Redetermination of elastic constants of single-crystals $CaMoO_4$

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Values of the elastic constant of $CaMoO_4$ obtained by Alton and Barlow are compared with those obtained using equations developed by Chung and Li. The velocities measured by Alton and Barlow were used in the computations.

In a previous paper, Alton and Barlow[1] (AB) did a complete analysis for the elastic constants of the tetragonal system with class 4/mmm. They also calculated the C_{ij}'s from the velocity measurements in single crystals of $CaMoO_4$. In this paper we present the results from a calculation with a different method.[2] Comparison of our calculated values with those of AB will be made.

Hoyte and Priestley[3] (HP) have independently measured ultrasonic velocities in single-crystal $CaMoO_4$ in about the same time as AB.[1] The values of velocities in different high-symmetry directions are comparable with those of AB, though the frequency used by HP is lower (45 MHz).

Here we are going to use the velocity values of AB in order to make a direct comparison. The detailed method of calculations is described in Ref. 2. Only the results will be presented here. We are particularly interested in the values of C_{11}, C_{66}, C_{12}, and C_{16}, since the other three (C_{33}, C_{44}, C_{13}) are identical to those of AB.

TABLE I. Values obtained for four elastic constants compared with those of AB (Ref. 1).

C_{11}	C_{66}	C_{12}	C_{16}
14.439(14.469)	4.545(4.514)	6.582(6.582)	1.272(1.34)
4.545(4.514)	14.439(14.469)	-25.566(16.54)	-1.272(1.34)
9.562(9.755)	9.422(9.229)	-4.328(-4.267)	5.107(5.14)
9.422(9.229)	9.562(9.755)	-14.656(-3.741)	-5.107(5.14)

The four sets of values obtained for four elastic constants are given in Table I (in units of 10^{11} dyn/cm^2). For easy comparison, the corresponding values obtained by AB[1] are given in parentheses. By the same reasoning used in Ref. 1, we believe that the first set is the correct one to choose. It is apparent that the results for these four elastic constants are slightly different from those of AB. The possible reason is that there was some numerical error in Table I of Ref. 1. The last two lines for the "Quantity obtained ···" should read

$$\tfrac{1}{4}C_{33}^2+\tfrac{5}{4}C_{44}^2+\tfrac{1}{2}A+\tfrac{1}{4}B',$$

$$C_{44}^2+B'+\tfrac{3}{8}D'+\tfrac{1}{2}\sqrt{3}F,$$

respectively, as one can easily verify from Eq. (5) of Ref. 1. With this correction, the results should agree with the one presented here. It should be noted that recently Farley and Saunders,[4] using their computer program for $CaMoO_4$, also found some deviation from the results of AB.[1]

Thus, we have redetermined some of the elastic constants for $CaMoO_4$ using a different method of calculation. We have also made some numerical corrections for the method used in Ref. 1.

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[3] A. F. Hoyte and B. W. Priestley, M. S. thesis (Howard University, 1969) (unpublished).
[4] J. M. Farley and G. A. Saunders, Solid State Commun. 9, 965 (1971).

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