Lattice specific heat and local density of states of Ni-based dilute alloys at low temperature

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Abstract. A detailed theoretical study of the low-temperature lattice specific heat of Ni-based dilute alloys has been carried out. Lattice Green's function method has been used to calculate the local density of states of substitutional impurities and lattice specific heat in different alloys. The resonance condition has been investigated for possible occurrence of resonance modes. Except in NiCr and NiMn, low-frequency resonance modes have been obtained in all the alloys. However, no localized mode was obtained. The impurity-induced increase in lattice specific heat is explained on the basis of the obtained resonance modes. The calculation shows an excellent agreement with the measured lattice specific heat in these alloys

1. Introduction

Theoretically, impurity-induced lattice specific heat at low temperatures has been discussed extensively taking into account the effect of mass and force-constant changes. Large number of experimental measurements on lattice specific heat has also been reported. Introduction of substitutional impurities in a metallic lattice normally gives rise to volume expansion whose effect must also be taken into account while calculating lattice specific heat of dilute alloys. Using appropriate contribution of volume effect along with the change in mass and force constant, the lattice specific heat has been studied [1–4].

As regards the Ni-based alloys, there have been a number of measurements [5–10] at different concentration of alloying impurities. Rene Caudron et al [11] have made detailed experimental measurements of specific heat of a large number of alloys where, in most of the cases the alloying element has been a transition metal.

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The contribution to the change in specific heat comes from different terms including the electronic and lattice part. These authors [11] have presented the results of measured lattice and electronic specific heat and discussed the electronic part of measured specific heat in considerable detail but no theoretical calculation of electronic or lattice part of change in specific heat was presented in these systems. Due to the limitations of our present low-concentration theory of specific heat, we have not considered the electronic part ($\Delta \gamma T$) of specific heat in our present calculation; our discussion is restricted to lattice part of change in specific heat and we compared our calculation to the measured $\Delta C_{\mathrm{L}}(= \Delta \beta T^3)$ only. In order to gain some insight into the dynamics of different impurity – host systems, it is of some interest to investigate the lattice specific heat of these alloys. In the present paper, therefore, we have calculated lattice specific heat of a number of dilute alloys and discussed the results in the light of measurements of Rene Caudron *et al* [11].

In the calculation of lattice specific heat, we have used a Green's function theory [12] and a nearest-neighbour impurity model involving only central force-constant changes has been utilized. Apart from central force-constant changes, near the impurity, the usual mass change and the effect of volume expansion have also been considered. The perfect lattice Green's functions have been calculated using a method due to Gilat and Raubenheimer [13]. The required perfect lattice phonons of Ni are calculated using a general 4 Th neighbour force model derived by Birgeneau *et al* [14], on the basis of Born Von Karman fit to the measured dispersion curves in neutron scattering experiments. A comparison of calculated and experimental lattice specific heat provides us an appropriate value of nearest-neighbour central force-constant change between impurity and host atom. In the comparison, we have utilized the experimental results of lattice specific heat pertaining to lowest concentration of impurities, since we used a low-concentration theory where single impurity t-matrix approximation is considered.

The obtained force-constant changes are used to calculate local density of states of individual impurities in the lattice for different alloys. In order to find out the occurrence of possible resonance and localized modes the behaviour of resonant denominator has been studied in detail. We get a resonance mode in all the dilute alloys except in NiMn and NiCr. The presence of resonance is reflected in the typical resonant peaks in the calculated local density of states of impurities. In fact, there is almost complete identity between the frequency of obtained resonance modes and resonant peaks in the calculated local density of states. The method of local density of states [15–19] is quite useful in the study of resonant vibrations and in understanding the thermodynamical properties of defects. In our recent papers [20,21] we have presented the results of local density of states of PdNi, AuAl and AgAl dilute alloys and theoretically discussed the change of lattice specific heat and role of localized modes in understanding the changes in lattice specific heat in these alloys at very low temperatures.

The theory of change in lattice specific heat of dilute alloys is discussed in brief in §2. The theory of local density of states and resonance condition are discussed in §3. The calculated results are presented and discussed in §4. The calculated results of change in lattice specific heat are interpreted in terms of the obtained resonance modes. An overall good agreement between theory and experiment is obtained.

2. Lattice specific heat of dilute alloys

The theory of lattice specific heat of alloys including the volume changes has been discussed in many papers (see [1]). The change in specific heat after the addition of a small fraction of impurities in the host crystal at very low temperatures may be due to two different factors: (i) due to change in volume and (ii) due to change in the mass and force-constants.

The lattice specific heat of alloys, therefore, can be expressed as

$$C_L^{\text{alloy}} = C_L^{\text{pure}} + \Delta C_L^{\text{im}} + \Delta C_L^{\text{loc}}, \tag{1}$$

where ΔC_L^{im} is the change in specific heat due to volume change corresponding to the homogeneous expansion of the lattice called the image expansion and gives rise to softening of forces throughout the lattice and ΔC_L^{loc} is the change due to local perturbation from mass defect and force-constant changes. According to Debye T^3-law which is valid in solids only at temperature $< \theta_D/60$ [11], lattice specific heat is given by

$$C_L(T) = (12/5)\pi^4 R(T/\theta_D)^3. \tag{2}$$

The values of Debye temperature for different alloys are taken from the experimental measurements [11] and the values of $\Delta\beta$ are known from the experimental results using the equation $\beta^{\text{alloy}} = \beta^{\text{pure}} + \Delta\beta$ where β^{alloy} can be expressed in terms of Debye temperature using $\beta = (12/5)\pi^4 R/\theta_D^3$. In the experimental determination of β [11], an error of only 0.1% at low-temperature region was reported and therefore, in the values of θ_D determined from β^{alloy} and given in table 1 for different alloys, an estimated error of 0.03% ($\theta_D \pm 0.15$) might occur. The change in Debye temperature due to uniform volume expansion of lattice is given in terms of Gruneisen constant

