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The Single Crystal Elastic Constants of Hexagonal SiC to 1000°C

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ABSTRACT

The relationships between the sound velocities in the cubic and hexagonal crystal structures and the tensor transformations for the two structures are applied to determine the elastic stiffnesses, C_{ij} *and* $(\mathrm{d}C_{ij}/T)$ *for the hexagonal structures of SiC to 1000°C. These results are then applied to calculate the polycrystalline elastic moduli, E and G, and their temperature variations. The calculated values for E and G at 20°C are 420 and 180 GPa and for* $(\mathrm{d}E/\mathrm{d}T)$ *and* $(\mathrm{d}G/\mathrm{d}T)$ *the values are* $-0{\cdot}020$ *and* $-0{\cdot}007$ *(GPa/°C), respectively. These agree well with published experimental values for E and G of dense polycrystalline alpha silicon carbides.*

INTRODUCTION

Silicon carbide can exist in a number of different crystalline polytypes which may be classified into the cubic (C), hexagonal (H) and rhombohedral (R) space groups.[1,2] The structural differences between these polytypes are in their stacking layer sequences. They are unique features which result in some of the physical properties of the numerous polytypes being quite similar.

Practical interest has recently intensified in the calculation of the thermal stresses which develop in ceramic or metal matrix composite materials using single crystal SiC grains or whiskers as the reinforcing component phase.[3,4] For determination of the thermal stresses at all temperatures, it is necessary

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to know, or to be able to reliably estimate the single crystal elastic constants of SiC and also their temperature dependencies. However, the single crystal elastic constants and their temperature dependencies have never been measured for a 'pure' hexagonal polytype.

This paper initially considers the similarities of the acoustic wave velocities in the cubic and the hexagonal polytypes of SiC, and then utilizes tensor transformations relating the single crystal elastic constants of the two structures to calculate the single crystal elastic constants and their temperature dependencies for all of the hexagonal SiC polytypes. These results are then utilized to estimate the polycrystalline elastic moduli of the hexagonal polytypes of SiC from room temperature to 1000°C applying appropriate averaging procedures. The calculated values are then compared with the published measurements of the polycrystalline elastic moduli for the alpha SiC polytypes.

SINGLE CRYSTAL ELASTIC CONSTANTS

Patrick has classified the different physical properties of SiC according to their wave-vector dependence.[2] Properties which depend on the axial and transverse wave vectors include the phonon dispersion spectrum and the acoustic wave velocities. The latter are directly related to the single crystal elastic constants. Properties which depend on the Brillouin zone boundary wave vector include the electron mobilities. Other properties depend on a weighted average over all of the wave vectors, including the thermal conductivity and the thermal expansion. These latter two groups of properties have been demonstrated to vary considerably with the different polytypes; however, the phonon dispersion spectra and the acoustic wave velocities are very similar for all of the polytypes.

Feldman *et al.* have measured the Raman spectra of a number of the SiC structures and have found that the phonon spectra in the axial direction is common to all of the polytypes.[5] Vetelino and Mitra have applied a rigid ion model to theoretically calculate the dispersion curves in the [111] direction of the (3C) cubic SiC polytype[6] and have obtained results which are in good agreement with the Feldman *et al.* experimental values. These studies confirm that the longitudinal and the transverse acoustic sound velocities along the hexagonal SiC polytype [0001] directions, V_L^h and V_T^h can be assumed to be identical to those along the cubic [111] direction, V_L^c and V_T^c.

