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THE FORCE CONSTANTS FOR Kr SINGLE CRYSTALS

C. Ruiz Mejía

Instituto de Física, Universidad Nacional de México

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ABSTRACT: We evaluate the force constants for Kr single crystals, using the experimental results of Daniels et al, and compare our values with those obtained directly from the calculation of the phonon spectrum.

INTRODUCTION

The angular distribution of neutrons which are coherently scattered by one phonon processes consists of peaks like delta-functions whose position is governed by the conservation laws[1]:

$$\mathbf{k} = \mathbf{k}' + \mathbf{G} + \mathbf{K}$$

$$\frac{\hbar^2}{2M_n}\, \mathbf{k} \cdot \mathbf{k} = \frac{\hbar^2}{2M_n}\, \mathbf{k}' \cdot \mathbf{k}' \pm \hbar\omega_{\mathbf{k}} \ ,$$

where $\mathbf{k}$ is the wave vector of the incident neutron, $\mathbf{k}'$ that of the scattered one, $\mathbf{G}$ is any reciprocal lattice vector and, $\mathbf{K}$ the wave vector of the phonon created (+) or absorbed (−) in the process. M_n is the mass of the neutron.

Studies of the phonon spectra have now been carried out for a number

of solids.[2] It can be seen that such an experiment provides a detailed survey of the phonon spectra, one which goes far beyond the information hitherto available, obtained by means of long-wave-length dispersion relations.

The purpose of this paper is to evaluate the force constants for Kr using the experimental results of Daniels et al[3] and to compare them with those obtained directly from the calculation of the phonon spectrum by Horton and Leech[4] using a Lennard-Jones interaction potential. For the first part we shall use the method proposed by Foreman and Lomer[5].

In the Born-von Karmán theory, restoring forces between atoms depend linearly on the relative displacements of the atoms. The equations of motion of the l-th primitive unit cell for a particular mode in a particular symmetric direction is[6]:

$$M\ddot{u}_{\alpha l} = - \sum_{l'} \Phi_{\alpha\alpha}(l, l')\, u_{\alpha l'} \qquad (1)$$

where $u_{\alpha l}$ is the displacement of atom l in the particular direction α (of polarization) considered, and M is the mass of the atoms. $\Phi_{\alpha\alpha}(l, l')$ represents the restoring force exerted on atom l in the direction α when atom l' is moved a unit distance also in direction α.