$$\gamma = -\mathrm{d}\ln\theta_D/\mathrm{d}\ln V \quad \text{or} \quad \gamma\Delta V^{\text{im}}/V = -\Delta\theta_D/\theta_D, \tag{3}$$

where ΔV^{im} is the so-called image expansion in the lattice related to the total volume change ΔV by the expression

$$\Delta V^{\text{im}} = [2(1-2p)/3(1-p)]\Delta V, \tag{4}$$

where p is the Poisson ratio (=0.28) for Ni. Having found $\Delta\theta_D$ due to volume change we can find out specific heat of expanded lattice and thus change in specific heat due to image expansion is $\Delta C_L^{\text{im}} = C_L^{\text{expanded}} - C_L^{\text{pure}}$, and change due to local perturbation (mass + force-constant change) is $\Delta C_L^{\text{loc}} = C_L^{\text{alloy}} - C_L^{\text{expanded}}$.

The change in specific heat in the presence of very low concentration of impurities at very low temperature may be expressed as

$$\Delta C_L(T) = N_d k \int \mathrm{d}\omega \Delta Z(\omega)(\hbar\omega/2kT)^2 \operatorname{cosech}^2(\hbar\omega/2kT), \tag{5}$$

where $\Delta Z(\omega)$ is the change in the density of states due to single impurity and $N_d = cN$ is the total number of impurities in the lattice and c is the impurity concentration.

Table 1. Debye temperature of pure Ni and its alloys, change in Debye temperature due to volume expansion $\Delta\theta_D$ (K), Debye temperature of expanded lattice ($\theta_D^{expanded} = \theta_D^{pure} + \Delta\theta_D$) along with the total relative volume change ($\Delta V/cV$), for unit concentration of impurities.

Alloys	$\Delta V/cV^c$	θ_D (K)^{pure} = 472.0^a θ_D (K)^b (alloys)	$\Delta\theta_D$ (K)	$\theta_D^{expanded}$
$Ni_{0.99}Pt_{0.01}$	+0.4568	465.42	−1.61	470.39
$Ni_{0.99}Os_{0.01}$	+0.0771	463.03	−0.27	471.73
$Ni_{0.99}W_{0.01}$	+0.3693	462.64	−1.30	470.70
$Ni_{0.99}Pd_{0.01}$	+0.4133	467.86	−1.45	470.55
$Ni_{0.995}Ru_{0.005}$	+0.2876	467.86	−0.51	471.49
$Ni_{0.993}Mo_{0.007}$	+0.2227	465.42	−0.55	471.45
$Ni_{0.993}Nb_{0.007}$	+0.5124	463.82	−1.26	470.74
$Ni_{0.99}Mn_{0.01}$	+0.2320	469.51	−0.82	471.18
$Ni_{0.985}Cr_{0.015}$	+0.1034	468.68	−0.55	471.45
$Ni_{0.0985}V_{0.015}$	+0.1334	465.42	−0.70	471.30
$Ni_{0.985}Ti_{0.015}$	+0.2943	464.62	−1.55	470.45

^{a}Ref. [23]; ^{b}ref. [11]; ^{c}ref. [24].

The change in density of states can be expressed in terms of phase shift $\theta(\omega)$, as

$$\Delta Z(\omega) = d\theta(\omega)/\pi d\omega. \tag{6}$$

Using the above expression in eq. (5) and integrating by parts, we get the change in lattice specific heat in terms of phase shift.

$$\Delta C_L(T) = -2N_d k/\pi \int_0^\infty d\omega (d\theta(\omega)/\omega)[\mathrm{cosech}^2(\hbar\omega/2kT)$$
$$\times \{(1 - (\hbar\omega/2kT))\coth(\hbar\omega/2kT)\}](\hbar\omega/2kT)^2. \tag{7}$$

The calculation of change in lattice specific heat is simplified by using the symmetry of impurity. The total phase shift $\theta(\omega)$ is the sum of phase shifts in different irreducible representation of the point group of impurity site. Therefore, the change in density of states and hence the change in specific heat may be expressed as

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

where $\Delta C_L^\nu(T)$ is the contribution due to νth irreducible subspace.

3. Resonance mode and local density of states

The density of states of individual atom which is either host or impurity, is called as the local density of that particular type of atom. The total density can be expressed as the sum of densities of states of all atoms present in the lattice. The local density

of states provides a convenient quantity to discuss the vibrational properties of a single atom e.g., a defect atom. Dederichs *et al* [16] have discussed the theory of local density of states and resonance in detail. The Green's function $G^0(\omega)$ for the perfect crystal is defined by

$$(\Phi^0 - M^0\omega^2)G^0(\omega) = 1. \tag{9}$$

While the Green's function $G(\omega)$ for the imperfect crystal is given by

$$(\Phi - M\omega^2)G(\omega) = 1, \tag{10}$$

where $\Phi^0(\Phi)$ and $M^0(M)$ are the force constant and mass number for the perfect (imperfect) lattice respectively. If we assume the presence of a single impurity, the Green's function of imperfect lattice may be written as

$$(\Phi^0 - M^0\omega^2 + P(\omega))G(\omega) = 1, \tag{11}$$

where $P(\omega) = \Phi - \Phi^0 - (M - M^0)\omega^2 = \Delta\Phi - \Delta M\omega^2$, is the perturbation matrix due to single impurity. Using eqs (9) and (11) the imperfect lattice Green's function can be expressed as

$$G(\omega) = [I + G^0(\omega)P(\omega)]^{-1}G^0(\omega). \tag{12}$$

From the expression of $G(\omega)$ it is clear that the condition of occurrence of resonance or localized mode is given by

$$\mathrm{Re}\, D(\omega) = \mathrm{Re}\,|1 + G^0(\omega)P(\omega)| = 0, \tag{13}$$

where $D(\omega)$ is the denominator of $G(\omega)$.