The hexagonal crystal structures of SiC have $P6_3mc$ symmetry and require five independent single crystal elastic constants for description. These can be expressed as either the elastic stiffnesses (C_{11}, C_{12}, C_{13}, C_{33}, and C_{44}) or the elastic compliances, the S_{ij}.[7] The relationships between the sound velocities in SiC and the elastic stiffnesses along the [0001] direction in a hexagonal crystal are expressed as:

$$\rho V_L^2 = C_{33}^h \tag{1a}$$

and

$$\rho V_T^2 = C_{44}^h \tag{1b}$$

where ρ is the density, and V_L and V_T are the longitudinal and transverse sound velocities, respectively. The relationships between the sound velocities and the elastic stiffnesses along the [111] direction in a cubic crystal are expressed by:[8]

$$3\rho V_L^2 = C_{11}^c + 2C_{12}^c + 4C_{44}^c \tag{2a}$$

and

$$3\rho V_T^2 = C_{11}^c - C_{12}^c + C_{44}^c \tag{2b}$$

As previously reported by Feldman *et al.* and Vetelino and Mitra, the sound velocities along the [0001] directions of the hexagonal SiC crystals are identical to those along the [111] directions of a cubic SiC crystal.[5,6] Since the crystalline densities are also equivalent, several of the single crystal elastic constants of the hexagonal and the cubic structures can be related through eqns (1) and (2) as has been discussed by Pandey and Dayal.[9] The two unique relationships are:

$$3C_{33}^h = C_{11}^c + 2C_{12}^c + 4C_{44}^c \tag{3a}$$

and

$$3C_{44}^h = C_{11}^c - C_{12}^c + C_{44}^c \tag{3b}$$

Equations (3a) and (3b) can also be derived from the tensor transformations for the two structures, which confirms that the other single crystal elastic constants of hexagonal SiC can also be calculated from the single crystal elastic constants of the cubic beta structure. Single crystal elastic constants are fourth order tensors and can be expressed in any arbitrary direction by:[10]

$$C'_{ijkl} = \alpha_{im}\alpha_{jn}\alpha_{ko}\alpha_{lp}C_{mnop} \tag{4}$$

where the α_{ij}, etc., are the directional cosines. The C_{mnop} are the elastic stiffnesses in the original crystallographic coordinates and the C'_{ijkl} are the stiffnesses in the new orientation. Since a hexagonal 'pseudocell' can be specified within any cubic structure with the hexagonal [0001] parallel to the cubic [111], the $[\bar{1}2\bar{1}0]$ parallel to the $[\bar{1}10]$, and the $[\bar{1}010]$ parallel to the

$[\bar{1}\bar{1}2]$, the single crystal elastic constants of the hexagonal structure of SiC can be estimated by utilizing eqn (4) and the transformation matrix:

$$\begin{bmatrix} X'_1 \\ X'_2 \\ X'_3 \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ -1/\sqrt{6} & -1/\sqrt{6} & 2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{3} & X_3 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \quad (5)$$

Where the X'_1, X'_2 and X'_3 are the axes of the hexagonal 'pseudocell' along the $[\bar{1}10]$, the $[\bar{1}\bar{1}2]$ and the [111] cubic directions, respectively, and X_1, X_2 and X_3 are the axes of the cubic crystal along the [100], the [010] and the [001] directions. Substituting the appropriate α_{ij} values yields the complete set of relationships between the hexagonal and the cubic single crystal elastic stiffnesses as:

$$2C^{h}_{11} = C^{c}_{11} + C^{c}_{12} + 2C^{c}_{44} \quad (6a)$$

$$3C^{h}_{33} = C^{c}_{11} + 2C^{c}_{12} + 4C^{c}_{44} \quad (6b)$$

$$6C^{h}_{12} = C^{c}_{11} + 5C^{c}_{12} - 2C^{c}_{44} \quad (6c)$$

$$6C^{h}_{13} = C^{c}_{11} + 2C^{c}_{12} - 2C^{c}_{44} \quad (6d)$$

and

$$3C^{h}_{44} = C^{c}_{11} - C^{c}_{12} + C^{c}_{44} \quad (6e)$$

Equations (6b) and (6e) are identical to eqns (3a) and (3b), which were determined from the sound velocity considerations.

