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Lattice dynamics of $Rb_{71}K_{29}$: Molecular dynamics study

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Interionic potentials have been constructed to describe the lattice dynamics of the alloy $Rb_{71}K_{29}$. Using these, computer-simulation molecular-dynamics calculations have been carried out for a system of 432 particles, periodic boundary conditions being used to approximate the infinite system. The results show that considerable local structural relaxation occurs around the K atoms. The dynamical structure factor $S(\vec{Q},\omega)$ has been calculated for selected wave vectors corresponding closely to those studied experimentally by Kamitakahara and Copley. There is excellent agreement with the experimental data where comparison is possible, both with respect to the local modes and to the host lattice frequencies.

I. INTRODUCTION

During the past few years a considerable effort has been expended in the study of various properties of alloys. Both theoretical and experimental investigations of electronic, magnetic, lattice-vibrational, mechanical, etc. properties have added a great deal to our understanding of these systems. Conceptually, the lattice-dynamical properties are possibly the easiest to understand upon alloying a material. Local modes are easily visualized, and a qualitative feeling for frequency shifts can often be otained by using simple mass defect arguments. But a detailed theoretical understanding of these features, particularly in the presence of anharmonic effects, can be very complicated. For many of the systems studied experimentally [e.g.,[1] Ni(Pd) and[2] Cu(Al)], a good theoretical treatment of the lattice dynamics of the pure constituents has not yet been obtained. Hence a quantitative theoretical understanding of these alloys is, at present, well-nigh impossible. However, there is one alloy system for which good data are available and which is within the scope of present-day theory. This is the Rb-K system. Kamitakahara and Copley[3] have used inelastic neutron scattering to study $[\xi\xi 0]L$ and $[\xi 00]T$ phonons of $Rb_{1-c}K_c$ at three concentrations ($c=0.06$, 0.18, and 0.29) and three temperatures (10, 85, and 190 K). A particularly interesting feature of these measurements is the presence of a local mode associated with both phonon branches at high frequencies. This mode, which grows in intensity as c is increased, appears to be associated with the motion of K ions ($M_{Rb}=2.18M_K$, where M is the ionic mass). Its position is virtually independent of temperature, and it exhibits some dispersion. A good test of a theoretical treatment would be to see whether these modes, as well as those of the host crystal, would be predicted at the correct frequencies, and whether the correct relative intensities would be obtained.

From a theoretical point of view, $Rb_{1-c}K_c$ is a good system to study. Both constituents are alkali metals which, because of their relatively simple band structure, are generally the least complicated of all metallic systems to deal with. There are, however, some difficulties with Rb which will be discussed in Sec. II. Assuming, then, that a good description of both Rb and K metals can be utilized, a study of the alloy system will shed a great deal of light on the general usefulness of the technique employed. One such technique that has been used by several authors[3-5] is the coherent-potential approximation (CPA). This is a mean-field type of approach that has frequently been successfully employed to describe electronic densities of states in random alloys. In the first attempt to use the CPA to describe the lattice dynamics of Rb-K, Kamitakahara and Copley[3] simply described the K ion as a mass defect, with no change of force constants. Qualitatively, their results showed the same features as the experimental data, but the calculated peaks were in the wrong positions as well as being poorly differentiated and not always having the right widths.

Mostoller and Kaplan[4] attempted to improve on the Kamitakahara and Copley calculations. They included nearest-neighbor radial force constant changes by using an extension of the CPA in which the forces superimposed linearly. The remainder of the force constants were treated in the virtual-crystal approximation. This resulted in better, but still not satisfactory, agreement with experiment. In particular, the local mode was rather poorly defined.

A further extension of the CPA approach has been employed by Grünewald and Scharnberg.[5] These authors used the microscopic description of Price *et al.*[10] for pure K and Rb, and recalculated the force constants at an electron density appropriate to the alloy. They then averaged the force constants to produce an effective force-constant matrix and an effective density of states for a periodic lattice. The procedure results in a further improved agreement with experiment, the peak positions being generally correct. However, neighboring peaks are not differentiated nearly so sharply as in the experiment. This appears to be a basic feature of any CPA calculation simply because of its mean-field character.

