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# Temperature Dependence of the Debye-Waller Factor for Copper and Aluminum

R. E. DEWAMES, T. WOLFRAM, AND G. W. LEHMAN
*North American Aviation Science Center, Canoga Park, California*

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The Debye-Waller factor for copper has recently been determined by Flinn *et al.* by making x-ray intensity measurements from 4–500°K. Flinn *et al.* were able to explain their results using a central force model for the copper lattice. However, it is well known that this model is inadequate in explaining the vibrational properties of the copper lattice over the entire wavelength region. Since various sets of force constants have been proposed for copper, we calculated the Debye-Waller factor for these sets. It is found that with the present experimental accuracy it is impossible to select between them. Calculations are also given for aluminum using Walker's atomic force constants.

## INTRODUCTION

RECENTLY, Flinn *et al.*[1] reported on the x-ray determination of the Debye-Waller factor for copper. They were able to interpret the experimental results in terms of a central force model (C.F.) including first- and second-neighbor interactions. Since the frequency spectrum is known for copper and was analyzed first by Jacobsen[2] using a full tensor model and second by Lehman *et al.*[3] using a special case of the full tensor model, it is interesting to compare the Debye-Waller factor predicted from these various sets of force constants. We have also calculated the Debye-Waller factor using the tensor force constants computed by White[4] from what amounts to a first-principles calculation using Feynman's theorem. Calculations of the Debye-Waller factor for aluminum are made using Walker's[5] tensor force constants which were determined from experimental dispersion curves. The method of calculation with the results is presented in Sec. II.

## RESULTS

The Debye-Waller factor for a cubic crystal can be written in the following manner:

$$f=e^{-2W}, \tag{1}$$

where

$$2W=RC(T), \tag{2}$$

and

$$C(T)=\frac{2}{3N}\sum_{\phi}(\bar{n}_{\phi}+\tfrac{1}{2})\frac{1}{\hbar\omega_{\phi}}. \tag{3}$$

$\phi$ stands for two indices $(q,j)$ where $\mathbf{q}$ is the propagation vector and $j$ the vibrational branch. $\bar{n}_{\phi}$ is the average number of phonons in a given mode $\phi$. $N$ refers to the total number of unit cells. $R$ is the recoil energy of a free emitting atom.

TABLE I. Atomic force constants for copper (in units of $10^4$ dyn cm$^{-1}$).

| Force constant | Jacobsen | White | A-S | C.F. |
|---|---|---|---|---|
| $\alpha_1$ | 0.87 | 1.71 | 1.12 | 1.477 |
| $\beta_1$ | 0.48 | −0.24 | −0.001 | 0 |
| $\gamma_1$ | 1.25 | 1.66 | 1.12 | 1.477 |
| $\alpha_2$ | 0.35 | −0.13 | −0.0227 | −0.2753 |
| $\beta_2$ | −0.072 | −0.07 | −0.0105 | 0 |
| $\alpha_3$ | 0.09 | −0.01 | 0.1122 | 0 |
| $\beta_3$ | −0.022 | +0.005 | 0.00345 | 0 |
| $\gamma_3$ | −0.015 | +0.02 | 0.03625 | 0 |
| $\delta_3$ | 0.06 | +0.01 | 0.0725 | 0 |

TABLE II. Atomic force constants for aluminum (in units of $10^4$ dyn cm$^{-1}$).

| Force constant | Walker | A-S |
|---|---|---|
| $\alpha_1$ | 0.845 | 0.845 |
| $\beta_1$ | −0.093 | −0.09 |
| $\gamma_1$ | 1.067 | 0.935 |
| $\alpha_2$ | 0.214 | 0.2 |
| $\beta_2$ | 0.04 | −0.1 |
| $\alpha_3$ | 0.027 | 0 |
| $\beta_3$ | −0.031 | 0 |
| $\gamma_3$ | 0.01 | 0 |
| $\delta_3$ | −0.019 | 0 |

In order to calculate the constant $C(T)$ the vibrational frequencies for an arbitrary propagation vector and branch are determined using a full tensor force model including third neighbors. The A-S (axially symmetric) calculation is done as a special case of the full tensor model.

Equation (3) is then evaluated by integrating over 1/48 of the Brillouin zone appropriate for the fcc structure. This portion of the Brillouin zone was divided into two regions. A triple Gaussian quadrature was used to evaluate the resulting integrals. The $3\times3$ dynamical matrix was diagonalized by $2\times2$ Jacobi rotation procedure at 1024 points in each region. Several checks were made to insure that the integration was independent of the order of the Gaussian quadrature. Table I gives the atomic force constants presently known for Cu which were used in the calculation of the Debye-Waller factor. Table II gives the atomic force constants

[1] P. A. Flinn, G. M. McManus, and J. A. Rayne, Phys. Rev. 123, 809 (1961).
[2] E. H. Jacobsen, Phys. Rev. 97, 654 (1955).
[3] G. W. Lehman, T. Wolfram, and R. E. DeWames, Phys. Rev. 128, 1593 (1962).
[4] H. C. White, Phys. Rev. 112, 1092 (1958).
[5] C. B. Walker, Phys. Rev. 103, 547 (1956).