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Low-temperature lattice specific heat of α-phase alloys based on gold

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The low-temperature lattice specific heat of Au-Cd, Au-Sn, and Au-Zn dilute alloys have been successfully explained on the basis of low-concentration Green's-function theory. The effects due to change in mass at the impurity site and the changes in the closest radial and angular force constants for the impurity—host-crystal interactions have been taken into account. The lattice contraction due to the introduction of Cd, Sn, or Zn impurities has also been included in the calculations. For Au—7.5-at. % Zn alloy the low-concentration theory has been modified. A reduction in the lattice specific heat due to substitution of these impurities has been observed. The calculated results compare well with the experimental data. The main contributions to the changed specific heat are caused by even-parity A_{1g}, E_g, F_{2g}, and F_{1g} symmetry modes, a feature which is not usually observed in other defect-induced physical properties.

I. INTRODUCTION

The measurement of the electronic specific heat provides one of the very useful methods for studying the electronic structure of metals. Its application to the study of the alloy phases based on the noble metals has become of particular interest following the determination, by means of a number of new techniques, of the topography of the Fermi surface in copper, silver, and gold.[1] In terms of simple models of the band structure,[2] the density of states at the Fermi level should decrease initially when the noble metals are alloyed with elements whose addition increases the electron concentration. The magnitude of the electronic specific-heat coefficient γ may be considered to give a measure of the density of states of the conduction electrons at the Fermi level. Therefore, measurements of the dependence of γ on alloying addition have been of special interest in testing the validity of the rigid-band model, and other factors such as the possible enhancement of the γ values by many-body effects and the effect of changes in the atomic volume.

In the last decade a number of low-temperature specific-heat investigations have been reported, with the specific goal of studying the band structure of the α phases, i.e., the terminal solid solutions based on the noble metals. There are a number of publications on the systems based on copper and silver.[3–8] However, only very few measurements of the low-temperature specific heat have been reported in the systems based on gold. The experimental work, particularly in the range of the terminal solid-solution α-phase alloys, has shown that systems based on Au differ in many respects from those based on Cu and Ag.[9]

The study of the lattice part of the specific heat of noble-metal alloys is also similarly very interesting, and of great use. In general the lattice specific-heat spectroscopy is universally applicable and involves all kinds of symmetry modes, whereas the application of several powerful methods like optical and inelastic neutron scattering measurements is restricted to particular classes of materials. For example, inelastic neutron scattering methods[10–12] are useful only when suitable neutron fluxes and specimen crystals are available. Similarly, the much celebrated technique of infrared absorption[13–15] may, usually, be employed only in the cases of electrically insulating crystals. Further, the infrared "sees" only the infrared-active modes. Thus, the study of a number of symmetry modes which is not readily feasible by any other experimental method, can be made by this technique. However, the resolution in specific-heat spectroscopy does not seem to be as large as in other methods.

It is well known that the substitutional impurities in the crystal produce special impurity modes, e.g., localized, resonance, or gap modes. The contribution of localized modes to the lattice part of the low-temperature specific heat is too small to be detected in the experimental measurements. On the other hand, the contribution of the low-frequency resonance modes to low-temperature specific heat is appreciable and is accessible to observation. The possibility of occurrence of a substantial enhancement due to low-frequency resonance modes was predicted by Lehman and De Wames[16] and independently by Kagan and Iosilevskii.[17] Recently, we have employed the experimental specific-heat data to investigate successfully the impurity modes in different systems, including the noble metals doped with different impurities.[18–22] Recent review articles[23] can be referred to for more details. However, no substantial lattice-dynamical work has been done on gold-based systems. In the case of Au-V alloys[24] we have observed a reduction in specific heat due to introduction of V impurities in Au, and a resonance is found in the F_{1u} irreducible representation near the maximum of the phonon frequency.

Recent measurements by Bevk *et al.*[25] on the specific heat of Au-Cd alloys prompted our lattice-dynamical study of these systems in detail. The results so obtained were compared with the specific-heat studies of Au-Sn and Au-Zn alloys, for which the experimental measurements already exist in the literature.[26,27] There is an additional interest in the study of these systems. As in some of the alloys, the Debye temperature shows an anomalous behavior due to alloying.

