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Dispersion of Phonon Waves in a Binary Alloy of Chromium and Tungsten

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Phonon dispersion relations along the three principal syminetry directions, [100], [110] and [111], are computed for tlie $Cr_{1-x}W_x$ alloys with tungsten concentration x = 0.3, 0.8 and 1.6% and compared with experimental results. **A** close agreement has been observed between tlie tlieoretical predictions and the experimental findings.

I. Introduction

In recent past enormous efforts have been done in the theoretical and experimental studies of the lattice dynamics of substitutional binary alloys. If we confine our attention to cubic crystals, experimental works on neutron scattering technique are available for some of tlie important alloys like $Cu_{1-x}Al_x$[1], $Ge_{1-x}Si_x$[2], $Rb_{1-x}K_x$[3], $Cu_{1-x}Au_x$[4] $Cr_{1-x}W_x$[5] and $Ni_{1-x}Pt_x$[6]. It is worth pointing out that the experimentalists faced more difficulty in obtaining the detailed structural information in the phonon spectra of alloys in contrast to pure crystals. On the other hand, theoreticians also have a fundamental difficulty in developing tlieir models due to the lack of perfect periodic structure in the alloy formation. In a definite manner the theoretical works have a proiiounced influence of the following aspects: (1) Whether the "host" crystal is liglit or heavy in comparisor to tlie impurity atom, and (2) Whether the atomic percent of the impurity atom in the alloy is low or high. It is found that heavy impurities in the light host lattice give rise to resonance modes corresponding to vibrations with rather low frequencies in comparision to the liost crystal. Systems with light impurities in heavy host lattices give rise to localized modes. From a theoretical point of view, the occurence of resonance rnodes or localized modes is predicted considering the mass defect and force constant changes as rigorously as possible. Some of tlie well known theories for binary allcys developed so far are those of Elliot and Maradudin[7], Taylor[8] and Mostoller and Kaplan[9]. It is noted that none of the aforesaid theories has equal success in interpreting the experimental phonon spectra for all the binary alloys combined together. We have developed a phenomenological model for $A_{1-x}B_x$ inetallic alloys[10]. In order to do that we followed completely tlie works of Kutty[11] and Garg et al.[12]. The basic ingredient in our theory was to select a good lattice dynamical inodel for tlie host and impurity atoms, A and B, which predicted experimental phonon spectra very well. The dynamical matrix for the $A_{1-x}B_x$ alloys have the following important features:

1. It is a 6 × 6 matrix and not a **3** x 3 as for pure metals A and B.
2. For all concentrations of the alloy in tlie host lattice, ie. 1% ≤ x ≤ 99%, this dynamical matrix gives only 3 eigenfrequencies for any particular phonon wavevector. The other 3 roots have zero frequency.
3. When x = 0% or x = 100%, the dynamical matrix of the alloy predicts tlie phonon frequency for tlie pure metals A and B. This shows that our clioice of an extended order dynamical matrix is not arbitrary but compatible with the theory.

In our previous study of the lattice dynarnics of $Rb_{1-x}K_x$ alloy[10] we had studied the case of a liglit impurity in tlie heavy host giving rise to localized modes. As a matter of fact localized modes are more complicated to interpret than the resonance mode. Following Garg et al.[12] we have, used a nonrandomiiess parameter λ to interpret the localized modes and dropped it out here for the study of resonance modes in $Cr_{1-x}W_x$ alloys. The phonon dispersion relations along the tliree

principal symmetry directions for tlie tliree different tungsten concentration in chromium, $x = 0.3\%$, 0.8% and 1.6% form the subject matter of tliis paper.

II. Theory

Tlie dynamical matrix necessary to calculate the phonon frequencies of tlie alloy $A_{1-x}B_x$ is given by[10]

$$\begin{vmatrix} (1-x)^2P - M_A\omega^2 & x(1-x)P \\ x(1-x)P & x^2P - M_B\omega^2 \end{vmatrix} = 0 \qquad (1)$$

where w is tlie phonon frequency, x is tlie alloy concentration, M_A and M_B are the masses of atom A and B, respectively. P is the dynamical matrix of tlie b.c c. system, previously introduced to study $Rb_{1-x}K_x$ alloys. In accordance with the earlier studies of phonons foi. the pure metals of tungsten and chromium[13], me have also considered tlic interionic interactions in alloys of chromium and tungsten to be effective between first two nearest neighbours.