Occurrence of resonance is possible if the impurity is heavier than the host atom $(M > M^0)$ or the coupling between host and impurity atom is weak. In such a situation, there is an increase in the crystal density of states and hence the increase in the lattice specific heat. On the other hand, there is a possibility of localized mode if the mass of impurity is less than the mass of the host atom or there is a strong increase in the force constants. Since in case of substitutional impurity the major contribution to the density of states comes from the F_{1u} mode, in which the motion of the impurity is involved, the resonance condition becomes

$$\mathrm{Re}\, D_{F_{1u}}(\omega) = 0. \tag{14}$$

The solution of this equation gives resonance or anti-resonance depending on whether the width

$$\Delta\omega = \mathrm{Im} D_{F_{1u}}(\omega)/\mathrm{d}(\mathrm{Re}\, D_{F_{1u}}(\omega))/\mathrm{d}\omega \tag{15}$$

is positive or negative. For resonance there is an increase in the density of states, while for anti-resonance there is a decrease in it.

The local density of states of the substitutional impurity atom can be expressed [19,22] as

$$Z_i^{\mathrm{d}}(\omega) = 2M\omega\, \mathrm{Im}\, G_{ii}^{\mathrm{dd}}(\omega)/\pi, \tag{16}$$

where $G_{ii}^{\mathrm{dd}}(\omega)$ is the appropriate defect Green's function and i denotes the Cartesian component.

4. Results and discussion

We have performed the calculation of change in lattice specific heat of different dilute alloys NiPt1.0%, NiOs1.0%, NiMo0.7%, NiW1.0%, NiPd1.0%, NiRu0.5%, NiNb0.7%, NiMn1.0%, NiCr1.5%, NiV1.5%, and NiTi1.5% at very low-temperatures (0–5 K). Rene Caudron *et al* 11] have done the measurements on these alloys at different concentrations, but we present the results of change in specific heat of different alloys at the lowest concentration of the impurities. In table 1, we have presented the Debye temperatures of alloys, change in Debye temperature due to image expansion, and Debye temperature of expanded lattice along with relative volume change. The Debye temperatures for alloys are from Rene Caudron *et al* [11], Debye temperature of pure Ni from Bower *et al* [23] while relative volume changes are taken from King [24]. The Green's functions used in the calculation are computed using the modified method of Gilat–Raubenheimer [13]. A nearest-neighbour perturbation model consisting of mass defect and central force-constant change is considered. The 39×39 Green's function and perturbation matrices are simplified using the O_h point group symmetry of the impurity site. The contribution to the lattice specific heat due to local perturbation is calculated by varying the central force-constant change. Results have been obtained by a set of force constant changes, which gives best fit to the experimental lattice specific heat. The derived force-constant changes are used to calculate the local density of states for the different substitutional impurities in Ni. Corresponding to these changes in the nearest-neighbour central force-constants the resonance denominator in F_{1u} mode, $D_{F_{1u}}(\omega)$, has been studied in detail to find out frequencies of resonance and localized modes. We have found resonance modes in all the alloys except in NiMn and NiCr but no localized mode was found. The frequencies of obtained resonance modes along with the relative force-constant changes and mass change parameter $\Delta M/M$ are presented in table 2. We observe that in NiPt, NiOs, NiW and in NiPd resonance modes are mass dominated whereas in NiRu, NiMo and NiNb the effect of mass change and force-constant change are equally important while in the remaining two systems NiV and NiTi the resonance modes are force-constant dominated. It may be seen that in the last two cases, i.e., in NiV and NiTi the host and impurities have similar masses and as such the resonances are induced by strong reduction in central force-constants near the impurities. In passing, we note that in NiMn, NiCr where resonance modes are not obtained, the masses of Ni and these impurities are almost equal, and the reduction in force-constants are not strong enough to cause resonant vibrations of impurities. It is further observed that at resonant mode frequencies we get typical resonant peaks in the calculated local density of states of impurities (see figures).

The calculated results for real and imaginary parts of resonant denominator $D_{F_{1u}}(\omega)$, local density of states of Pt along with local density of host Ni atom, and the change in lattice specific heat, in NiPt alloy have been plotted in figures 1–3. We plot all the calculated change in lattice specific heats and local density of states of impurities along with the local density of host nickel, alternatively in figures 4–23 for the remaining ten alloys. We discuss the results of various alloys individually.

Table 2. Relative force-constant changes ($\Delta f/f^0$), resonance frequency (ω_r), and relative change in masses of host and defect atoms ($\Delta M/M^0$).