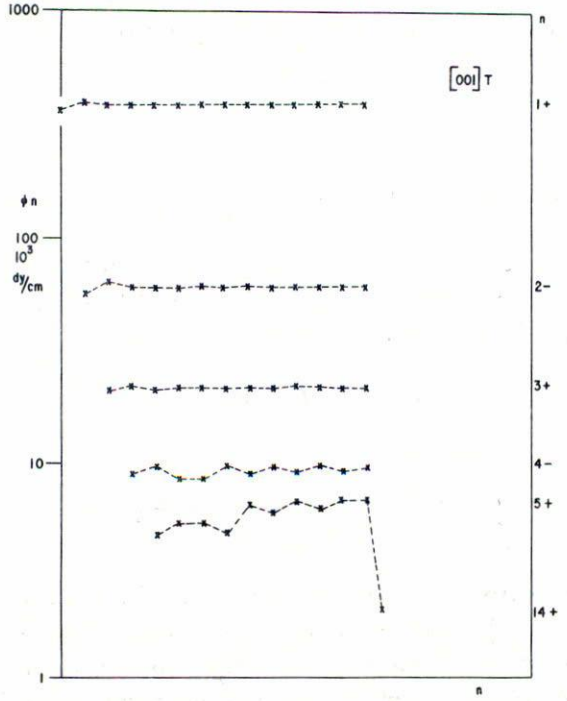


Fig. 1. Dependence of Φ_n with the number of planes Branch [001] T

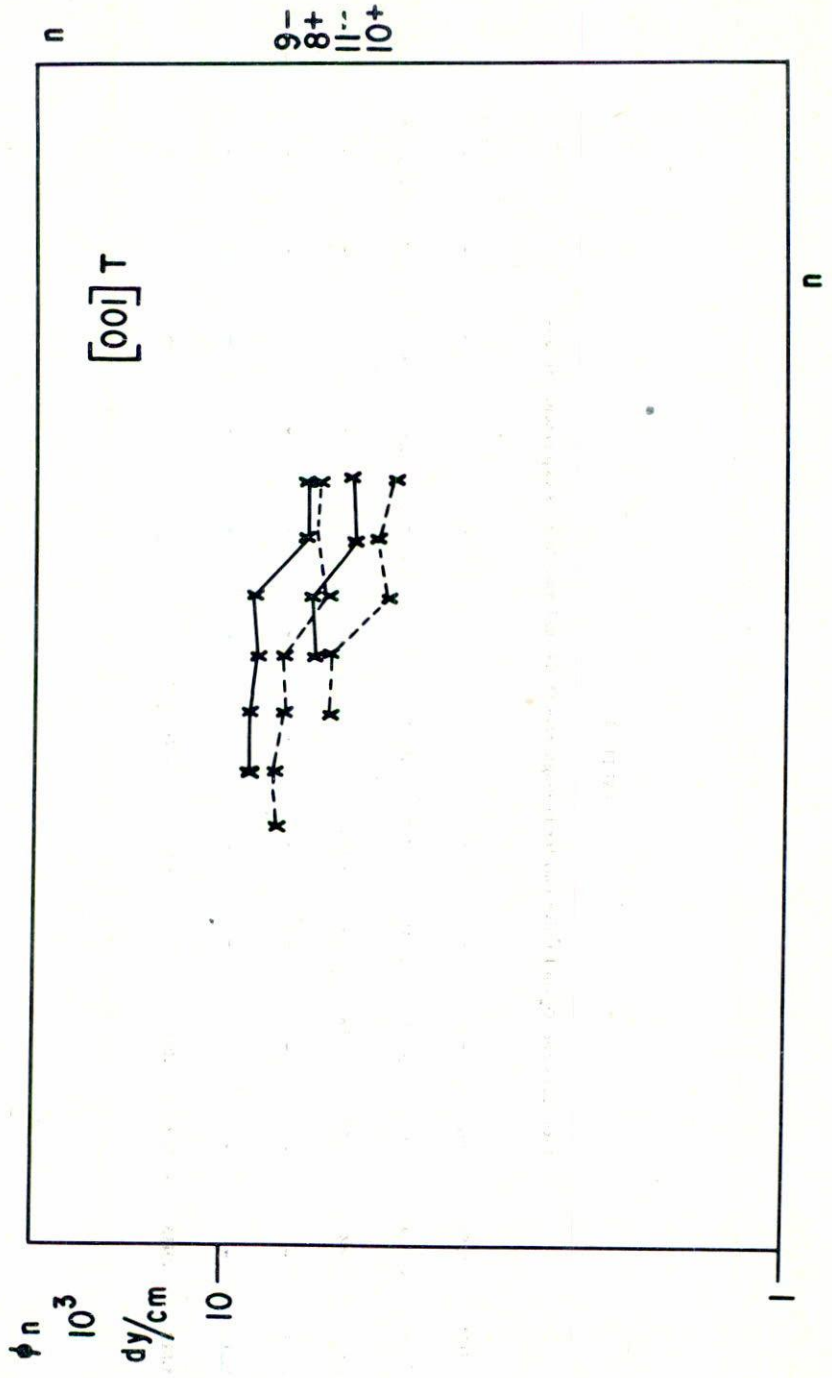


Fig. 2. Dependence of Φ_n with the number of planes Branch [001] T

TABLE 1

Force constants Φ_n (in 10^3 dyn/cm) for Kr single crystal obtained from Daniel's experimental results

[110] L	4.2111	.5258	-.1881	-	-	-	-	-	-	-	-	-	-	-
[110] T	3.904	-.5914	.221	-.0922	.0641	-.0747	.0207	.05703	-.0701	.0501	-.059	.086	-.06701	.021
[001] T	2.534	.0031	.0406	.0058	.0180	-.0047	-.0114	-.0127	.012	-	-	-	-	-
[111] T	0.1259	-	-	-	-	-	-	-	-	-	-	-	-	-
[001] L	5.21	-	-	-	-	-	-	-	-	-	-	-	-	-
[111] L	5.828	.0436	-.0262	.042	.0092	-.013	.021	-	-	-	-	-	-	-

Let the solution of (1) have the form of a traveling wave:

$$u_{\alpha l'} = U_\alpha \exp(i\mathbf{q}\cdot\mathbf{R}_l)\exp(i\mathbf{q}\cdot\mathbf{R}_{ll'} - i\omega t) \qquad (2)$$