Tlie typical diagonal aiid non diagonal part of the dynamical matriccs P_{ii} and P_{ij} are giveii by:

$$\begin{aligned} P_{ii} &= \frac{8}{3}A_1(1 - C_iC_jC_k) \\ &+ 2A_2(1 - C_{2i}) + 8B_1(1 - C_iC_jC_k) + 2B_2(3 - C_{2i} - C_{2j} - C_{2k}) \\ &+ \frac{a^3\lambda^2K_e}{4}\sum_h \left| \frac{(q_1 + h_i)^2}{|\vec{q}+\vec{h}|^2 + \frac{a^2\lambda^2}{4\pi^2}f(t_1)}g^2(u_1) - \frac{h_i^2}{h^2 + \frac{a^2\lambda^2}{4\pi^2}f(t_2)}g^2(u_2)\right|, \end{aligned} \qquad (2)$$

and

$$\begin{aligned} P_{ij} &= \frac{8}{3}A_1S_iS_jC_k \\ &+ \frac{a^3\lambda^2K_e}{4}\sum_h \left| \frac{(q_i + h_i)(q_j + h_j)}{|\vec{q}+\vec{h}|^2 + \frac{a^2\lambda^2}{4\pi^2}f(t_1)}g^2(u_1) - \frac{h_ih_j}{h^2 + \frac{a^2\lambda^2}{4\pi^2}f(t_2)}g^2(u_2)\right| \end{aligned} \qquad (3)$$

Tlie parameters in the above equations are given by $S_i = \sin(\pi aK_i)$, $C_i = \cos(\pi aK_i)$ $q_i = \frac{aK_i}{2\pi}$, $\lambda = 0.353\left(\frac{r_s}{a_o}\right)^{1/2}k_F$,

$$g(u) = 3.(\sin\ u - u\ \cos\ u)/u^3, \qquad (4)$$

$$f(t) = \frac{1}{2} + \frac{1-t^2}{4t}\ln\left|\frac{1+t}{1-t}\right|, \qquad (5)$$

$$t_1 = \frac{\pi|\vec{q}+\vec{h}|}{ak_F}, \qquad (6)$$

$$t_2 = \frac{\pi h}{ak_F}, \qquad (7)$$

$$u_1 = \frac{2\pi r_s}{a}(\vec{q}+\vec{h}), \qquad (8)$$

$$u_2 = \frac{2\pi r_s h}{a}, \qquad (9)$$

where **Ir',**, and h, (i = 1, 2, 3) are respectively tlie cartesian components of the wavevector and tlie reciprocal lattice vector: a is tlie lattice parameter; k_F represent tlie Fermi wavevector: r, is tlie radius of atomic sphere; a_0 is the Bohr radius aiid k_e represents tlie bulk modulus of tlie electron gas.

III. Numerical Computations

There are five disposable parainеters in our model and these are A,, $B_i(i = 1, 2)$ and K_e. The model parainеters for the pure inetal tungsten and chromium are taken from the earlier work by one of us[13]. In order to evaluate the moclel parameters of tlie alloy we have used the linear interpolation sclieme

$$(A_i, B_i, K_e)_{alloy} = (1-x)(A_i, B_i, K_e)_{Cr} + x(A_i, B_i, K_e)_W$$

Tlie input data to calculate the phonon frequencics of tlie alloys at tlie three different concentrations is shown in Table 1.

Table 1
Inp ıt data (in units of 10^3 dyn/cm)

Chromium Concentration	A_1	B_1	A_2	B_2	ake
0.3 *at* %*W*	24.711	28.100	4.230	2.101	15.877
0.8 *at* %*W*	24.844	28.128	4.233	2.108	16.035
1.6 *at* %*W*	25.057	28.174	4.238	2.119	16.287

We have solved the dynamical matrix for the three principal symmetry directions. [ξ00], [[(O] and [ξξξ], and plotted the computed aiid experimental frequencies iii figure? 1 to 3. hlso given in Table 2 aiid 3 are tlie calculated aiid experimental frequencies and deviations between them for those wavevectors for which experimental results were available.