Alloys	Relative change in mass ($\Delta M/M^0$)	Relative change in force-constant $\Delta f/f^0$ ($f^0 = 36319$ dynes/cm)[a]	Obtained resonance mode frequency (THz)
$Ni_{0.99}Pt_{0.01}$	2.3235	$+0.26$	3.37
$Ni_{0.99}Os_{0.01}$	2.2402	-0.40	2.37
$Ni_{0.99}W_{0.01}$	2.1320	-0.35	2.45
$Ni_{0.99}Pd_{0.01}$	0.8126	-0.10	3.73
$Ni_{0.995}Ru_{0.005}$	0.7218	-0.72	2.41
$Ni_{0.993}Mo_{0.007}$	0.6344	-0.85	1.89
$Ni_{0.993}Nb_{0.007}$	0.5827	-0.95	1.13
$Ni_{0.99}Mn_{0.01}$	-0.0641	-0.31	$-$
$Ni_{0.985}Cr_{0.015}$	-0.1176	-0.36	$-$
$Ni_{0.0985}V_{0.015}$	-0.1322	-0.58	3.81
$Ni_{0.985}Ti_{0.015}$	-0.1840	-0.59	3.73

[a]Ref. [14].
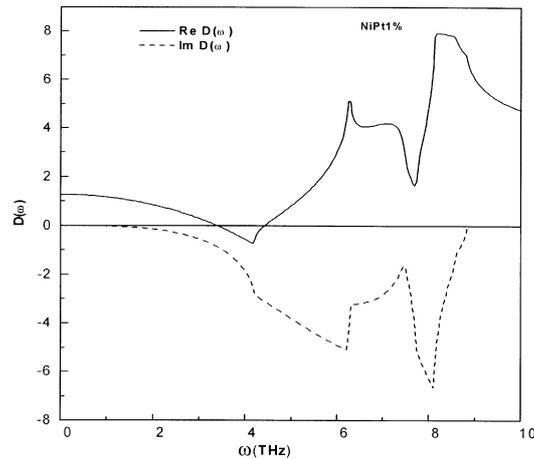
Figure 1. Real and imaginary parts of resonant denominator of NiPt.

(i) *NiPt*1.0%: The experimental measurements on NiPt alloy shows an increase in the lattice specific heat in the presence of impurity. Therefore, taking the central force-constant change, the best agreement of our calculated results with the experimental data is obtained at $\Delta f = 0.26f^0$, where $f^0 = 36319$ dynes/cm is the central force-constant for the ideal lattice. The increase in lattice specific heat, largely due to the resonance mode, may be attributed to heavy mass of the impurity atom of platinum. The fact is also clear from the local density of states where a strong peak at low frequency (figure 2) is obtained. The solid curve in figure 2 represents
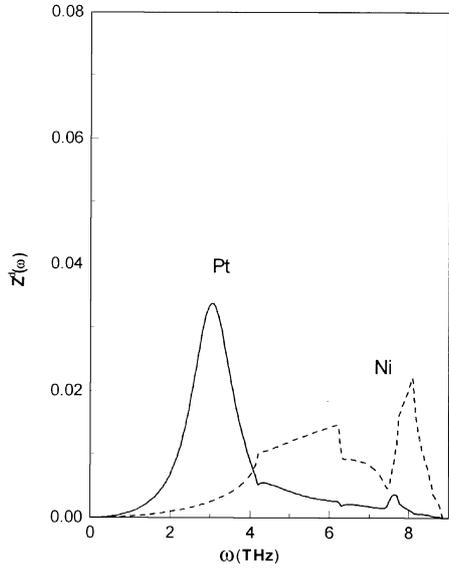
Figure 2. Local density of states of Pt and host Ni.
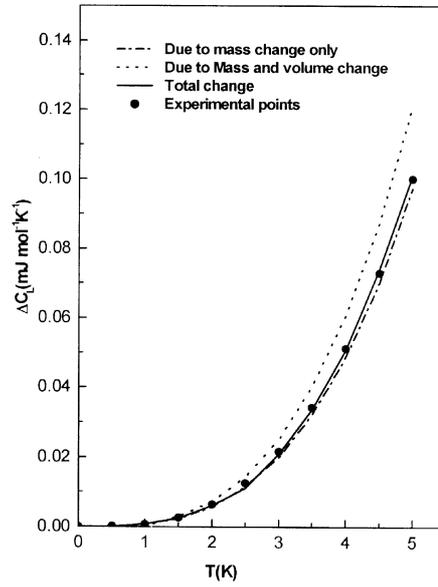
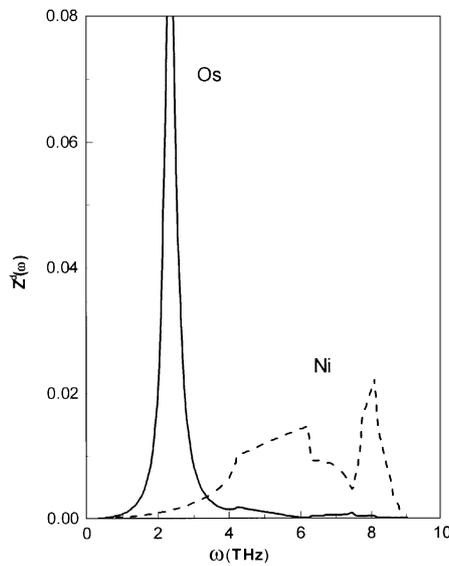**Figure 3.** Change in lattice specific heat of NiPt1.0%.

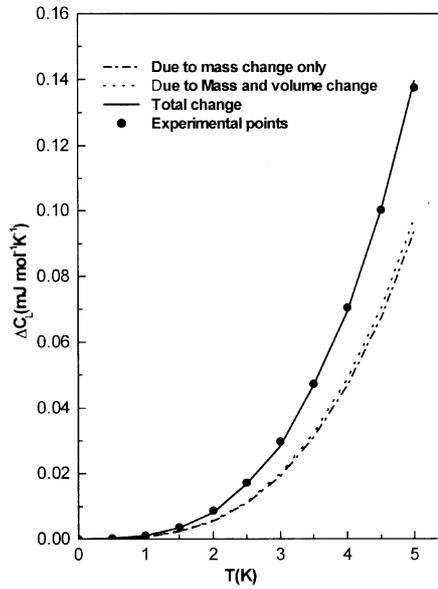**Figure 4.** Local density of states of Os and host Ni.

