included in columns 2 and 3) are given in column 4.

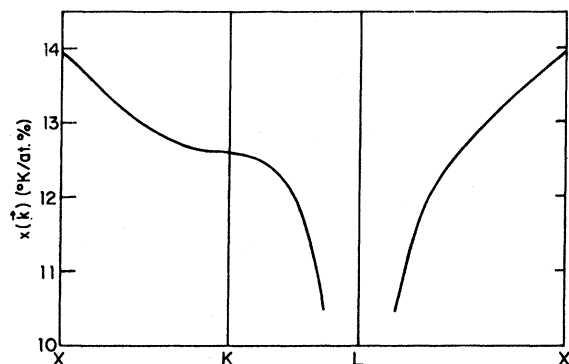| | $(1/c)(\Delta A/A)$ per at.% × 10^{-2} | | | | Dingle temperature (x) K/at.% | | m^*x K/at.% | |
Orbit	CPA	RB	Expt.	Latt. corr. (theoretical)	CPA	Expt.	CPA	Expt.
Neck	4.84	5.04	4.92 ± 0.46	0.68	10.5	18.5 ± 1.0	4.1	8.2 ± 0.4
B100	0.52	0.54	0.56 ± 0.01	0.11	13.1	18.1 ± 0.5	16.1	24.3 ± 0.7
B111	0.56	0.58	0.59 ± 0.02	0.11	12.3	17.8 ± 1.0	15.8	24.5 ± 1.4

FIG. 3. Anisotropy of the local Dingle temperature (Ref. 45) $x(\vec{k})$ in (010) and (110) planes of the Brillouin zone.

all spectra of alloys [e.g., absence of the virtual bound state in CuNi (Ref. 53)] and is inadequate in understanding the current experiments concerning Fermi-surface geometry of alloys [e.g., nonuniform response of the hole and electron orbits in α-PdH$_x$ (Ref. 54)].

ACKNOWLEDGMENTS

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[26]We note that these corrections are also obtainable to

a high degree of accuracy in $Cu_{1-c}Zn_c$ by considering the Fermi surface of Cu for normal and 2% expanded lattice. (See also Ref. 1.)

[27]Physically, these semiempirical adjustments were associated in Ref. 1 with transfer of charge between the constituent atoms. The fact that such adjustments were not required in the present calculations does not imply absence of charge transfer, but simply that it is difficult to address this question within the scope of this article (or Ref. 1), since the charge density in the A and B atom cells in the alloy is not computed.

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[35]It may also be noted here that the impurity bands derived from the Zn d levels possess a weight of $10c$ in $Cu_{1-c}Zn_c$. Therefore, these bands may be viewed as accommodating all the Zn $3d$ electrons.

[36]Another example would be the "sinking band" model of Refs. 37 and 38. This sort of sinking of the conduction bands, however, arises naturally in a proper calculation of the electronic spectrum because, on the average, the crystal potential in $Cu_{1-c}Zn_c$ becomes more attractive with increasing c.

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of energy) can lead physically to the transfer of charge between the atoms (Ref. 1). For these reasons, we have also considered the effects of a 0.5-Ry shift in the muffin-tin zero.

[40]Three such computations were considered: (i) the $d^{10}s$ Herman-Skillman charge densities, used to construct the present Cu potential (see Ref. 20) were overlapped on a 2% expanded lattice and the corresponding Fermi surface was obtained, (ii) the results for the "renormalized atom" potentials for the normal and expanded lattice given in Ref. 1, and (iii) the results of a calculation by Davis, Faulkner, and Joy [Phys. Rev. 167, 601 (1968)].

[41]Note that the ATA results reported earlier in Ref. 1 employed a semiempirical adjustment (within the "shifted-muffin-tin" and the "charge-renormalized" models), which forced the energy of the edge of the optical spectrum of α-brasses (with respect to Cu) by approximately 0.2 eV for 30-at. % Zn, in accord with the then existing experimental data (Refs. 42 and 43). More recent differential optical reflectivity measurements (Refs. 8 and 9), however, show this change to be 0.38 eV (as is the case in the present work) instead of 0.2 eV. In fact, if a value of 0.38 eV is used in making the adjustments in Ref. 1, a rather good agreement is obtained between such ATA and the present CPA results.

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[50]The present framework *requires* a value of the alloy muffin-tin zero, which is commonly defined as the average of the muffin-tin zeros of the constituent atoms. Therefore, the scattering of electrons arising from differences in potentials of the constituent atoms in the muffin-tin region is inherently excluded. Using perturbation theory (Ref. 51), we estimate the magnitude of this effect to be 4–7 – K/at. % Zn. Such a correction would increase the theoretical Dingle temperatures and substantially explain the discrepancy between theory and experiment in Table II.

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