Table 2
Calculated aiid experimental values of phonons frequencies in tlie traiisversal branch $[\xi, 0, 0]$ direction

$x = 0.3\%$

ξ	Exp. values [TH]	Calc. values [TH]	$\frac{(W_{exp}-W_{calc})}{W_{exp}}$
0.15	1.94	1.93	0.00
0.20	2.62	2.54	0.02
0.25	3.29	3.14	0.05
0.30	3.93	3.71	0.06
0.35	4.53	4.25	0.06
0.40	5.09	4.76	0.06
0.45	5.58	5.23	0.06
0.50	5.94	5.66	0.05

$x = 0.8\%$

ξ	Exp. values [TH]	Calc. values [TH]	$\frac{(W_{exp}-W_{calc})}{W_{exp}}$
0.15	1.04	1.91	0.01
0.20	2.61	2.52	0.03
0.25	3.25	3.11	0.04
0.30	3.86	3.68	0.05
0.35	4.53	4.21	0.07
0.40	5.13	4.71	0.08
0.45	5.55	5.18	0.07
0.50	6.00	5.61	0.06

$x = 1.6\%$

ξ	Exp. values [TH]	Calc. values [TH]	$\frac{(W_{exp}-W_{calc})}{W_{exp}}$
0.15	1.91	1.88	0.01
0.20	2.54	2.48	0.02
0.25	3.16	3.07	0.03
0.30	3.83	3.62	0.05
0.35	4.46	4.15	0.07
0.40	5.10	4.64	0.09
0.45	5.57	5.10	0.08
0.50	5.94	5.53	0.07

Table 3
Calculated aiid experimental values of phonons frequencies in the transversal branch along $[\xi, \xi, 0]$ direction

$x = 0.3\%$

ξ	Exp. values [TH]	Calc. values [TH]	$\frac{(W_{exp}-W_{calc})}{W_{exp}}$
Q15	3.10	3.12	0.01
0.20	4.12	4.04	0.02
0.25	5.00	4.86	0.03
0.30	5.78	5.56	0.04
0.35	6.41	6.12	0.04
0.40	G.95	6.54	0.06
0.45	7.27	6.79	0.07
0.50	7.52	6.87	0.09

$x = 1.6\%$

ξ	Exp. values [TH]	Calc. values [TH]	$\frac{(W_{exp}-W_{calc})}{W_{exp}}$
0.15	2.99	3.03	0.01
0.20	4.00	3.93	0.02
0.25	4.93	4.73	0.04
0.30	5.74	5.41	0.06
0.35	6.43	5.96	0.07
0.40	6.95	6.36	0.09
0.45	7.23	6.61	0.09
0.50	7.49	6.69	0.10

IV. Discussions and Conclusions

A critical analysis of Fig. 1-3 reveals tliat Cunnigham et al.[5] have measured only tlie transverse branches of tlie phonons along tlie [ξ00] and [ξξ0] directions, for tlie alloy concentrations x = 0.33% aiid $x = 1.6\%$ and for tlie concentration $x = 0.8\%$ only tlie branch along tlie [ξ00] was measured. Note tliat although a small amount of measurements is available

they provide a relatively good test for the theory. The tl-ieoretical predictions are very close to the experimental ones. In order to show quantitative differences between the calculated and experimental phonons we have given in Table 2 and 3 these results. The maximum percentage deviation between the calculated and experimental values is of the order of 10% which represents a good agreement.