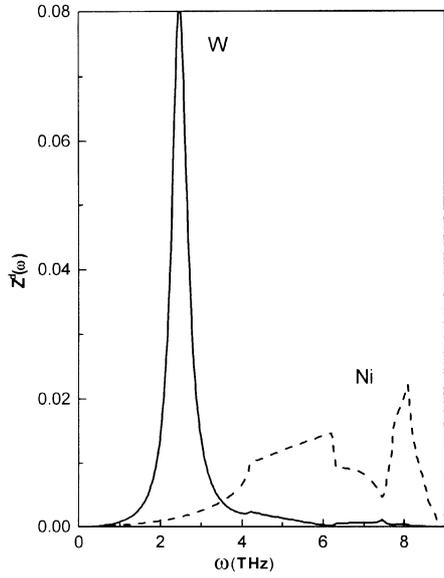**Figure 5.** Change in lattice specific heat of NiOs1.0%.

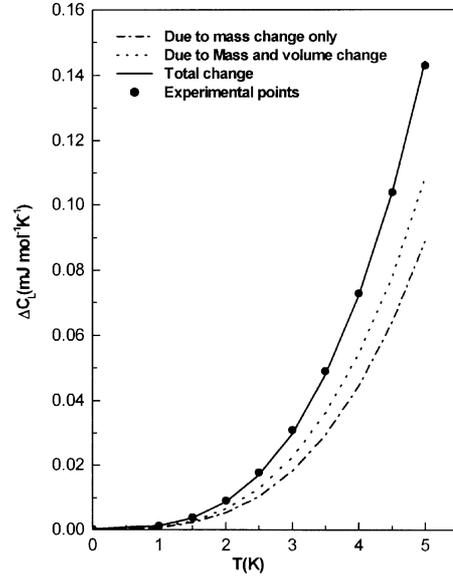**Figure 6.** Local density of states of W and host Ni.

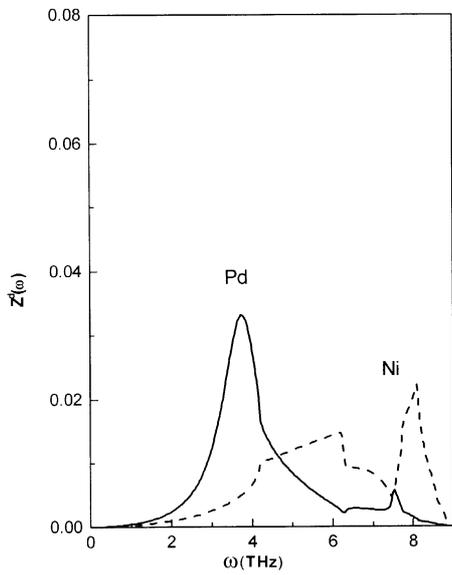**Figure 7.** Change in lattice specific heat of NiW1.0%.

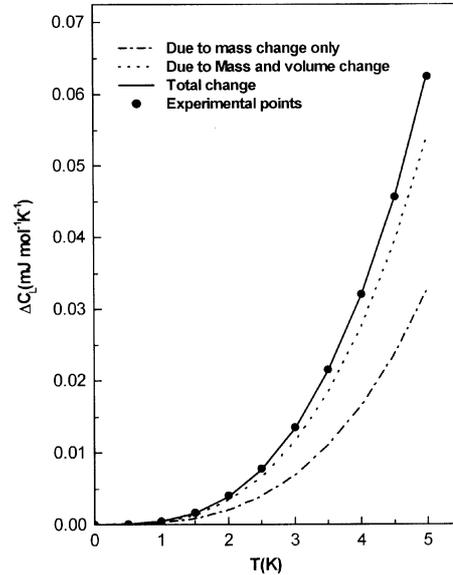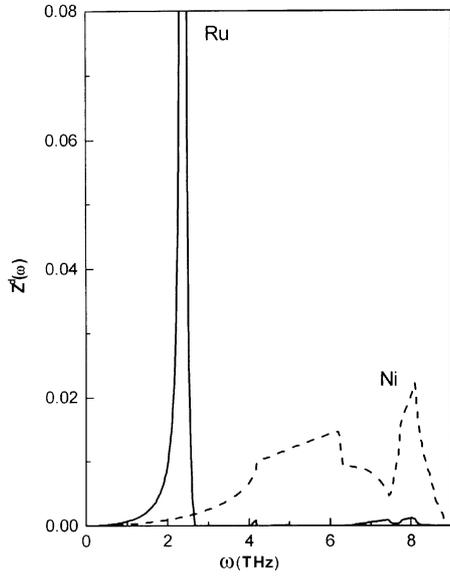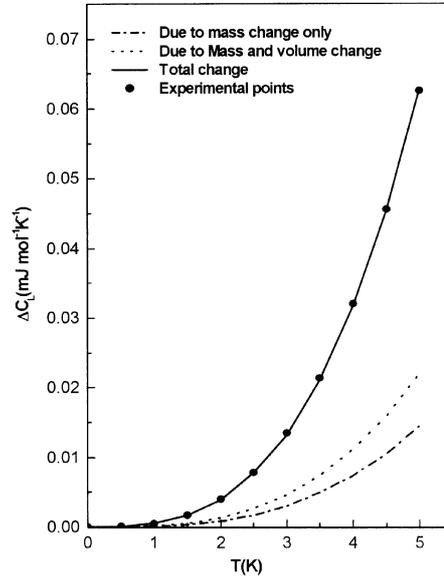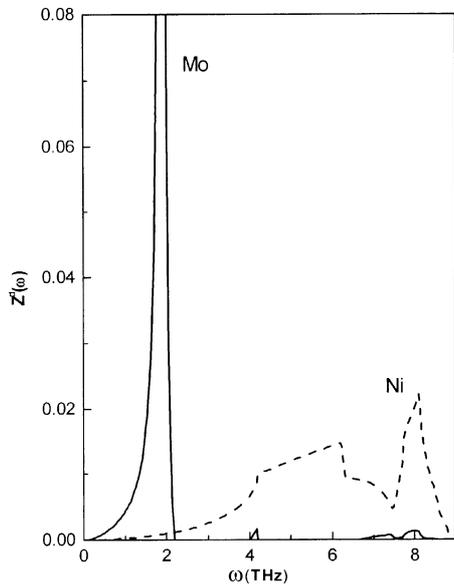**Figure 8.** Local density of states of Pd and host Ni.

