

of the Grüneisen parameter calculated from the single crystal and the polycrystal TOEC with that calculated from bulk data. Using values for the linear expansion coefficient, $\alpha = 7.02 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$, and specific heat, $C_v = 0.065 \text{ cal g}^{-1} \text{ } ^\circ\text{C}^{-1}$ obtained from handbooks and the density $\rho = 8.578 \text{ g/cm}^3$, and isothermal bulk modulus, $K^T = 1.687 \times 10^{12} \text{ dyn/cm}^2$ obtained in the present study in the relation

$$\gamma_B = 3\alpha K^T / C_v \rho \quad (4)$$

gives the value for the bulk Grüneisen parameter of $\gamma_B = 1.52$. Using the methods of Ref. 4 for obtaining the Grüneisen parameter from the elastic constants by averaging the contribution of 39 pure-mode phonons to that parameter results in values of $\gamma_{\text{SC}} = 1.511 \pm 0.026$ and $\gamma_{\text{PC}} = 1.546 \pm 0.092$ for the single crystal and the polycrystal, respectively. A useful calculational equation for the polycrystal Grüneisen parameter which can be obtained from the equations of Brugger⁴ by imposing isotropy conditions is

$$\gamma_{\text{PC}} = (K^T m_1' - \Delta K) / 6C_{11}^S + (K^T m_2' - \Delta K) / 3C_{44}^S, \quad (5)$$

where m_1' and m_2' are the measured hydrostatic pressure slopes for the polycrystal and $\Delta K = K^S - K^T$ is the difference between the adiabatic and isothermal bulk moduli.

A second check on the values of the TOEC determined here is to compare the measured polycrystal constants with values calculated from the single-crystal constants. Recently, equations permitting this

comparison were derived³⁰ using strain-energy density considerations with the approximation that a uniform state of strain acting on the surface of a homogeneous, quasi-isotropic, polycrystalline body produces a uniform strain throughout the body. This development, analogous to that of Voigt relating the second-order elastic constants,³¹ leads to the following relations between the TOEC:

$$\nu_1 = \frac{1}{3^{\frac{1}{2}}} (C_{111} + 18C_{112} + 16C_{123} - 30C_{144} - 12C_{166} + 16C_{456})$$

$$\nu_2 = \frac{1}{3^{\frac{1}{2}}} (C_{111} + 4C_{112} - 5C_{123} + 19C_{144} + 2C_{166} - 12C_{456})$$

$$\nu_3 = \frac{1}{3^{\frac{1}{2}}} (C_{111} - 3C_{112} + 2C_{123} - 9C_{144} + 9C_{166} + 9C_{456}). \quad (6)$$

Using the values of C_{ijk} for columbium given in Table III in these equations results in $\nu_1 = -4.59 \pm 0.38$, $\nu_2 = -3.80 \pm 0.15$, and $\nu_3 = +0.78 \pm 0.09$, all in units of 10^{12} dyn/cm^2 . These values are seen to be in very good agreement with the values measured for the polycrystal sample B shown in Table V which provides an indirect check on both sets of TOEC.

ACKNOWLEDGMENTS

We are grateful for the excellent work in sample preparation done by Robert G. Herron who polished the samples and Paul C. Romo who performed the x-ray orientations.

³⁰ R. Chang, *Appl. Phys. Letters* **11**, 305 (1967).

³¹ W. Voigt, *Lehrbuch der Kristallphysik* (B. G. Teubner, Leipzig, 1928), p. 962.