

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  $\gamma_{SC} = 1.511 \pm 0.026$  and  $\gamma_{PC} = 1.546 \pm 0.092$  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 Brugger<sup>4</sup> by imposing isotropy conditions is

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

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 derived<sup>30</sup> 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,<sup>31</sup> leads to the following relations between the TOEC:

$$\begin{aligned} \nu_1 &= \frac{1}{3^5} (C_{111} + 18C_{112} + 16C_{123} - 30C_{144} - 12C_{166} + 16C_{456}) \\ \nu_2 &= \frac{1}{3^5} (C_{111} + 4C_{112} - 5C_{123} + 19C_{144} + 2C_{166} - 12C_{456}) \\ \nu_3 &= \frac{1}{3^5} (C_{111} - 3C_{112} + 2C_{123} - 9C_{144} + 9C_{166} + 9C_{456}). \end{aligned} \quad (6)$$

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  $10^{12} \text{ dyn/cm}^2$ . 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.

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<sup>30</sup> R. Chang, *Appl. Phys. Letters* **11**, 305 (1967).

<sup>31</sup> W. Voigt, *Lehrbuch der Kristallphysik* (B. G. Tuebner, Leipzig, 1928), p. 962.