In this paper, we apply the classical molecular-dynamics (MD) procedure to the Rb-K alloy problem. This avoids the concentration averaging implicit in the CPA approach, and also allows for the inclusion of anharmonic and multiphonon effects. This technique is particularly useful where the constituents are of a different size, giving rise to size effect distortions and destroying the lattice periodicity. The chief disadvantage of a MD calculation is the cost involved. This has the effect of limiting the size of the cluster of Rb and K ions considered, and, therefore, the number of phonon modes that can be analyzed. Also, in our case, we were able to afford to study only one concentration ($c = 0.29$), one temperature (80 K), and one random disposition of ions in the lattice. This was still sufficient to provide a meaningful test of our description of the alloy, and to allow us to compare our results with the CPA calculations. Not surprisingly, we found that the peaks in the MD run were more clearly defined than in the CPA results. In general, the agreement with experiment was very good, and we feel that our results provide a good understanding of phonons in the Rb-K system.

Another motivation for performing a MD calculation is that it provides a good, direct test of the CPA. The model is well defined, and a meaningful comparison of techniques becomes possible if the same force constants are employed. Our force constants for all three types of interactions in the alloy are available from the authors on request.

In Sec. II, we give the details of our description of the alloy and our calculations. We then present our results in Sec. III, with a summary in Sec. IV.

II. DETAILS OF CALCULATION

A. Interionic potentials for the alloy

To describe the Rb-K alloy system, three pair potentials were required. For the K-K interaction $V_{K\text{-}K}(r)$, we used the potential of Dagens *et al.*[6] (DRT), recalculated at the appropriate electron density for the alloy. This potential has been shown to give an excellent account of the lattice dynamics of pure K.[6-9]

A good description of Rb is rather more complicated than that of K. The problem stems from the fact that at pure Rb density the compressibility of the electron gas is close to zero, and is conceivably negative. Hence the normal approach of a pseudopotential-perturbation calculation, based on the electron gas as the zero-order approximation, is rather dubious. This is because one is starting with a thermodynamically unstable system to provide a description of one which is thermodynamically stable. The way out of this dilemma, adopted by Price *et al.*,[10] was to scale the electron gas density parameter r_s by the band-structure effective mass m^*, which then meant that one was dealing with an effective density for which the electron gas compressibility was large and positive. The physical meaning of this approach is not clear, but it bears a close resemblance to Kukkonen's[11] suggestion that the effect of the large core polarization of Rb could be taken into account by a suitable scaling of r_s, also in the direction of large, positive compressibility. These ideas clearly warrant further investigation, but the interesting feature is that by use of the Ashcroft pseudopotential, with suitable choice of the model radius parameter R_c and adjustment of m^*, Price *et al.*[10] obtained a good fit to the observed Rb phonon dispersion curves. Also, their potential was found by Rahman[12] to be in excellent accord with the collective excitations in liquid Rb. Hence despite the obvious objections, we have taken the pragmatic route of performing a similar calculation to that of Price *et al.*, our reasoning being that, for the problem at hand, such a description of Rb should be adequate. To be precise, we chose $R_c = 2.45$, $m^* = 0.852$, and used the Geldart and Taylor[13] dielectric function to screen the Ashcroft model potential.

For the Rb-K interaction $V_{Rb\text{-}K}$, the appropriate Rb and K model potentials were combined, with m^* scaled to a value of 0.926, to produce an impurity potential as described by DRT and as applied previously to impurity problems[14] and alloys.[15]

B. Quasiharmonic lattice dynamics of Rb

As a test of our description of Rb, we have calculated quasiharmonic frequencies for a lattice

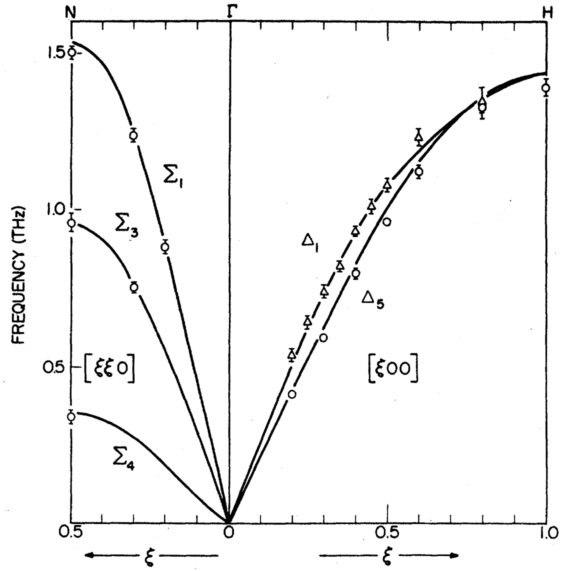

FIG. 1. Phonon dispersion curves for symmetry directions in solid Rb. Experimental points (Ref. 16) and quasiharmonic calculations (solid curve are for $T=12$ K ($a=5.585$ Å).

