The single-crystal elastic constants of cubic (3C) SiC to 1000°C

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Experimental measurements of the polycrystalline elastic moduli of the cubic (3C) beta polytype of SiC at elevated temperatures and the room-temperature single-crystal elastic constants were combined through equations that relate the two to determine the stiffnesses C_{ij} and the compliances S_{ij} to 1000°C. The results demonstrate a general method for estimating the elevated temperature single-crystal constants of cubic crystals and illustrate that the cubic (3C) beta polytype of SiC becomes more elastically anisotropic at elevated temperatures.

1. Introduction

Many single-crystal mechanical property calculations which involve the residual stresses which develop during cooling [1], the elastic strain energy [2], and numerous other thermomechanical situations [3] require a knowledge of the single-crystal elastic constants of the material (either the stiffnesses C_{ij} or the compliances S_{ij}) at the temperature of interest. The extensive summary of Simmons and Wang [4] provides that type of information for the familiar halides and a few metals, but only for Al_2O_3 [5] and MgO [6] of all of the common oxides. In particular, no elevated-temperature information exists for carbides, nitrides or borides. This dilemma is understandable, for the experimental studies can be formidable undertakings. It is, however, especially unfortunate for the case of SiC, since single-crystal cubic (3C) beta polytype SiC whiskers are currently being incorporated into both metal matrix [7] and ceramic matrix composites [8]. For those situations, the temperature dependencies of the single-crystal elastic constants, either the C_{ij} or S_{ij}, are required if the residual stresses in the fibres and in the matrix, or the stress concentrations at the fibre–matrix interfaces, are to be accurately calculated. This paper reports the determination of the C_{ij} of the cubic (3C) beta polytype of SiC for elevated temperatures to 1000°C, utilizing the room-temperature single-crystal C_{ij} values and the experimentally measured temperature dependencies of the polycrystalline elastic moduli. It utilizes a method which can also be readily applied to other cubic structures for which similar information exists for both the single-crystal and the polycrystalline ceramic elastic properties.

2. Results and discussion

There are three independent elastic constants for cubic single crystals, which may be expressed as either the stiffnesses (C_{11}, C_{12} and C_{44}), or the compliances (S_{11}, S_{12} and S_{44}). The C_{ij} and S_{ij} are related [9]. For the cubic (3C) beta polytype of SiC at room temperature these single-crystal elastic constants have been

reported by Tolpygo [10] as 352.3, 140.4, 232.9 GPa and 3.673×10^{-3}, -1.047×10^{-3} and 4.294×10^{-3} GPa^{-1}, respectively. Note that the S_{12} value is negative. Since polycrystalline ceramic materials consist of randomly oriented crystals, unless they are highly textured, description of their elastic properties requires only two independent elastic constants including either Young's modulus (E), the shear modulus (G), the bulk modulus (K) or Poisson's ratio (v). Relationships between the single-crystal elastic constants and the polycrystalline ceramic elastic moduli have been developed by a number of researchers and have been summarized by Mura [11]. Among them, the Voigt relation is a simple one which is the average of the elastic stiffnesses. The Voigt averages for Young's modulus and the shear modulus are given by

$$E_V = \frac{(C_{11} - C_{12} + 3C_{44})(C_{11} + 2C_{12})}{2C_{11} + 3C_{12} + C_{44}} \quad (1)$$

and

$$G_V = (C_{11} - C_{12} + 3C_{44})/5, \quad (2)$$

while the Reuss averages for the moduli from the compliances are

$$\frac{1}{E_R} = \frac{3S_{11} + 2S_{12} + S_{44}}{5} \quad (3)$$

and

$$\frac{1}{G_R} = \frac{4S_{11} - 4S_{12} - 3S_{44}}{5} \quad (4)$$

The Voigt and Reuss averages are generally accepted to define the upper and lower bounds of the polycrystalline elastic constant averages, respectively. However, there are reports of polycrystalline moduli which exceed these bounds [12]. The bulk modulus, K, unlike E and G, is an unambiguous value which is not dependent upon the averaging procedure. It is expressed by

$$K = K_V = K_R = \frac{(C_{11} + 2C_{12})}{3}$$

$$= \frac{1}{3(S_{11} + 2S_{12})} \quad (5)$$

or in term of the polycrystalline technical engineering elastic moduli

$$K = \frac{EG}{3(3G - E)} \qquad (6)$$

The temperature dependencies of the elastic moduli of numerous materials have been expressed by empirical equations over wide temperature ranges. However, above room temperature most ceramic materials exhibit a region of linear decrease of the elastic constants with increasing temperature [13]. The Young's modulus and shear modulus of high-density SiC polycrystals have been measured by several different researchers [14–17]. The results ascribe to straight lines and can be expressed in the forms