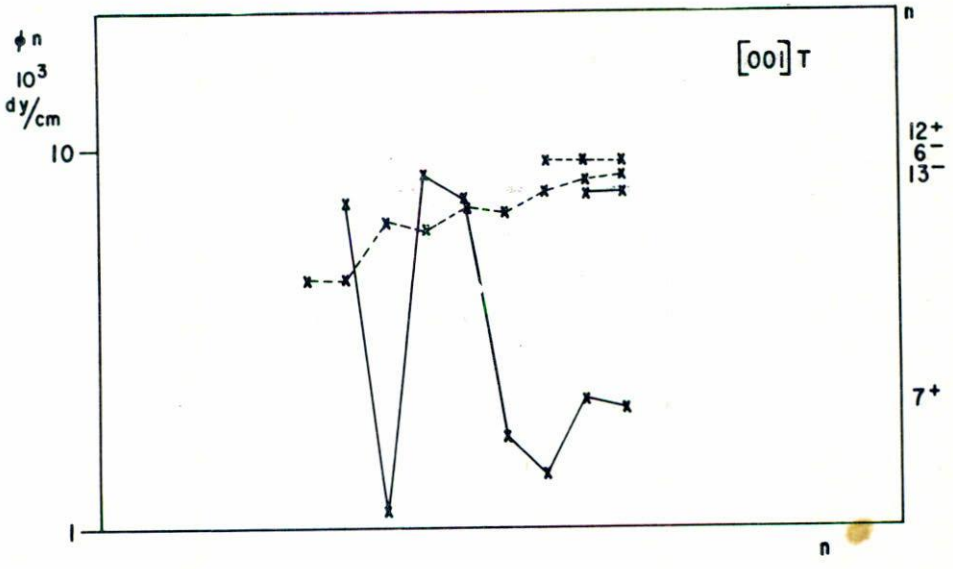
where $\mathbf{R}_l$ is the vector distance of the l-th atom from the origin and $\mathbf{R}_{ll'}$ is the vector distance from l-th atom to l'-th one. Substituting Eq. (2) in Eq. (1) we obtain,

$$M\omega^2 = \sum_{l'}\Phi_{\alpha\alpha}(l,l')\exp(i\mathbf{q}\cdot\mathbf{R}_{ll'})\,. \qquad (3)$$

This can be written as

$$M\omega^2 = \sum_{n=1}^{N}\Phi_n\left[1-\cos(nq\pi/q_m)\right], \qquad (4)$$

where q_m is half the distance to the nearest reciprocal lattice point in the direction of $\mathbf{q}$, $q = |\mathbf{q}|$ and Φ_n is a linear combination of $\Phi_{\alpha\alpha}(l,l')$ for which the phase $\mathbf{q}\cdot\mathbf{R}_{ll'}$ is a constant. Φ_n effectively represents a force between



Dependence of Φ_n with the number of planes Branch [001] T

a particular atom and the (two) planes of atoms normal to q and n planes away. The sum is taken up to a number of terms N such that $\Phi \simeq 0$ for $n > N$.

Using Eq. (4) and Daniel's results we obtained the values of Φ_n for the direction [001], [110], [111] and the transversal and longitudinal branches of the phonon spectrum of Kr. These results are presented in Table 1.

In Figs. 1, 2 and 3 we show the values of the coefficients for the [001] T-branch as a function of the number of terms used in Eq. (4); and for the same branch, Fig. 4 shows the interplanar force constants. For the theoretical calculations of the Φ_n the following potential was used,[4]

$$\phi(z) = c' \{z^{-m}/m\} \tag{5}$$

with

$$c' = \epsilon \left(\frac{6m}{m-6} \right) \tag{6}$$

$$z = r/\sigma \tag{7}$$

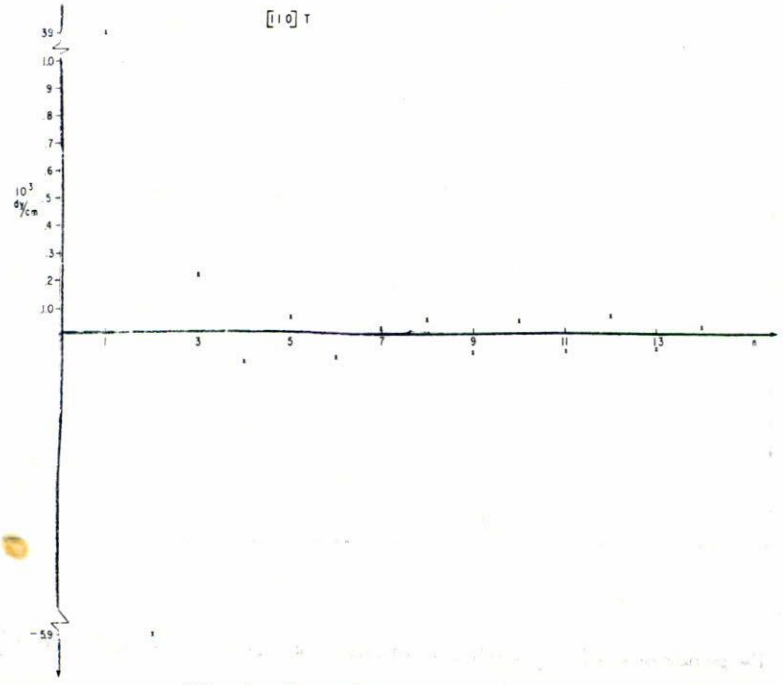


Fig. 4. Interplanar force constants.