In earlier studies[18–20,22,24] the low-concentration Green's-function theory has been used taking the effect of single impurity and then multiplying by the concentration of impurities. This study is taken to be valid only for the concentration of impurities not exceeding 5 at. %. In the present work we have also studied the Au–7.5-at. % Zn alloy by using the approximations of Elliott and Taylor.[28] This approximation has been successfully applied by Kesharwani and Agrawal[12,29] in the study of phonon-frequency shifts and phonon-frequency widths of dilute alloys, and by us in lattice specific-heat studies of α-phase alloys based on copper and silver.[21] The present model includes the change in mass at the impurity site and the changes in the nearest-neighbor radial and angular force constants. The effect of lattice contraction due to the introduction of impurities (Cd, Sn, or Zn in Au) has also been accounted for. It is to be pointed out that the force-constant changes evaluated under this formulation can be used to explain other defect-induced properties.[19,22]

II. THEORY

A. Lattice specific heat

Owing to the presence of impurities, the change in the vibrational specific heat of a crystal (per g mole) at temperature T can be expressed as

$$\Delta C_L(T) = \frac{\hbar^2}{4k_B T^2}\int_0^\infty \omega^2 \Delta N(\omega)\operatorname{csch}^2(\hbar\omega/2k_B T)d\omega \,, \tag{1}$$

where k_B is Boltzmann's constant, $\hbar$ is Planck's constant, and ω is the phonon frequency. $\Delta N(\omega)$ denotes the change in the phonon density of states $N(\omega)$ which is defined as the number of normal modes in the interval ω and $\omega + d\omega$ in the limit as $d\omega \to 0$. $N(\omega)$ is related to a similarly defined function $N(\omega^2)$, which is a more common function in the theory of crystal-lattice dynamics as

$$N(\omega) = 2\omega N(\omega^2) \,.$$

The evaluation of $\Delta N(\omega^2)$ is very difficult for a general defect, but the problem is tractable if the perturbation caused by a defect exhibits some symmetry. For instance, one observes a point-group symmetry of the host lattice for a point defect substituted at a lattice site and considers only the impurity space of dimension $3b \times 3b$ where b is the total number of ions directly affected by a defect, including itself. A group-theoretical analysis may be performed for the change in the phonon density of states in such cases. For a crystal containing a single defect, one may therefore write

$$\Delta N(\omega^2) = \sum_\nu \Delta N_\nu(\omega^2) \,, \tag{2}$$

where $\Delta N_\nu(\omega^2)$ is the contribution made by the symmetric motion ν and is given by

$$\Delta N_\nu(\omega^2) = -\frac{l_\nu}{\pi}\operatorname{Im}\left[\frac{1}{D_\nu(z)}\frac{dD_\nu(z)}{d\omega^2}\right] . \tag{3}$$

Here l_ν is the dimension of the irreducible representation ν, $z = \omega^2 + 2i\omega\xi$ is the complex squared frequency in the limit $\xi \to 0$, and $D_\nu(z)$ is the resonance denominator corresponding to the irreducible representation ν. The expression for $D_\nu(z)$ is given by

$$D_\nu(z) = |\underline{I} + \underline{g}_\nu(z)\underline{p}_\nu(\omega^2)| \,, \tag{4}$$

where $\underline{I}$ is the unit matrix, and $\underline{p}_\nu(\omega^2)$ and $\underline{g}_\nu(z)$ are the perturbation and Green's-function matrices projected onto the subspace of irreducible representation ν.

The frequency of an impurity mode, i.e., resonance or localized mode in the symmetric motion ν may be determined by the solution of the equation

$$\operatorname{Re}D_\nu(z) = 0 \,. \tag{5}$$

The problem is simplified if we introduce the phase shifts δ_ν, a concept used extensively in solid-state scattering theory.[30] In present notation δ_ν can be defined as

$$\tan\delta_\nu = -\frac{\mathrm{Im}D_\nu(z)}{\mathrm{Re}D_\nu(z)} . \tag{6}$$

In terms of phase shift the contribution towards the change in density of states due to symmetry mode ν can be written as

$$\Delta N_\nu(\omega^2) = \frac{1_\nu}{\pi}\frac{d\delta_\nu}{d\omega^2} . \tag{7}$$