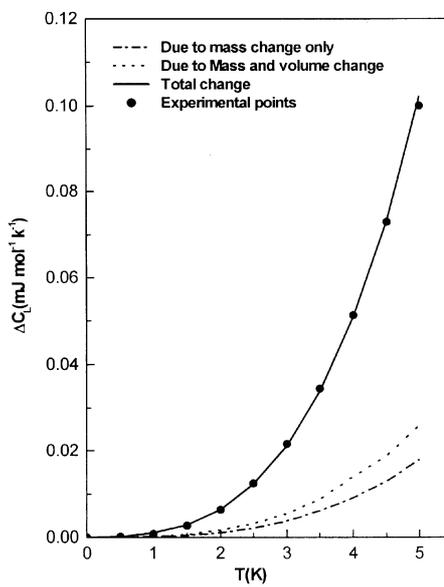**Figure 9.** Change in lattice specific heat of NiPd1.0%.

Figure 10. Local density of states of Ru and host Ni.

Figure 11. Change in lattice specific heat of NiRu0.5%.

Figure 12. Local density of states of Mo and host Ni.

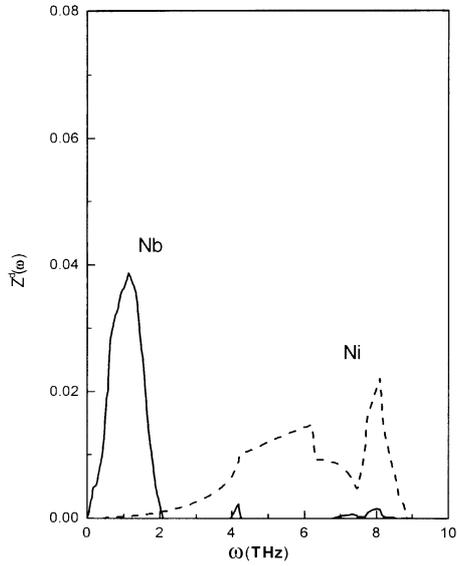**Figure 13.** Change in lattice specific heat of NiMo0.7%.

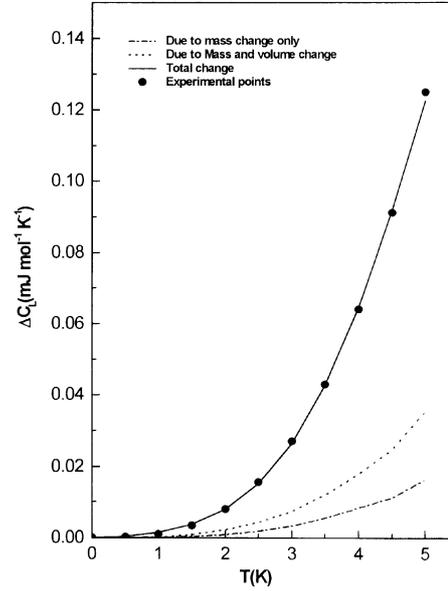**Figure 14.** Local density of states of Nb and host Ni.
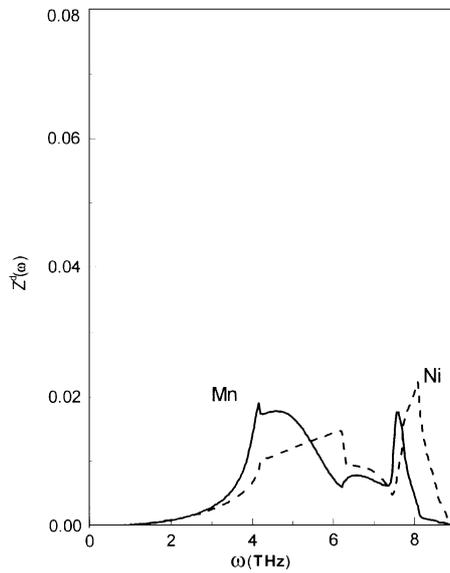

Figure 15. Change in lattice specific heat of NiNb0.7%.
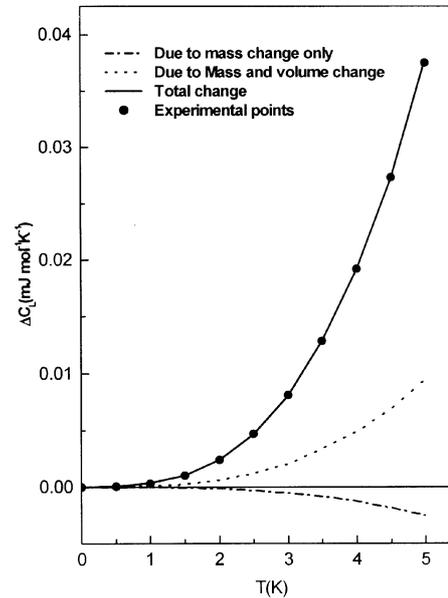