and where, for brevity, we have used the notation

$$\{f(m)\} \equiv f(m) - f(6) . \tag{8}$$

Clearly $\phi(1) = -\epsilon$, $\phi'(1) = 0$. Here m is a parameter which measures the steepness of the repulsive part of the potential well; for numerical work we have used $m = 14$. In Eq. (7) r is the distance between atoms, σ and ϵ are constants with the values $\sigma = 4.056$ Å, $\epsilon = 236.7 \times 10^{-16}$ ergs, and $b = 2.8235$ Å is the interplanar distance[4].

We now put

$$\Phi_{\alpha\beta} = \left. \frac{\partial^2 \phi(r)}{\partial u_\alpha \partial u_\beta} \right|_{r = R_{ll'}} \tag{9}$$

from which we obtain

$$\Phi_{\alpha\beta} = \left(\frac{u_\alpha u_\beta}{r^2} \left[\phi''(r) - \frac{1}{r} \phi'(r) \right] + \delta_{\alpha\beta} \frac{1}{r} \phi'(r) \right) \Bigg|_{r = R_{ll'}} \tag{10}$$

and

$$\Phi_{\alpha\alpha} = \left. \frac{u_\alpha^2}{r^2} \phi''(r) \right|_{r = R_{ll'}}$$

$$= \frac{u_\alpha^2}{r^2} \frac{\epsilon}{\sigma^2} \cdot \frac{6m}{m-6} \left[(m+1) \left(\frac{\sigma}{r} \right)^{m+2} - 7 \left(\frac{\sigma}{r} \right)^8 \right] \Bigg|_{r = R_{ll'}} \tag{11}$$

Taking into account the fact that the

$$u_\alpha \Big|_{r = R_{ll'}}$$

has different values for different symmetry directions, the following formulas for the interplanar force constants are obtained:

For the [100] direction,

$$\Phi_n = \frac{\epsilon}{\sigma^2} \cdot \frac{6m}{m-6} \sum_{l_1 l_2 l_3} \left[\left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{m+2} (m+1) - 7 \left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{8} \right] \times \frac{l_1^2}{(l_1^2 + l_2^2 + l_3^2)}$$

with the condition

$$l_1 + l_2 + l_3 = 2n$$

where l_1, l_2, l_3 are all integers.

In the [110] direction,

$$\Phi_n = \frac{\epsilon}{\sigma^2} \cdot \frac{6m}{m-6} \sum_{l_1 l_2 l_3} \left[\left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{m+2} (m+1) - 7 \left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{8} \right] \times \frac{l_1^2 + l_2^2 + 2 l_1 l_2}{2 (l_1^2 + l_2^2 + l_3^2)}$$

with the condition

$$l_1 + l_2 + l_3 = 2n .$$

For the [111] direction

$$\Phi_n = \frac{\epsilon}{\sigma^2} \cdot \frac{6m}{m-6} \sum_{l_1 l_2 l_3} \left[\left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{m+2} (m+1) - 7 \left(\frac{\sigma}{b (l_1^2 + l_2^2 + l_3^2)^{1/2}} \right)^{8} \right] \times \frac{l_1^2 + l_2^2 + l_3^2 + 2 l_1 l_2 + 2 l_1 l_3 + 2 l_2 l_3}{3 (l_1^2 + l_2^2 + l_3^2)}$$

with the condition

$$l_1^2 + l_2^2 + l_3^2 = 6n .$$

TABLE 2

Calculated force constants Φ_n (in 10^3 dyn/cm) for single crystal using a Horton-Leech potential.

001	1.935	-.071	-.0035	-.0003
011	3.875	-.023	-.002	-.0002
111	-.023	-.0009		

It can be seen that the experimental values for the interplanar force constants show the same qualitative and quantitative behavior as in the case of Pb[4] and Al[4]. The results for the force constants obtained directly from the Horton and Leech potential are very similar to those found for the transverse branches of identical crystal directions, calculated from the experimental values. The results for the theoretical model are shown in Table 2. For the [111] branch the disagreement between the calculation and the experimental results is evident. Probably a better agreement could be achieved by using the anharmonic approximation.

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