Substituting for $\Delta N(\omega)$ in Eq. (1) and integrating once by parts, the change in specific heat due to a single defect can be written as

$$\Delta C_L(T) = \sum_\nu \Delta C_L^\nu(T) , \tag{8}$$

where the contribution of each irreducible representation is

$$\Delta C_L^\nu(T) = -\frac{2k_B B'^2}{3N\pi}\int_0^\infty \delta_\nu \omega \,\mathrm{csch}^2(B'\omega) \times [1 - B'\omega\coth(B'\omega)]d\omega , \tag{9}$$

where $B' = \hbar/2k_B T$ and N is the number of unit cells in a crystal.

In the low-concentration limit we assume that the impurities do not interact among themselves and therefore the change in the density of states that is due to a small concentration of impurities in a crystal may be determined by multiplying the change due to a single defect by the impurity concentration. The total change in specific heat due to a fractional concentration c of point defects is, thus, given by

$$\Delta^{\mathrm{total}}C_L(T) = cN\Delta C_L(T) . \tag{10}$$

B. Perturbation model

The noble metal gold and its alloys, with low concentrations of cadmium, tin, and zinc, crystallize in α phase (fcc structure). For the atom Cd, Sn, or Zn occupying the substitutional site, the symmetry is seen to be O_h type. Along with a changed mass at the impurity site we consider also the changes in the radial and angular nearest-neighbor impurity—host-crystal interactions. The perturbation matrix is of dimension 39 × 39. For a monatomic fcc lattice, the pertinent expressions for the various irreducible representations are given in an earlier paper[20] in the low-concentration limits. The irreducible representations appearing in the problem are F_{1u}, F_{1g}, F_{2g}, F_{2u}, A_{1g}, A_{2g}, A_{2u}, E_g, and E_u. As the concentration of impurities increases the above expressions do not remain valid. The next simplest approximation is that of Elliott and Taylor[28] which replaces Eq. (4) by

$$D_\nu(z) = |\underline{I} + (1-c)\underline{g}_\nu(z)\underline{p}_\nu(\omega^2)| . \tag{11}$$

This approximation has taken into account exactly the scattering of phonons on single impurities and neglected scattering of clusters of impurities; i.e., we have neglected the possibility of neighboring defects interfering with the scattering on a particular defect. Although the results can be taken in a better approximation, e.g., in the coherent potential approximation[31–33] where essentially single-site self-consistent scatterings are considered after taking into account proper multiple occupancy corrections, the expressions are more involved and are intractable to computation for the case of a more complex defect. Also at higher concentrations of impurities the alloys concerned change their phase and are no longer in the α phases.

The expressions for the resonance denominators for a monatomic fcc lattice in the approximation of Elliott and Taylor can be obtained from the earlier expressions[20] if λ and λ' are replaced by $(1-c)\lambda$ and $(1-c)\lambda'$, respectively. We get resonance in the F_{1u} mode only, hence we give the expression for the resonance denominator in this particular mode. The simplified expression for $D_{F_{1u}}(z)$ for radial forces only, can be written as

$$\begin{aligned} D_{F_{1u}}(z) = 1 &- (1-c)[\epsilon\omega^2 g_1 - \tfrac{1}{2}\lambda(8A_1 - A_2 + A_3)] \\ &+ \tfrac{1}{2}(1-c)\lambda\epsilon\omega^2[g_1(A_2 - A_3) \\ &\qquad - 8A_1(g_2 - g_4)] , \end{aligned}$$

where

$$A_1 = g_1 - g_2 + g_4 ,$$

$$\begin{aligned} A_2 = &-g_1 + 8g_2 - 2g_3 - g_5 - g_6 \\ &+ g_7 + g_9 - 2g_{10} + 2g_{12} , \end{aligned}$$

and

$$A_3 = g_1 + 10g_4 - g_5 - g_6 + g_7 - g_9 - 2g_{12} - 2g_{13} .$$

When we consider nearest-neighbor angular forces also, the resonance denominator $D_{F_{1u}}(z)$ is