$$E = E_0 + bT \qquad (7)$$

and

$$G = G_0 + b'T \qquad (8)$$

where E_0 and G_0 are the 0°C values. These may be dependent upon the material's microstructure, such as the density, porosity, grain size, etc. Reported values for E_0 and G_0 for polycrystalline beta (3C) SiC are 400 to 470 and 170 to 200 GPa, respectively, encompassing a rather wide range of values for each. However, the values of b and b' which have been reported for polycrystalline (3C) beta SiC by the different researchers are essentially identical. For the cubic (3C) SiC polycrystalline beta structure, the b and b' values are -0.020 and $-0.007\,\text{GPa}\,(^\circ\text{C})^{-1}$, respectively. The bulk modulus of polycrystalline cubic (3C) beta SiC, calculated from Equation 6, can also be expressed as a linear equation. The value of dK/dT is $-0.016\,\text{GPa}\,(^\circ\text{C})^{-1}$.

It is a reasonable first approximation to assume that the temperature dependencies of the polycrystalline Young's modulus, shear modulus, and bulk modulus calculated from the single-crystal elastic stiffnesses, the C_{ij}, can also be expressed by simple linear equations such as Equations 7 and 8. In the Voigt form, the E_0, G_0 and K_0 values are 425.2, 182.5 and 211.4 GPa, respectively. The temperature derivatives dE/dT, dG/dT and dK/dT may be expected to be similar to the experimental polycrystalline values, -0.020, -0.007 and $-0.016\,\text{GPa}\,(^\circ\text{C})^{-1}$, respectively. These can be related to and applied to determine the dC_{ij}/dT. However, since the single-crystal elastic constants exist as three independent parameters, it is necessary to develop additional relationships between the single-crystal elastic constant and the polycrystalline ceramic elastic moduli temperature dependencies.

As previously noted, a number of the elastic constants for cubic single crystals have been measured at elevated temperatures and are summarized by Simmons and Wang [4]. The elastic constants, E_V, G_V, C_{11} and C_{44}, for a number of those materials were calculated as a function of temperature from that tabulation. Table I illustrates the temperature derivatives of the elastic constants for those cubic materials. The E and G values listed in Table I are the Voigt averages, although the Reuss averages would probably also be equally satisfactory. The results illustrate that all

TABLE I Temperature derivatives of the elastic constants of some cubic crystals

Crystal	dC_{11}/dT	dE/dT	dC_{44}/dT	dG/dT	T (°C)
CaF$_2$	−0.039	−0.031	−0.012	−0.012	20 to 420
LiF	−0.091	−0.071	−0.020	−0.022	20 to 800
CsBr	−0.017	−0.018	−0.009	−0.007	20 to 450
TlBr	−0.027	−0.022	−0.009	−0.009	25 to 427
MgO	−0.078	−0.056	−0.016	−0.021	20 to 1200
SbIn	−0.019	−0.028	−0.003	−0.003	27 to 327
Al	−0.069	−0.041	−0.015	−0.015	20 to 500
Ag	−0.035	−0.028	−0.013	−0.010	27 to 527
Au	−0.035	−0.028	−0.013	−0.011	27 to 527
Fe	−0.055	−0.045	−0.021	−0.017	25 to 500
Ge	−0.014	−0.015	−0.007	−0.007	20 to 300
Ni	−0.063	−0.081	−0.039	−0.035	27 to 487
Ti	−0.022	−0.028	−0.013	−0.011	25 to 500

are well fitted by a first-order linear equation as the correlation coefficients are larger than 0.99 for each of the results. A comparison of the single-crystal and polycrystalline elastic constant calculations for the materials listed in Table I reveals that most of the values of dC_{44}/dT and dG/dT for each of these cubic materials are nearly identical, and in every instance the value is much smaller than the value of dE/dT. On the basis of the results of this tabulation, the assumption can be made that the temperature dependencies, dC_{44}/dT and dG/dT, for the cubic (3C) beta polytype of SiC are also identical and are equal to $-0.007\,\text{GPa}\,(^\circ\text{C})^{-1}$.

