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STABILITY, LATTICE PARAMETERS, AND THERMAL EXPANSION OF β -CRISTOBALITE: A DISCUSSION

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Aumento (1966) has stated that I "erroneously calculated" a value of 8.53×10^{-6} °C⁻¹ for the linear coefficient of expansion of high cristobalite. This unfortunate remark carries with it a disparaging implication of arithmetical ineptitude. The figure is incorrect in the reference, Lukesh (1942), to be sure, but had Aumento quoted a correct value (one based on the data which were available and which he presumably correctly calculated) of 8.93×10^{-6} , the high probability of a typographical error would have been quite obvious to the discerning reader. The reference cited was the abstract of a paper read by title only at the 1941 meeting of the Mineralogical Society of America held in Boston. Since pre-publication proofs of such abstracts are not provided to the authors, the error could not be noted and, hence, remained uncorrected.

That Aumento did not report the correct value is, perhaps, because the rather low values of the lattice constants "seem unacceptable" to him. The fact that the constants were smaller than any previously reported was commented on in the abstract. So, too, was the synthetic origin of the material studied in the earlier work noted, although it was not mentioned there that it was prepared by devitrification of a high quality, laboratory grade vitreous silica. This latter point is of importance because it suggests that the product was considerably less cluttered with impurities than was that used by Aumento. His method of preparation from stilbite was hardly conducive to the formation of pure silica, and he himself admits that his product "is stuffed with aluminum in solid solution." From the apparent relative purities of the two samples, one can well suspect that the "unacceptable" low values of the lattice constants are more representative of the true constants of pure silicon dioxide in the high cristobalite phase than are the appreciably larger ones of Aumento. Indeed, the constants reported by Büssem *et al* (1935), which were also unacceptable to Aumento, lie between his and mine. The wide scatter in values found throughout the literature is most easily explained by variations in impurity content from sample to sample. In addition to causing lattice expansion, solid solute atoms also are capable of stabilizing a phase below its normal displacive transformation temperature, a fact noted by Aumento in connection with the persistence of his high phase at room temperature. The unacceptability of my lattice constants has not been adequately demonstrated.

It is of interest and also informative to compare the value (non-erroneously calculated, of course) of the coefficient, 8.93×10⁻⁶, °C⁻¹, to that of Aumento. He finds a coefficient of 10.9×10^{-6} for the temperature range 100°C to 500°C, and it is presumed that this is an average over the range, just as the smaller value is an average over the range from 275°C to 480°C. (I was unable to extend the range to a lower temperature because the cristobalite transformed to the low phase in the manner of pure, well-crystallized material.) Aumento further states that the value decreases to " 1.7×10^{-6} between 500°C and 1000°C," and it is reasonable to assume that the decrease is close to a straight line function of temperature, a notion that is not incompatible with the diagram of Sosman (1927, p. 394). Now the effect of solid solutes on the expansion coefficient of a host crystal is of a lower magnitude than is their effect on the lattice constants so that it is quite in order to make a first approximation comparison of the two values. A simple straight line plot drawn through the value of 10.9 at the median temperature of 300°C and through 8.93 at 377.5°C will pass through 1.7 somewhere "between 500°C and 1000°C." This is admittedly a crude device, but it does serve to show that the two coefficients are far from incompatible.

It is not necessary or proper to discard my linear coefficient of expansion; the later work of Aumento serves as confirmation of its basic validity. Nor should the lower values of the lattice constants be summarily dismissed simply because they "seem unacceptable" unless and until they have been shown to be incorrect through further and more definitive work with specimens, of known purity, thermal history and perfection of crystallinity, which also behave in the manner shown in the classic work of Fenner (1913).