Tolpygo has theoretically calculated the C_{11}, C_{12} and C_{44} values of the cubic (3C) beta polytype of SiC at room temperature (20°C) to be 352·3, 140·4 and 232·9 GPa, respectively.[11] Utilizing Tolpygo's theoretical C_{ij} values and eqns (6a–e), the room temperature single crystal elastic stiffnesses of the hexagonal structures of SiC can be determined. The calculations are summarized in Table 1 along with the experimental elastic stiffnesses which have been reported for a mixed, but predominantly (6H) hexagonal polytype specimen of SiC by Arlt and Schodder.[12] Comparison of these results illustrates that they are in satisfactory agreement, especially considering that the (6H) polytype SiC crystal which was experimentally measured by Arlt and Schodder also contained some of the (15R) polytype.

It is appropriate to further compare this analytical approach with the experimental results for zinc sulphide, ZnS, which also exists in similarly related cubic (3C) and hexagonal (2H) polytype structures. The single crystal elastic constants of both the (3C) cubic structure (sphalerite) of ZnS and the (2H) hexagonal structure (wurtzite) of ZnS have been measured by different researchers.[13,14] The values are listed in Table 1. The elastic stiffnesses of cubic (3C) ZnS were transformed to those of the hexagonal ZnS polytype by using eqns (6a–e) and are also listed in Table 1. It is evident that the

TABLE 1

Room Temperature Single Crystal Elastic Stiffnesses of SiC and ZnS (GPa)

	SiC[a]					*ZnS*[b]				
	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}
Cubic values	352·3	—	140·4	—	232·9	104·6	—	65·3	—	46·1
Hexagonal values	500	564	92	—	168	124	140	60	45	286
Transformed values[c]	479	521	98	56	148	131	140	56	48	285

[a] Cubic values;[11] hexagonal values.[10]

[b] Cubic values;[13] hexagonal values.[14]

[c] After eqns (6a–e).

transformed values are in excellent agreement with the reported experimental values which further supports the validity of the transformation procedures.

TEMPERATURE DEPENDENCIES OF THE C_{ij}

The temperature dependencies of the single crystal and polycrystalline elastic constants of numerous crystalline solids have been expressed by different empirical equations over wide temperature ranges. Above room temperature, most ceramic materials exhibit an extensive region of linear decrease of the elastic constants with increasing temperature.[15] These can be expressed as:

$$C_{ij} = C^0_{ij} + b_{ij}T \tag{7}$$

where the C^0_{ij} are the 0°C values and the b_{ij} are constants which are equal to $(\mathrm{d}C_{ij}/\mathrm{d}T)$.

The b_{ij} and temperature dependencies of the C_{ij} for the cubic (3C) beta SiC have been determined from room temperature to 1000°C.[16] The $(\mathrm{d}C^c_{11}/\mathrm{d}T)$, $(\mathrm{d}C^c_{12}/\mathrm{d}T)$ $(\mathrm{d}C^c_{44}/\mathrm{d}T)$ values for the cubic (3C) beta SiC polytype are $-0{\cdot}025$, $-0{\cdot}011$, and $-0{\cdot}007$ GPa/°C, respectively. To calculate the temperature dependencies of the C^h_{ij} values, the $(\mathrm{d}C^h_{ij}/\mathrm{d}T)$ for the hexagonal SiC structures, eqns (6a–e) can be differentiated with respect to temperature. For example eqn (6a) yields:

$$\left(\frac{\mathrm{d}C^h_{11}}{\mathrm{d}T}\right) = \frac{1}{2}\left(\frac{\mathrm{d}C^c_{11}}{\mathrm{d}T}\right) + \frac{1}{2}\left(\frac{\mathrm{d}C^c_{12}}{\mathrm{d}T}\right) + \left(\frac{\mathrm{d}C^c_{44}}{\mathrm{d}T}\right) \tag{8a}$$

and eqn (6b) yields:

$$\left(\frac{\mathrm{d}C^{\mathrm{h}}_{33}}{\mathrm{d}T}\right)=\frac{1}{3}\left(\frac{\mathrm{d}C^{\mathrm{c}}_{11}}{\mathrm{d}T}\right)+\frac{2}{3}\left(\frac{\mathrm{d}C^{\mathrm{c}}_{12}}{\mathrm{d}T}\right)+\frac{4}{3}\left(\frac{\mathrm{d}C^{\mathrm{c}}_{44}}{\mathrm{d}T}\right) \qquad (8b)$$

The other stiffness relationships (6c–e) can be similarly differentiated so that by applying previously determined $(\mathrm{d}C^{\mathrm{c}}_{\mathrm{ij}}/\mathrm{d}T)$ values for the cubic (3C) beta SiC polytype,[16] the $(\mathrm{d}C^{\mathrm{h}}_{\mathrm{ij}}/\mathrm{d}T)$ values for the hexagonal SiC structures can be estimated.