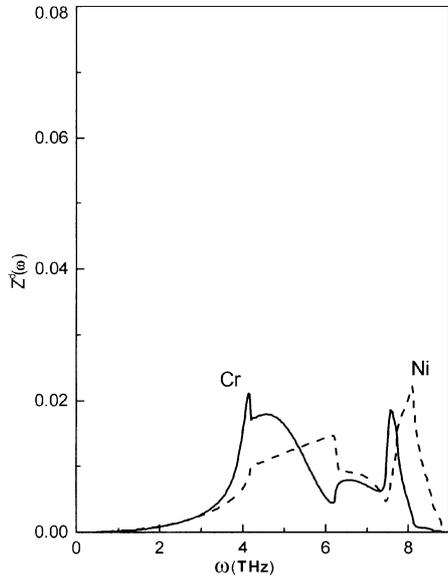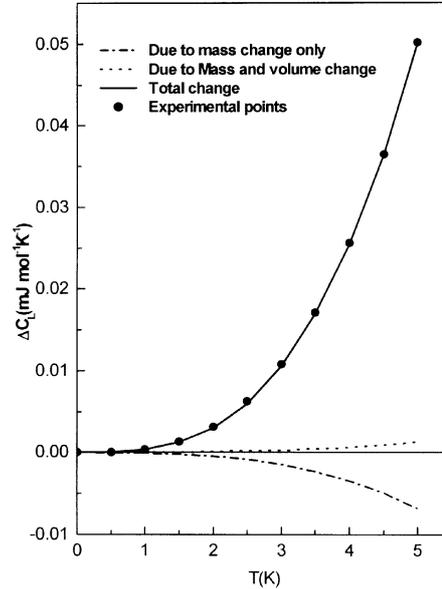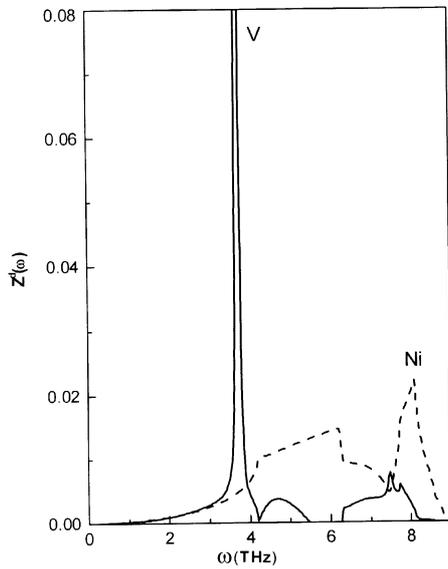**Figure 16.** Local density of states of Mn and host Ni.

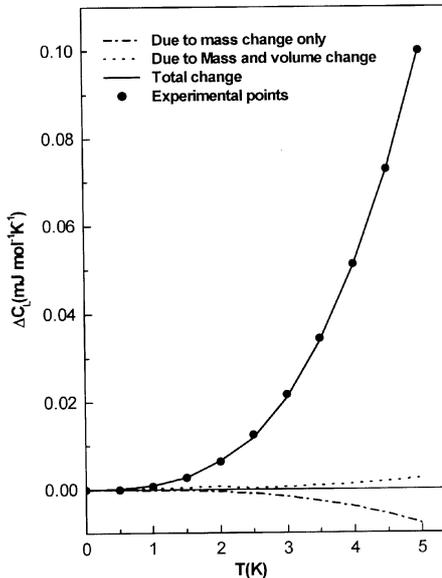**Figure 17.** Change in lattice specific heat of NiMn1.0%.

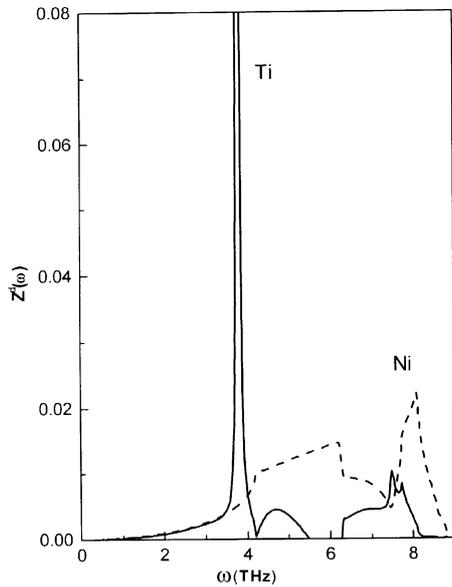**Figure 18.** Local density of states of Cr and host Ni.

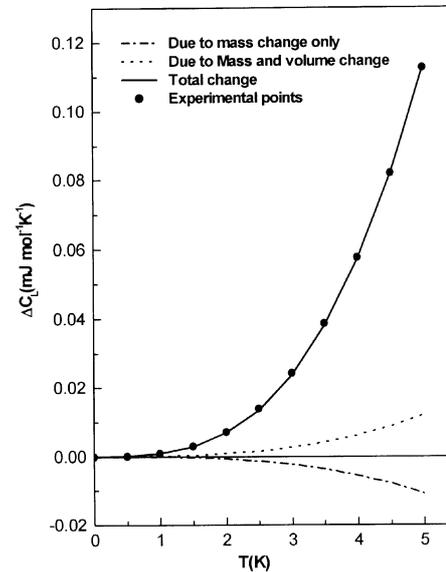**Figure 19.** Change in lattice specific heat of NiCr1.5%.

Figure 20. Local density of states of V and host Ni.

Figure 21. Change in lattice specific heat of NiV1.5%.