parameter of $a=5.585$ Å for eight shells of interacting neighbors. The results are shown in Fig. 1 and compared with the measured frequencies of Copley and Brockhouse[16] at 12 K for the [ξξ0] and [ξ00] directions. There seems to be good overall agreement, with a small systematic error for the [ξ00]T branch, the calculations being about 0.04 THz too high at the zone boundary. This discrepancy may reflect the fact that we used only a local pseudopotential description of Rb. It may also be due, in part, to anharmonic effects, since it is known that this Δ_5 branch, and H_{15} point in particular, has the largest anharmonic shifts.[17]

Copley *et al.*[18] have measured the temperature and volume dependence of selected phonons in solid Rb. Using data at four temperatures (80, 150, 230, and 295 K) they computed average values for the zero-pressure mode Grüneisen parameters $\gamma_i = -(\partial \ln\omega_i/\partial \ln V)$. These are listed in Table I along with our calculated values, which seem to be systematically smaller. Nevertheless, the calculations give a rather faithful reproduction of the relative values. A detailed examination of the actual shift in phonon frequency, induced by a given volume change, appears to generate data in good agreement with the actual measurements of Copley *et al.*[18] Hence we believe that their error bars are somewhat optimistic.

The interest in obtaining Grüneisen parameters is due to the fact that our model must be able to account for volume changes and their effects on the lattice dynamics. For example, a 1% change in the Rb-K nearest-neighbor separation would generate approximately a 4% shift in a phonon frequency (cf. Table I). As we shall see, important local relaxations do occur in the alloy. We conclude from these results that the description of pure Rb is very satisfactory.

C. Structure of the alloy

The system consisted of 432 particles arranged on a bcc lattice, 125 of which were randomly chosen to be K atoms. Periodic boundary conditions were used to simulate an infinite system. The atoms interacted with the appropriate interatomic potentials described earlier, namely, $V_{\text{K-K}}$, $V_{\text{Rb-K}}$, or $V_{\text{Rb-Rb}}$, truncated after eight shells of neighbors ($2.5a$). In this way, a given atom interacted with 112 atoms. Previous studies of solid Na and K have shown that such a procedure represents the optimum compromise between accuracy and computer time.[19,20] The classical equations of motion for this system were integrated using the Verlet algorithm and a time step of 3×10^{-14} sec. An initial run of 1000 time steps was carried out at a temperature of about 80 K. This temperature is much less than the melting point (330 K), but yet greater than the Debye temperature, so that classical mechanics should apply on the one hand, and anharmonic effects should be relatively unimportant on the other. The molecular-dynamics data were stored every fourth time step on a magnetic tape. At the end of this initial run, certain properties of the system were examined. For example, the rms amplitudes of the K and Rb atoms were

TABLE I. Mode Grüneisen parameters for rubidium. Experimental values are taken from Copley *et al.* (Ref. 18).

Direction	Polarization	Reduced wave vector $\xi = aq/2\pi$	γ(expt)	γ(calc)
[ξ00]	L	0.20	2.15 ± 0.23	1.5
[ξξ0]	L	0.20	1.65 ± 0.07	1.3
[ξξ0]	T_1	0.30	1.31 ± 0.25	1.0
[ξ00]	T	0.20	0.99 ± 0.13	0.7

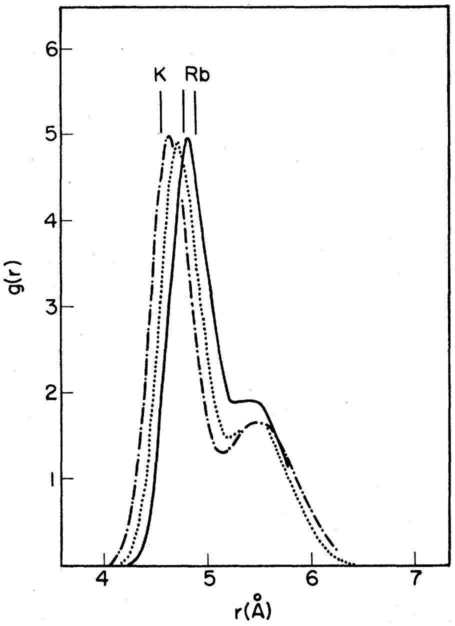

FIG. 2. Spherically averaged radial distribution functions for the alloy at 80 K, $g_{\text{Rb-Rb}}(r)$ (solid curve), $g_{\text{Rb-K}}(r)$ (dotted curve), $g_{\text{K-K}}(r)$ (dash-dot curve). Vertical lines refer to the nearest-neighbor separations for pure Rb, the alloy, and pure K at 80 K.

found to be 8.1% and 7.8%, respectively, of the mean nearest-neighbor separation of the alloy (4.768 Å). The spherically averaged radial distribution functions, $g_{\text{Rb-Rb}}(r)$, and $g_{\text{Rb-K}}(r)$, and $g_{\text{K-K}}(r)$, were examined and results for the two closest shells of neighbors are shown in Fig. 2.