Using the $(\mathrm{d}C^{\mathrm{c}}_{\mathrm{ij}}/\mathrm{d}T)$ values and the transformed room temperature $C^{\mathrm{h}}_{\mathrm{ij}}$ values, rather than the experimental measurements by Arlt and Schodder which do not contain a C_{13} value, the single crystal elastic stiffnesses for the hexagonal SiC structure were calculated through 1000°C. The results are illustrated in Fig. 1 and are summarized in Table 2. The elastic compliances, the $S^{\mathrm{h}}_{\mathrm{ij}}$, can also be readily calculated,[7] and are listed in Table 2 from room temperature through 1000°C.

The polycrystalline Young's modulus and shear modulus of hexagonal SiC can be estimated at elevated temperatures from the $C^{\mathrm{h}}_{\mathrm{ij}}$ and $S^{\mathrm{h}}_{\mathrm{ij}}$ values and the mean value of the Voigt and Reuss averages.[17] Other averaging schemes may also be applied. Utilizing the elastic constants for the hexagonal SiC structure listed in Table 2, the average polycrystalline elastic moduli at elevated temperatures were calculated and their temperature

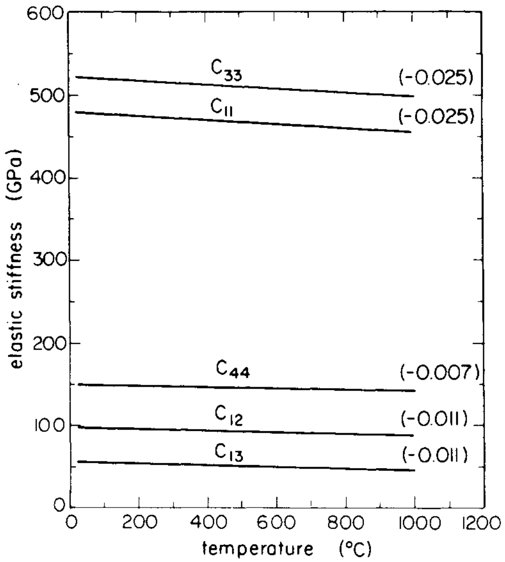

Fig. 1. Single crystal elastic stiffnesses of hexagonal SiC as a function of temperature. Figures in parentheses are the gradients $(\mathrm{d}C_{\mathrm{ij}}/\mathrm{d}T)$ in GPa/°C.

TABLE 2

Calculated Elastic Stiffnesses and Compliances of Hexagonal SiC at Elevated Temperatures

T (°C)	*Stiffnesses (GPa)*					*Compliances* ($\times 10^{-3}$/*GPa*)				
	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}	S_{11}	S_{33}	S_{12}	S_{13}	S_{44}
20	479·3	521·6	98·1	55·8	148·3	2·196	1·958	−0·427	−0·189	6·743
200	474·8	517·1	96·1	53·8	147·0	2·214	1·973	−0·427	−0·186	6·801
400	469·8	512·1	93·9	51·6	145·6	2·234	1·989	−0·426	−0·182	6·866
600	464·8	507·1	91·7	49·4	144·2	2·254	2·007	−0·426	−0·180	6·933
800	459·8	502·1	89·5	47·2	142·8	2·276	2·024	−0·425	−0·174	7·001
1 000	454·8	497·1	87·3	45·0	141·4	2·297	2·042	−0·424	−0·170	7·070

dependencies determined. The results are summarized in Table 3 and are presented graphically in Fig. 2. The resulting (dE/dT) and (dG/dT) are −0·020 and −0·007 GPa/°C, respectively. These values are in good agreement with the experimental polycrystalline values that have been reported by several different researchers[18−21] for commercial alpha SiC materials that are mixtures of hexagonal and rhombohedral polytypes. Those high-density hexagonal SiC (dE/dT) and (dG/dT) experimental values range from 0·016 to 0·021 and from 0·006 to 0·009 GPa/°C, respectively.