$$D_{F_{1u}}(z) = |\underline{I} + (1-c)\underline{g}_{F_{1u}}(z)\underline{p}_{F_{1u}}(\omega^2)| , \tag{12}$$

where

$$g_{F_{1u}}(z)=\begin{bmatrix} g_1 & 2g_3 & \sqrt{8}g_2 & -\sqrt{8_4} \\ 2g_3 & g_1+2g_5+g_8 & \sqrt{8}(g_2+g_{11}) & -\sqrt{8}g_{12} \\ \sqrt{8}g_2 & \sqrt{8}(g_2+g_{11}) & g_1+2g_3+g_5+g_6+g_7+2g_{10} & -(2g_2+g_9) \\ -\sqrt{8}g_4 & -\sqrt{8}g_{12} & -(2g_2+g_9) & g_1+2g_4-g_5-g_6+g_7-2g_{13} \end{bmatrix}$$

$$p_{F_{1u}}(\omega^2)=\begin{bmatrix} -\epsilon\omega^2+4(\lambda+2\lambda') & -2\lambda' & -\sqrt{2}(\lambda+\lambda') & \sqrt{2}(\lambda-\lambda') \\ -2\lambda' & \lambda' & 0 & 0 \\ -\sqrt{2}(\lambda+\lambda') & 0 & \frac{1}{2}(\lambda+\lambda') & -\frac{1}{2}(\lambda-\lambda') \\ \sqrt{2}(\lambda-\lambda') & 0 & -\frac{1}{2}(\lambda-\lambda') & \frac{1}{2}(\lambda+\lambda') \end{bmatrix} .$$

$g_\mu(\mu=1,13)$ represent the various Green's functions appearing in the present problem and the expressions for them are given elsewhere.[20] The change in mass ϵ at the impurity site is given by $\epsilon=(M_{\text{imp}}-M_{\text{Au}})/M_{\text{Au}}$. M_{imp} and M_{Au} denote the masses of the impurity and gold atoms, respectively. The force-constant-change parameters λ and λ' are given as $\lambda=\Delta f/M_{\text{Au}}$, and $\lambda'=\Delta f'/M_{\text{Au}}$, where $f=f_0+\Delta f$ and $f'=f_0'+\Delta f'$ are the radial and angular force constants between the impurity and its twelve gold atoms defined in de Launay's lattice-dynamical model; Δf and $\Delta f'$ are the changes due to an impurity and f_0 and f_0' are the corresponding force constants in the host gold lattice.

C. Volume-change effects

The need of considering the volume-change effects in the study of defect-induced properties has been discussed by many workers,[3,7,8,12,29] including the present author.[21,22] The substitution of heavy impurities causes the expansion of the matrix, whereas alloying with a less massive element dilates.[34] The masses of all three substitutional impurities Cd, Sn, and Zn are light, hence a contraction in the gold lattice is expected. In the low-concentration limit and in α phases the behavior of the Debye temperatures of Au-Cd and Au-Zn alloys are as expected, i.e., the Debye temperatures increase due to introduction of Cd and Zn in gold, whereas in the case of Au-Sn systems we see an unusual behavior of the change in the measured Debye temperatures as a function of concentration. However, when we consider the volume-contraction effects, then the behavior of the changed specific heat is similar for the three systems.

The volume-change effect can be accounted for if we know the Grüneisen constant γ which is related to the Debye temperature as

$$-\frac{\partial\ \ln\Theta_D}{\partial\ \ln V}=\gamma\,. \tag{13}$$

Bevk *et al.*[25] have calculated the value of the Grüneisen constant for Au and have found two values (3.03 and 8.6) from two different methods of calculation. There is a wide discrepancy between the two values, which may be due to the much more complex nature of the phonon spectrum for Au as compared to Cu and Ag. We have taken the lower value of γ in the present calculations. The reason is that two other noble metals, Cu and Ag, have the corresponding values 1.9 and 2.5, respectively, and these values are nearer to 3.03. Using relation (13) we have corrected the Debye temperatures for the three systems for different concentrations of impurities. The values of Debye temperatures for pure gold after taking lattice dilation effects due to introduction of different impurities and the experimentally measured values are given in Table I. The difference between the two values are accounted for by the impurity effects which are considered later. The present method for considering the volume-change effect is not as accurate as the

TABLE I. Values of Debye temperatures Θ_p for pure gold after taking the volume-change effects and experimentally measured Θ_m.