From this figure we see that considerable local relaxation occurs and that the alloy is far from homogeneous in density. Recall that our choice of lattice parameter, 5.506 Å, was taken from a linear interpolation between that for pure K $a = 5.251$ Å and pure Rb $a = 5.610$ Å at 80 K, previous experiments having shown that this K-Rb alloy followed closely such a law, at least at room temperature.[21] The corresponding nearest-neighbor separations for bcc K and Rb are 4.548 and 4.858 Å, respectively, and these distances are indicated in Fig. 2 along with the mean nearest-neighbor separation, 4.768 Å, expected for the alloy. The actual nearest-neighbor separations found in our computer simulation are seen to differ considerably from the mean value. The alloy thus appears to undergo local relaxations such that the environment of a K atom tends to be compressed, while that of a Rb atom is expanded. To appreciate the importance of these relaxations, we note that equivalent dilations of pure Rb and K crystals would lead to approximately a 5% softening of the Rb zone-boundary frequencies and a 7% hardening in K. These figures are based on the calculated Grüneisen parameters of Table I for Rb and Ref. 9 for K. Since the total measured shift of the local K mode out of the host band is about 20% at the zone boundary, in principle these dilations can account for half of the effect. To date, such effects have not been incorporated in analytical theories of the dynamics of alloys.

Certain preliminary studies were also carried out on the dynamical properties, and these indicated reasonable accord with observed phonon frequencies.[22] The molecular-dynamics run was then extended for approximately 15 000 steps in order to improve the statistics for the calculation of phonon frequencies. This course was chosen rather than, say, averaging the results of three clusters run for 5000 steps, because it was felt that at the 29% concentration little was to be gained from averaging over additional random dispositions, whereas it was important to average out as much noise as was practical.[7] The results are described in Sec. III.

III. DYNAMICAL STRUCTURE FACTOR $S(\vec{Q}, \omega)$

The experimental neutron scattering study of Kamitakahara and Copley[3] revealed the existence of a well-defined local mode for the $Rb_{71}K_{29}$ alloy for the high-frequency phonons of the $[001]T$ and $[110]L$ branches. As indicated in the Introduction, CPA calculations have not given an entirely satisfactory description of the measured $S(\vec{Q}, \omega)$. One reason for this would appear to be because the mean-field character of the CPA cannot take account of the local relaxations described in Sec. II. The MD computer simulation, in allowing for this effect as well as avoiding other mean-field approximations, goes beyond the CPA. Our preliminary study[22] of $Rb_{71}K_{29}$ revealed the clear differentiation of peaks that was observed experimentally, and demonstrated the usefulness of the technique as well as the importance of the effects that cannot be included via a CPA approach. Encouraged by these results, we have carried out the detailed study reported here.

The neutron scattering experiments are related to the dynamical structure factor $S(\vec{Q}, \omega)$, where $\vec{Q}$ and ω are the momentum and energy transferred to the crystal by the neutrons. Following van Hove, this can be related to the Fourier transform of the intermediate scattering function $F(\vec{Q}, t)$:

$$S(\vec{Q}, \omega) = \int_{-\infty}^{\infty} F(\vec{Q}, t) e^{i\omega t}\, dt,$$

where the intermediate scattering function is given by the following ensemble average, which is evaluated by molecular dynamics:

$$F(\vec{Q},t)=\langle\rho_{\vec{Q}}(t)\rho_{-\vec{Q}}(0)\rangle,$$

with

$$\rho_{\vec{Q}}(t)=\sum_{l} b_l e^{-i\vec{Q}\cdot\vec{r}_l(t)}.$$

The summation over l extends over all the atoms of the system (both K and Rb atoms), whose positions at time t are given by $\vec{r}_l(t)$ and whose scattering lengths for the neutrons are given by $b_{\mathrm{Rb}} = 0.708$, $b_{\mathrm{K}}=0.37$. Because of the presence of the two kinds of atoms, $S(\vec{Q},\omega)$ can be decomposed into three contributions:

$$S(\vec{Q},\omega)=S_{\mathrm{K\text{-}K}}(\vec{Q},\omega)+2S_{\mathrm{K\text{-}Rb}}(\vec{Q},\omega)+S_{\mathrm{Rb\text{-}Rb}}(\vec{Q},\omega).$$

We often found it helpful in identifying the local mode to examine $S_{\mathrm{K\text{-}K}}$ and $S_{\mathrm{Rb\text{-}Rb}}$ separately.