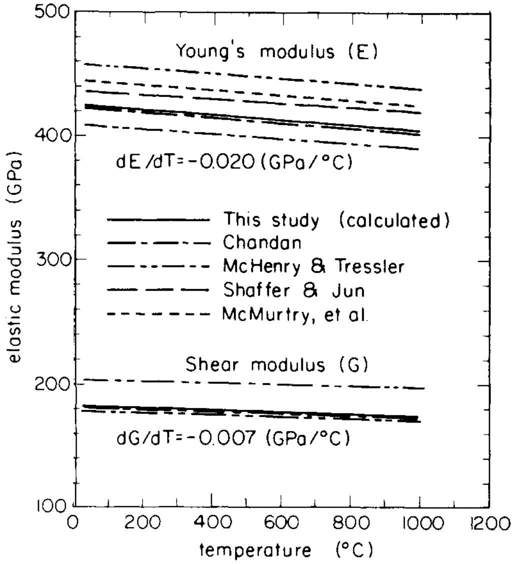

Fig. 2. Polycrystalline elastic moduli of hexagonal SiC as a function of temperature.

TABLE 3
Calculated Elevated Temperature Polycrystalline Values of Young's Modulus, Shear Modulus and Poisson's Ratio for Hexagonal SiC

T (°C)	*Young's Modulus E (GPa)*	*Shear Modulus G (GPa)*	*Poisson's Ratio* ν
20	420	180	0·17
200	416	178	0·17
400	412	177	0·17
600	408	175	0·16
800	404	174	0·16
1 000	400	173	0·16

STACKING LAYER SEQUENCE EFFECTS

The tensor transformation method discussed for estimating the single crystal elastic constants and their temperature dependencies for hexagonal SiC is based on the assumption that the effects of the stacking layer sequences in the [0001] directions of the hexagonal SiC structures on those structures' elastic constants are the same as along the [111] direction for the cubic SiC structure. The results of Feldman *et al.*[5] and those of Vetelino and Mitra[6] substantiate that this is indeed the case. However, the stacking layer sequences of the various hexagonal polytypes of SiC in the [0001] direction are different. The cubic (3C) polytype of SiC has the pure cubic stacking layer sequence of ABCABC, while the hexagonal (2H) polytype of SiC has the pure hexagonal stacking layer sequence of ABABAB. It is possible to describe the remainder of the hexagonal SiC polytypes on a percentage of hexagonal stacking fraction. On that basis, the percentage of hexagonal stacking layer sequence for the (4H), (6H), and (8H) polytypes are 50%, 33%, and 25%, respectively. It is obvious that the longer period polytypes are all less hexagonal in stacking layer sequence content than the (2H) polytype. Since the previous derivation of the 'pure' hexagonal layer stacking sequence (2H) polytype single crystal elastic constants from the (3C) cubic values have been demonstrated to yield excellent agreement for the ZnS case, it may be assumed that the results achieved in this study for the (2H) SiC will apply equally well to the other hexagonal SiC polytypes. On this basis it is concluded that the SiC hexagonal single crystal stiffnesses, C_{ij}^{h}, which have been determined in this study can be applied to all of the hexagonal polytypes of SiC.

The single crystal elastic constants of the rhombohedral (R) structure polytypes of SiC and their temperature dependencies can also be estimated using this same tensor transformation approach. However, besides C^r_{11}, C^r_{33}, C^r_{12}, C^r_{13}, and C^r_{44} values, the C^r_{14} value is not equal to zero for the rhombohedral polytypes. This general approach can also be readily extended beyond the polytypes of SiC as similar procedures can also be applied to all other polytype structures with similar, or different structural relationships.[22]

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