Systems	Θ_p (K)	Θ_m (K)
Au–4-at. % Cd	153.3	164.4
Au–1.21-at. % Sn	159.6	160.6
Au–2.31-at. % Sn	157.1	159.1
Au–3.21-at. % Sn	155.0	157.9
Au–4.59-at. % Sn	151.7	157.7
Au–2.5-at. % Zn	156.6	162.5
Au–5.0-at. % Zn	150.7	163.8
Au–7.5-at. % Zn	144.8	166.3

Green's-function theory for considering the impurity effects. However, the approximation is valid in the low-concentration limits.

III. NUMERICAL COMPUTATIONS AND RESULTS

A. Green's functions

The lattice dynamics of gold in Kreb's model[35] has been discussed by us earlier.[24,36] In this model one takes into account the effects of electrons on the motion of ions via screened Coulombic-interaction and umklapp processes to satisfy the symmetry requirements, whereas most of the elastic force models used in the lattice dynamics of gold do not satisfy the symmetry requirements. We also consider the repulsive ion-ion interactions between closed-ion shells extending out to two neighbors. We have taken the expression for the screening parameters (which is not well defined in this model) given by Langer and Vosko[37]:

$$k_c^2 = K_c^2(\mathrm{TF}) f(t) ,$$

where

$$f(t) = \tfrac{1}{2} + \frac{1-t^2}{4t} \ln \left| \frac{1+t}{1-t} \right| .$$

k_c is the screening parameter and $K_c(\mathrm{TF}) = \beta'(r_0/a_0)^{1/2} k_F$ (β' is the Langer-Vosko parameter). The interelectronic spacing is $r_0 = (\frac{3}{4}\pi n_e)^{1/3}$, n_e is the electronic density, a_0 is the Bohr radius, and $k_F = (3\pi^2 n_e)^{2/3}$ is the Fermi radius and $t = \vec{q}/2k_F$, where $\vec{q}$ is the electron wave vector in the electron liquid.

Langer-Vosko parameter β' is adjusted with the elastic constants of Neighbours and Alers[38] and was found to be 0.81. The eigenfrequencies and eigenvectors are determined by diagonalizing the 3×3 dynamical matrix using Jacobi's method. The use of a grid which includes 8000 points in the first Brillouin zone was seen to give reasonably good results. The calculated dispersion curves in the main symmetry directions were seen to be in good agreement with the experimental results of Lynn *et al.*[39] The Green's functions were calculated by a staggered-bin averaging procedure.[40] The pertinent integrations were performed after dividing the phonon frequency range into 60 equal bins, each of width 0.25 in the unit of bin width.

B. Changed lattice specific heat

The low-temperature specific heat of gold and its alloys with cadmium, tin, and zinc have been measured by Bevk *et al.*,[25] by Will and Green,[26] and by Martin,[27] respectively. The electrons, as well as phonons, contribute to the specific heat of the metal. The electronic specific heat shows a T-dependent behavior whereas the lattice part exhibits T^3 and T^5 variation in all the three systems studied here. A reduction in the lattice specific heats due to presence of Cd, Sn, or Zn atoms was observed. The impurity contribution to the lattice specific heat has been calculated using Eqs. (8), (9), and (10) by varying the nearest-neighbor radial and angular force-constant change parameters λ and λ' for the systems in which the concentration of impurities are below 5 at. %. The present formulation has been found to give good agreement with the experiment in a number of systems.[18–21,24] The parameters (λ,λ') found in the specific-heat studies give good results in other defect-induced vibrational properties of solids.[19,22,41] The systems studied with this formulation were Au – 4-at. % Cd, Au – 1.21-at. % Sn, Au – 2.31-at. % Sn, Au – 4.59-at. % Sn, Au – 2.5-at. % Zn, and Au – 5-at. % Zn. The calculated change in the lattice specific heat of the above systems shows good agreement with the experimental results. In all cases we get a reduction in the specific heat due to introduction of impurities.