For estimating C_{11} and C_{12} at elevated temperatures, Equations 2 and 5 can be differentiated to yield

$$\frac{dG}{dT} = \frac{1}{5}\left(\frac{dC_{11}}{dT}\right) - \frac{1}{5}\left(\frac{dC_{12}}{dT}\right) + \frac{3}{5}\left(\frac{dC_{44}}{dT}\right) \qquad (9)$$

and

$$\frac{dK}{dT} = \frac{1}{3}\left(\frac{dC_{11}}{dT}\right) + \frac{2}{3}\left(\frac{dC_{12}}{dT}\right) \qquad (10)$$

Since the values of dK/dT, dG/dT and dC_{44}/dT from room temperature to 1000°C are already known as -0.016, -0.007 and $-0.007\,\text{GPa}\,(^\circ\text{C})^{-1}$, respectively, both dC_{11}/dT and dC_{12}/dT can be easily determined from the above two equations. The values are equal to -0.025 and $-0.011\,\text{GPa}\,(^\circ\text{C})^{-1}$, respectively. The
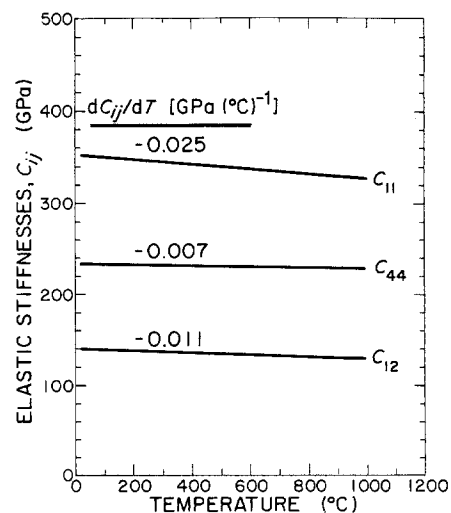

Figure 1 Single-crystal elastic stiffnesses of cubic (3C) beta SiC as a function of temperature.

TABLE II Calculated elastic stiffnesses, compliances and Zener ratios of cubic SiC at elevated temperatures

T (°C)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	A	S_{11} (GPa^{-1})	S_{12} (GPa^{-1})	S_{44} (GPa^{-1})
RT	352.3	140.4	232.9	2.198	3.673×10^{-3}	-1.047×10^{-3}	4.294×10^{-3}
200	347.7	138.8	231.6	2.212	3.718×10^{-3}	-1.058×10^{-3}	4.317×10^{-3}
400	342.6	136.0	230.2	2.229	3.770×10^{-3}	-1.071×10^{-3}	4.343×10^{-3}
600	337.5	133.7	228.8	2.245	3.823×10^{-3}	-1.085×10^{-3}	4.370×10^{-3}
800	332.4	131.4	227.4	2.263	3.877×10^{-3}	-1.099×10^{-3}	4.397×10^{-3}
1000	327.4	129.2	226.0	2.281	3.933×10^{-3}	-1.113×10^{-3}	4.424×10^{-3}

$\mathrm{d}C_{ij}/\mathrm{d}T$ values between room temperature and 1000° C for the cubic (3C) beta polytype of SiC are then -0.025, -0.011 and $-0.007\,\mathrm{GPa}\,(°\mathrm{C})^{-1}$, for C_{11}, C_{12} and C_{44}, respectively. These values compare favourably with those for the other cubic crystals which are summarized in Table I.

Using the temperature derivative values, the $\mathrm{d}C_{ij}/\mathrm{d}T$, and the room-temperature C_{ij} values after Tolpygo [10], the elastic stiffnesses of the cubic (3C) beta polytype of SiC were calculated to 1000° C. The results are summarized in Table II and are illustrated in Fig. 1. The elastic compliances, the S_{ij}, can also be calculated using the equations listed by Nye [9]. They are also listed in Table II. Substituting the above C_{ij} values into Equation 1, the Voigt average for the polycrystalline Young's modulus against temperature was determined and then the temperature derivative was calculated. The $\mathrm{d}E/\mathrm{d}T$ value is $-0.020\,\mathrm{GPa}\,(°\mathrm{C})^{-1}$, which is identical to the experimental polycrystalline values. The consistency of this internal check confirms that the above assumptions and calculation procedures are satisfactory for the $\mathrm{d}C_{ij}/\mathrm{d}T$ values.

The cubic (3C) beta polytype of SiC is quite elastically anisotropic when compared to most other cubic crystals. For example, at room temperature $E_{\langle100\rangle}$ is 272.3 GPa, while $E_{\langle111\rangle}$ is 510.8 GPa, nearly twice as large [18]. It is of further interest to examine this anisotropy as the change of the Zener ratio with increasing temperature. The Zener ratio can be expressed as

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \qquad (11)$$

The Zener ratio values are also summarized from room temperature to 1000° C in Table II and they show that the elastic anisotropy of cubic (3C) beta SiC increases with increasing temperature, as the Zener ratio increases about 5% from 2.2 at room temperature to 2.3 at 1000° C.

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