Finally, if we introduce weightings $b_{\mathrm{Rb}}=+1$, $b_{\mathrm{K}}=-1$, then the resulting dynamical structure factor can be related to the spectrum of concentration fluctuations occuring in the system,[23,24] $S_{CC}(\vec{Q},\omega)$ and this too was calculated.

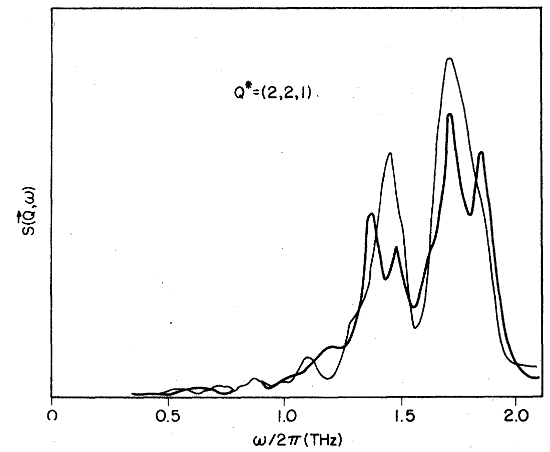

FIG. 3. One-phonon approximation to $S(\vec{Q},\omega)$, $S_1(\vec{Q},\omega)$ for $Q^*=(2,2,1)$. Heavy line is $S_1(\vec{Q},\omega)$ averaged over 1000 time steps and thin line is $S_1(\vec{Q},\omega)$ averaged over the full run.

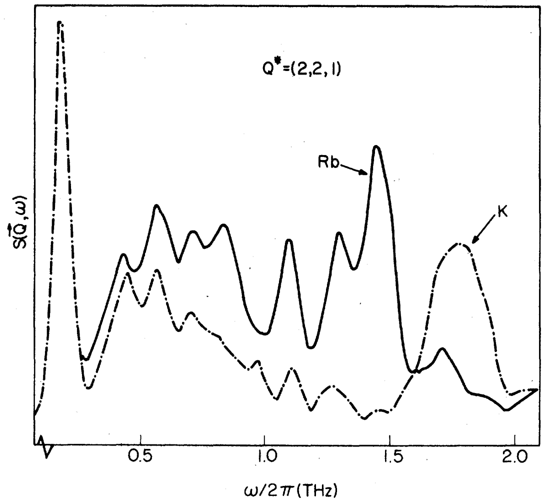

FIG. 4. $S_{\mathrm{K\text{-}K}}(\vec{Q},\omega)$ (dash-dot curve) and $S_{\mathrm{Rb\text{-}Rb}}(\vec{Q},\omega)$ (solid curve) for $Q^*=(2,2,1)$.

Since our system consisted of 432 atoms this restricts the allowable $\vec{Q}$ vectors that can be studied. The smallest allowable vector is $(2\pi/6a)(1,0,0)$. We note that in the $[\xi\xi0]$ direction only the three points $(2\pi/a)(\zeta,\zeta,0)$ with $\zeta=\frac{1}{6}$, $\frac{1}{3}$, and $\frac{1}{2}$ can be studied, but fortunately, experiments showed that the latter two should both give the local mode. Defining $\vec{Q}^*=\vec{Q}/(2\pi/a)$, we chose to study in detail the six wave vectors $Q^*=(2,2,\frac{1}{6})$, $(2,2,\frac{2}{3})$, $(2,2,1)$, $(2\frac{1}{3},2\frac{1}{3},0)$, $(2\frac{1}{2},2\frac{1}{2},0)$, and $(1\frac{1}{2},1\frac{1}{2},1)$. The last wave vector was included not to study the local mode, but because previous studies[25] in solid K had shown that a large positive anharmonic shift from the quasiharmonic frequency should be expected for this, the slowest zone-boundary transverse mode propagating in the $[\xi\xi0]$ direction. As in previous work, we found it helpful also to examine $S_1(\vec{Q},\omega)$ the one-phonon approximation to $S(\vec{Q},\omega)$. This follows from writing $\vec{r}_l(t)=\vec{R}_l+\vec{u}_l(t)$, where $\vec{u}_l(t)$ represents the time-dependent displacement of the lth atom from its mean lattice position $\vec{R}_l$. In detail we calculate

$$S_1(\vec{Q},\omega)=\int_{-\infty}^{\infty} e^{i\omega t}F_1(\vec{Q},t)\,dt,$$

with

$$F_1(\vec{Q},t)=\langle\tilde{\rho}_{\vec{Q}}(t)\tilde{\rho}_{-\vec{Q}}(0)\rangle.$$