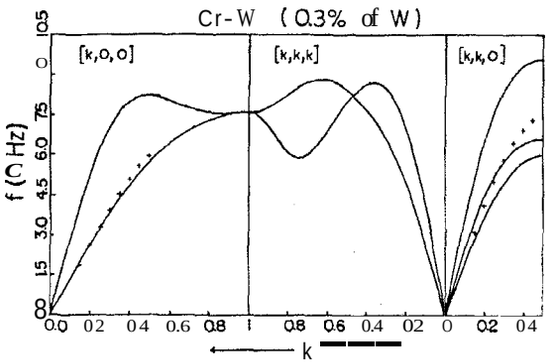

Figure 1: Phonon dispersion curves in $Cr-$W (0.3% at W) along the $[\xi,0,0]$, $[\xi.\xi,0]$ and $[\xi,\xi,\xi]$ directions. Tlie solid lines represent the theoretical results for longitudinal and transversal modes. The points represent tlie experimental results.

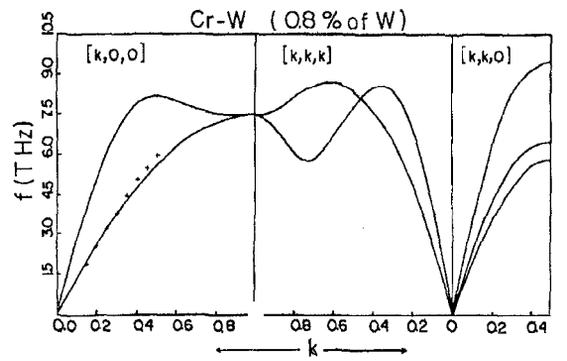

Figure 2: Phonon dispersion curves in $Cr-$W (0.8% at W) along the $[\xi,0,0]$, $[\xi,\xi,0]$ and $[\xi,\xi,\xi]$ directions. The solid lines represent the tlieoretical results for longitudinal and transversal modes. The points represent tlie experimental results.

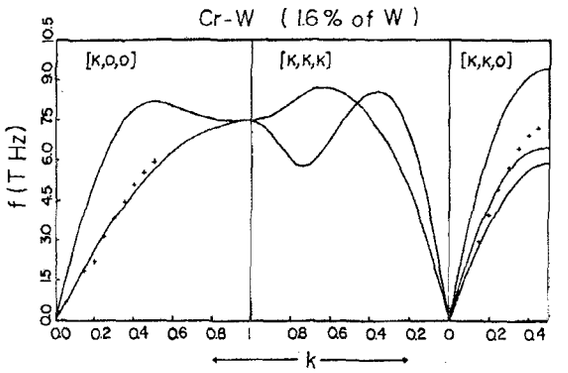

Figure 3: Plionon dispersion curves in $Cr-$W (1.6% at W) along tlie $[\xi,0,0]$,$[\xi,\xi,0]$ and $[\xi,\xi,\xi]$ dircctions. Tlie solid lines represent tlie tlieoretical results for longitudinal and transversal modes. The points represent the experimental results.

Tliis paper is the second one studying b.c.c. inetallic alloys based on our scheme of adopting a model for alloys. The first one was for $Rb_{1-x}K_x$ alloys[10]. We have obtained liere almost the same success as obtained in $Rb_{1-x}K_x$. Our work is based on a modification over the scheme of Garg et al.[12,14] for $Rb_{1-x}K_x$ and $Cr_{1-x}W_x$ but we have obtained definitively an improvement upon their their results because we have used a better model for the individual metals. Our model takes into account the electron-ion interaction which was ignored by tl-iose authors and preserves the periodicity in tlie calculated phonon frequencies in the reciproca1 space. We would like to point out that we have no means to check tlie validity of tlie theoretical calculations for the longitudinal branches of the phonon dispersion relations along [ξ00], [ξξ0] and [ξξξ]. On the other hand in our theoretical study of $Rb_{1-x}K_x$ we could not verify tlie transversal plionon frequencies. Another point to empliasize in our study of tlie two alloys is that one work is coinplementary to tlie other as in one we have studied the resonance mode and in otlier the local inode. To conclude we note that further detailed experimental measurements of the phonon frequencies of tlie two alloys studied by us is still necessary to allow a better comparison with our theoretical approach.

Finally, we comment that our theoretical scheme[15] was also applied for f.c.c alloys of $Ni_{1-x}Co_x$ and an excellent agreement was found.

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