We have tried a number of sets (λ,λ') to obtain good fit with the experimental results. A unique set of λ and λ' has been obtained to explain the experiments successfully. The obtained values of force-constants changes in the different host-impurity systems are given in Table II. The percentage changes of the force constants in the vicinity of the impurity of the contracted lattice with the force constants of pure gold lattice are also shown in this table. It is observed that the relative change in force constants decreases as the mass of the impurity increases. The relative change in both the force constants (radial and angular) due to tin impurity is approximately equal. Computations were also performed assuming the above impurities as mass defects. The mass-defect contribution to the changed specific heat is found to be on the average 35% due to Cd, 38% due to Sn, and 57% by Zn impurities, respectively.

To compute the lattice specific heat for α- phase Au – 7.5-at. % Zn we have taken the resonance denominators given by Eqs. (11) and (12) instead of Eq. (4). The modified expressions for the resonance denominators in the various irreducible representa-

TABLE II. Values of radial and angular force constants and resonant frequencies. The percentage change of calculated λ and λ' with the force constant f and f' of pure gold is also given.

Systems	$\lambda(10^{26}\ \mathrm{sec}^{-2})$	Percentage change	$\lambda'(10^{26}\ \mathrm{sec}^{-2})$	Percentage change	$\omega_r(\mathrm{cm}^{-1})$
Au-Cd	0.410	36%	−0.078	40.6%	147.0
Au-Sn	0.521	45.7%	−0.087	45.3%	152.3
Au-Zn	0.382	33.5%	−0.051	26.5%	159.0

tions are taken into account. The phase shifts shown by Eq. (6) as well as the lattice specific-heat equation are modified accordingly. The computed results compare well with the experiments. We have also calculated the changed specific heat when Elliott and Taylor's approximations were neglected. It is observed that when this approximation is not taken into consideration, the calculated results differ from the experimental data. The deviation is larger at comparatively higher temperatures. The same behavior was also observed in silver- and copper-based alloys[21].

Martin[27] expected that the smooth rise in Debye temperature due to alloying of zinc in gold produces high-frequency impurity modes, i.e., the low-frequency end of the lattice vibrational spectrum is depleted as zinc is added to gold. We have seen the resonances appearing in all the systems near the maximum frequency of the pure gold. But out of nine irreducible representations involved in the calculations, the high-frequency resonance modes occur only in the infrared-active irreducible representation F_{1u}, in which the impurity atom moves. The obtained values of resonance frequencies corresponding to fitted values of force-constant changes are given in Table II. At very low temperatures these resonance modes will not be excited and the contribution of the F_{1u} representation will not be very large.

Out of nine irreducible representations involved in the calculation, the main contribution to the specific heat arises due to the F_{1u}, F_{1g}, F_{2g}, A_{1g}, and E_g symmetry motions. The maximum contributions come from the irreducible representations A_{1g} and F_{2g} which are similar in magnitude and negative throughout the full temperature range. The contribution of the F_{1u} irreducible representation is positive and dominates in the lower-temperature side (~ 2 K) of the specific-heat curve. The contributions of irreducible representations E_g and F_{1g} are approximately temperature independent and are similar in magnitude but opposite in sign. The contribution of another odd-parity mode A_{2u} becomes appreciable at comparatively higher temperatures.

IV. CONCLUSIONS

The temperature dependence of the lattice specific heat of Au doped with Cd, Sn, and Zn impurities can be well understood on the basis of a localized perturbation model which considers mass change at the defect site as well as changes in the nearest-neighbor radial and angular force constants. Elliott and Taylor's approximation has been used for Cu−7.5-at.% Zn alloy. The effects of the volume change caused by the impurity atoms on the specific heat has also been taken into account. In Au-Cd and Au-Sn alloys the contribution due to force-constant changes is quite large, whereas in Au-Zn alloys it is 43%. The main contribution to the specific heat does not arise due to F_{1u} symmetry modes, but instead is due to even-parity A_{1g}, F_{1g}, F_{2g}, and E_g modes. This behavior is quite different from that observed earlier in other systems,[19–22] where the F_{1u} irreducible representation dominates over all others. It is hoped that the force-constant changes obtained in this study will be useful for future experiments on these alloys.

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