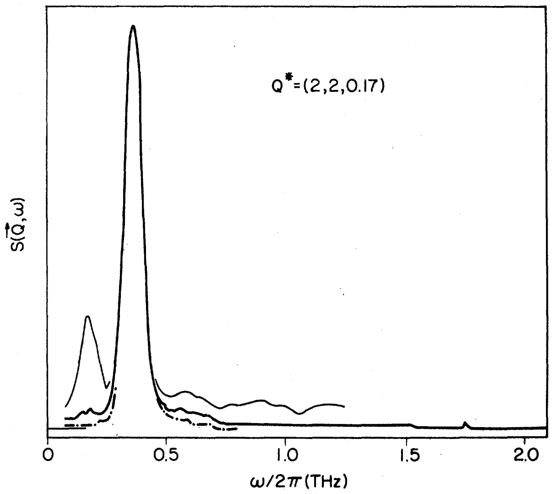

FIG. 5. $S(\vec{Q},\omega)$ (heavy curve) for $Q^*=(2,2,\frac{1}{6})$. Dash-dot curve is the one-phonon approximation and thin curve is $S_{CC}(\vec{Q},\omega)$ the spectrum of concentration fluctuations.

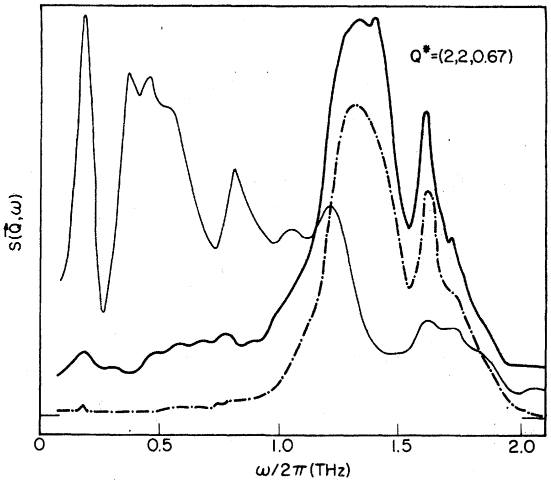

FIG. 6. $S(\vec{Q},\omega)$ (heavy curve) for $Q^*=(2,2,\frac{2}{3})$. See Fig. 5 for the definitions of the other curves.

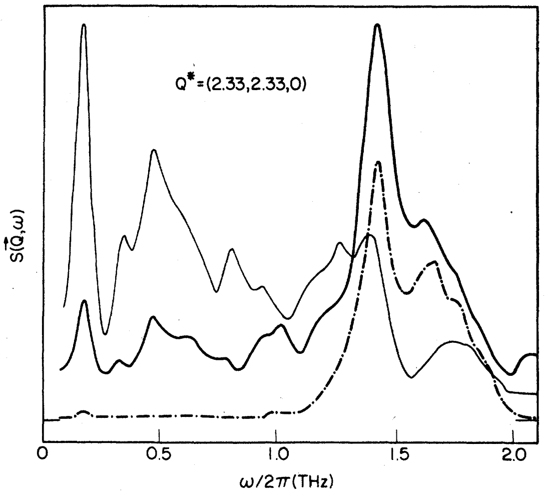

FIG. 8. $S(\vec{Q},\omega)$ (heavy curve) for $Q^*=(2\frac{1}{3},2\frac{1}{3},0)$. See Fig. 5 for the definitions of the other curves.

The one-phonon approximation to the density operator can be written

$$\tilde{\rho}_Q(t)=d_l(\vec{Q})\sum_l b_l e^{-i\vec{Q}\cdot\vec{R}_l}\, i\vec{Q}\cdot\vec{u}_l(t),$$

and the Debye-Waller factor is given as usual by

$$d_l(\vec{Q})=\langle e^{i\vec{Q}\cdot\vec{u}_l(t)}\rangle\simeq e^{-1/6Q^2\langle u_l^2\rangle},$$

for a cubic crystal.

The spectra $S_1(\vec{Q},\omega)$, since they are devoid of the multiphonon contribution, are often much easier to interpret.