Figure 22. Local density of states of Ti and host Ni.

Figure 23. Change in lattice specific heat of NiTi1.5%.

the local density of Pt impurity atom and dashed curve shows the local density of individual host Ni atom. Thus, we see that low frequency modes are prominent in impurity spectrum, which are instrumental in enhancing the lattice specific heat at low temperatures the contribution of low frequency modes are quite important compared to high frequency modes. This is largely due to the presence of the factor $\mathrm{cosec}^2(\hbar\omega/2kT)$ in the expression of lattice specific heat (eq. (7)). However, the calculated peak in local density of states in NiPt is at somewhat lower frequency compared to obtained resonance mode frequency (3.37 THz) from resonance condition (eq. (14)) in the F_{1u} mode. This type of variation could be attributed to the motion of neighbours of the impurity in the resonant vibration of the lattice. An increase in central force-constant in this system is expected to reduce the specific heat. However, the heavy mass of the impurity overcompensates any such reduction and we get an increase in the lattice specific heat. In addition, there is a positive change due to volume expansion also.

(ii) *NiOs*1.0%: From figure 4 we see that the volume and mass defect contributions to the lattice specific heat are positive but to account for total enhancement observed in the experimental measurements reduction of 40% of nearest-neighbour central force-constant in the ideal lattice is required. A strong mass change and reduction in force-constant is the cause of the resonance mode observed in this alloy. A peak at resonant frequency (2.37 THz) is also observed in the local density of states. The local density of states of Os (solid curve) along with the local density of host nickel (dashed curve) is plotted in figure 4. Again, the dominant contribution to the lattice specific heat is due to motion of impurity and resonance mode as is

evident from the resonance peak in the local density of states where modes of host frequencies are almost absent.

(iii) *NiW*1.0%: In this case also, the major contribution to the lattice specific heat is due to mass change and the contribution due to volume change is positive and quite significant. The best agreement with the experiment is found at $\Delta f = -0.35 f^0$. The resonance is obtained at 2.45 THz in the resonance denominator and the local density of states shows the resonance peak (figure 6) at the same frequency, which results in the increase in the lattice specific heat in this dilute alloy. Host modes are almost absent in this case also.

(iv) *NiPd*1.0%: The increase in the lattice specific heat of NiPd dilute alloy is largely due to mass change but the volume change is also contributing significantly to the enhancement of lattice specific heat. Only 10% reduction in the nearest-neighbour force-constant is required to get the best fit to the experimental results. The resonance peak in the local density of states (figure 8) of Pd is obtained at 3.73 THz.

(v) *NiRu*0.5%: In this alloy the increase in the lattice specific heat is due to significant reduction $(-0.72 f^0)$ in the central force-constant. The contribution to the lattice specific heat due to force-constant change is more than 50% and the remaining contribution is due to mass and volume change together. The local density of states showing the resonance condition at 2.41 THz is plotted in figure 10. Here again we see that low-frequency resonance modes are prominent in the local frequency spectrum of Ru and complete absence of host modes is seen.

(vi) *NiMo*0.7%: The major contribution to the lattice specific heat in this system comes from the large reduction in the central force-constant. The contribution due to mass change is nearly 25% and the volume change contribution is positive but less than due to mass change. The local frequency spectrum shows the resonance at 1.89 THz in figure 12.

(vii) *NiNb*0.7%: The enhancement in the lattice specific heat is dominantly (70%) due to strong decrease in the central force-constant and the remaining contribution due to mass and volume change, where, contribution due to mass change is less than 15% and the remaining contribution comes from the volume change. In the local spectrum of Nb the resonance is shown as a peak in the low-frequency region at 1.13 THz (figure 14).

(viii) *NiMn*1.0%: In this case, we have not found any resonance; it is an expected result since the mass of Mn is less than the mass of host Ni. The increase in the lattice specific heat is mainly due to reduction in the central force-constant but the contribution due to volume change is also quite significant. The best agreement with the experimental results of specific heat is obtained at $\Delta f = -0.31 f^0$.

(ix) *NiCr*1.5%: In the case of this alloy also, the resonance is absent as the mass of Cr impurity is less than the mass of the host Ni. Therefore increase in the lattice specific heat is largely due to change in central force constant. The negative contribution due to mass change and positive contribution due to volume change almost cancel each other. The obtained force-constant change is $\Delta f = -0.36 f^0$.

(x) *NiV*1.5%: Although the mass of vanadium is slightly less than the mass of Ni, resonance is observed in the local frequency spectrum as a sharp peak at 3.81 THz and hence, there is an increase in the lattice specific heat. The contribution to the lattice specific heat due to mass change and volume change together is negligible

and therefore resonance is possible because of strong reduction in the central force-constant. The obtained force-constant change is $\Delta f = -0.58 f^0$.

(xi) *NiTi*1.5%: Similar to NiV, the NiTi system also shows a sharp resonance peak at the frequency 3.73 THz in local spectrum of impurity Ti (figure 22). An increase in the lattice specific heat is attributed mainly due to large decrease in central force-constant. The combined contribution to the lattice specific heat due to mass and volume change is very small. There is a strong (59%) reduction in central force-constant, which is mainly responsible for the increase in the lattice specific heat.

5. Conclusion

A simple nearest-neighbour force-constant change model for the impurity is successfully applied to explain the observed lattice specific heat of Ni-based dilute alloys. The impurity-induced increase in the lattice specific heat is attributed to low-frequency resonance modes found in most of the alloys. The calculated local density of states shows typical resonant peaks at resonance mode frequencies. The local density of states corroborated the dominant contribution of resonance modes in enhancing the lattice specific heat at low temperatures.

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