To improve the statistics we averaged over all possible independent wave vectors and used 14 500 time steps. Figure 3 shows the $S_1(\vec{Q},\omega)$ spectrum for $Q^*=(2,2,1)$ averaged over the full run and the last 1000 time steps only. The comparison of the two calculations gives some idea of our probable uncertainty. There seems little doubt that the spectrum consists of two main peaks. Figure 4 shows $S_{\mathrm{K-K}}(\vec{Q},\omega)$ and $S_{\mathrm{Rb-Rb}}(\vec{Q},\omega)$ for $Q^*=(2,2,1)$, from which we see that the high-frequency peak is due to the K atoms.

Figures 5–10 show the various spectra $S(\vec{Q},\omega)$ for the six Q^* given above. Also shown in these figures are the $S_1(\vec{Q},\omega)$ spectra and $S_{CC}(\vec{Q},\omega)$. The latter appears always to contain a contribution from the low-frequency $[\xi\xi 0]T$ branch. All spectra have been convoluted with a Gaussian filter function with FWHM of 0.063 THz; this serves as

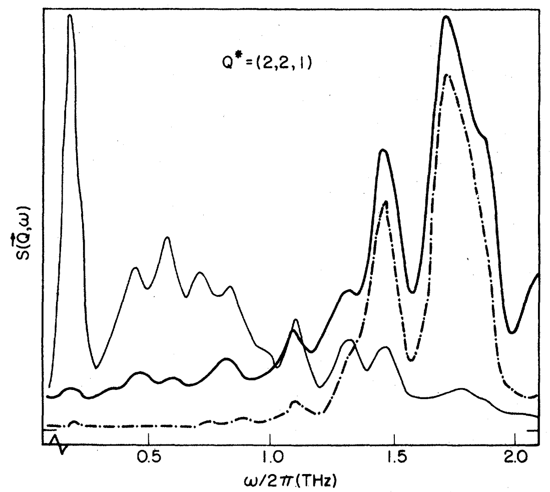

FIG. 7. $S(\vec{Q},\omega)$ (heavy curve) for $Q^*=(2,2,1)$. See Fig. 5 for the definitions of the other curves.

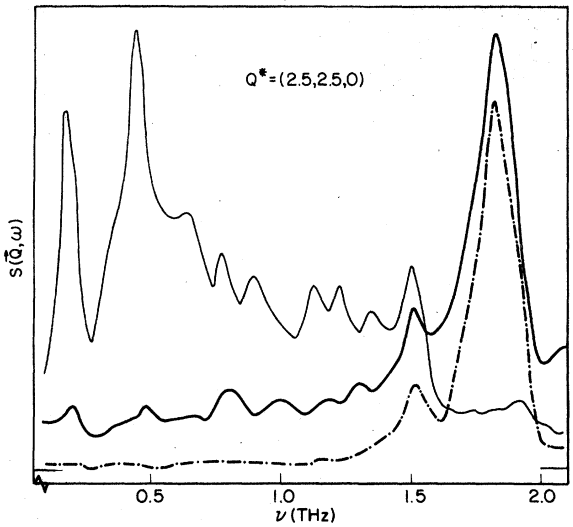

FIG. 9. $S(\vec{Q},\omega)$ (heavy curve) for $Q^*=(2\frac{1}{2},2\frac{1}{2},0)$. See Fig. 5 for the definitions of the other curves.

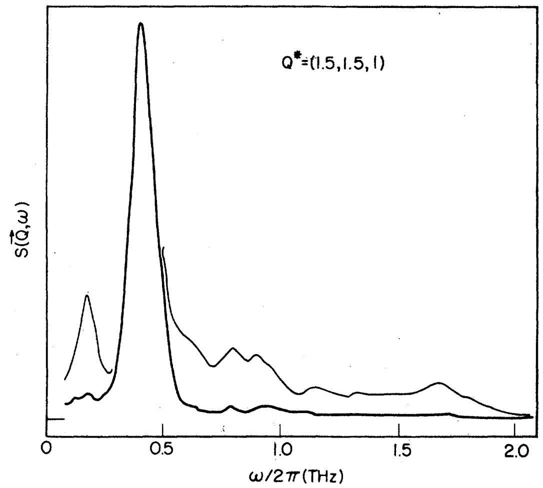

FIG. 10. $S(\vec{Q},\omega)$ (heavy curve) for $Q^* = (1\frac{1}{2}, 1\frac{1}{2}, 1)$. See Fig. 5 for the definitions of the other curves.

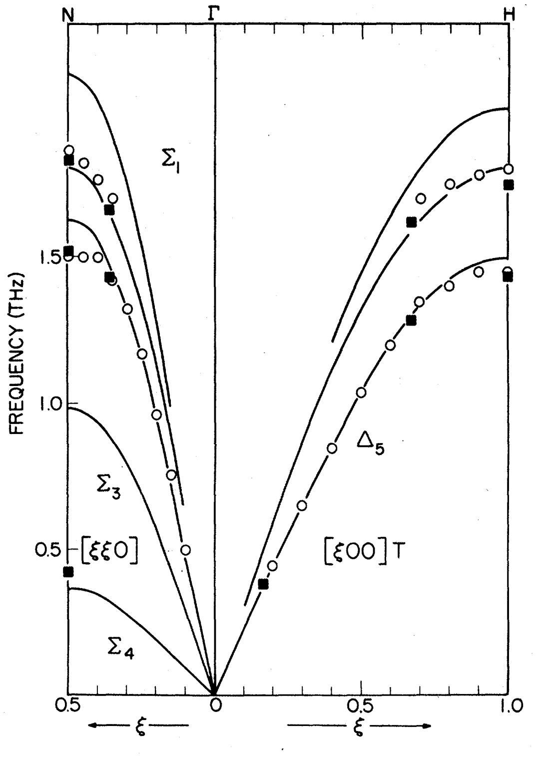

FIG. 11. Phonon dispersion curves for the $Rb_{71}K_{29}$ alloy. Calculations are for $T = 80$ K ($a = 5.506$ Å) and experimental points (Ref. 3) (open circles) are for $T = 10$K. Solid squares are the results of the MD computer simulation. For the Σ_3 and Σ_4 modes the solid lines are the quasiharmonic calculation for pure Rb at the alloy lattice parameter. For the Σ_1 and Δ_5 modes the solid lines are the quasiharmonic calculation for, in order of increasing magnitude, pure Rb, pure K, and K in Rb, all at the alloy lattice parameter.

an approximation to the experimental resolution function and also reduces our noise level somewhat. Comparison of the one-phonon approximation with the full $S(\vec{Q},\omega)$ for the wave vectors in question shows that at this temperature, 80 K, multiphonon effects appear to do little except provide a background with little structure. We have made no specific comparisons with the $S(\vec{Q},\omega)$ data since these will be published later, but reference to the unpublished work[3] shows excellent agreement between theory and experiment.

The most striking features of the simulations are the large widths calculated for the host lattice mode with $Q^* = (2, 2, \frac{2}{3})$ (Fig. 6) and also the (FWHM of ~ 0.2 THz) large width for the local mode $Q^* = (2, 2, 1)$ (Fig. 7). With reference to the latter figure we should point out that this differs somewhat from our preliminary results,[22] because in that work we made use of an outdated value of the RB scattering length.[26]

The molecular-dynamics results for the host lattice and local mode frequencies are shown as squares on Fig. 11. Also shown in this figure are the harmonic frequencies calculated for Rb and K at a lattice constant of 5.506 Å. It can be seen that the dispersion in the local mode and its frequency correlates quite strongly with the harmonic calculations for a pure K lattice at the appropriate density. Shown in the figure as circles are the experiment peak positions taken from the work of Kamitakahara and Copley. The agreement between our molecular-dynamics simulation and experiment is remarkably good, particularly for the large negative shift in the host lattice frequency for the $Q^* = (2, 2, 1)$ point.

IV. SUMMARY

We have carried out detailed calculations of $S(\vec{Q},\omega)$ for the alloy $Rb_{71}K_{29}$ at 80 K. For input we have used descriptions of Rb and K which give an excellent account of the lattice dynamics of the pure systems. The Rb-Rb and K-K potentials were recalculated at the appropriate alloy electron density and the cross interaction $V_{Rb\text{-}K}$ was calculated using a standard approach with no adjustment of parameters to fit alloy properties. The local mode associated with the motion of the K atoms is clearly seen and identified for $Q^* = (2, 2, 1)$, $(2, 2, \frac{2}{3})$, $(2\frac{1}{2}, 2\frac{1}{2}, 0)$, and $(2\frac{1}{3}, 2\frac{1}{3}, 0)$. There is good agreement with the 10-K experimental results of Kamitakahara and Copley, both with respect to the host lattice frequencies and the position of the local mode. Our calculations show that important local relaxations do occur in the alloy. We feel that any theory of the dynamics must necessarily incorporate such effects if a good account of the real system is to be expected.

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