

It may be seen from the above analytical expressions and also from Figs. 1 and 2 that with increasing temperature the lattice spacing increases in a non-linear manner, the non-linearity being slightly enhanced for the Cu-9.25 at.% Ge alloy (Fig. 2). From Fig. 3 as well as from the analytical expression it is apparent that for Ag-Ge alloys there is a gradual linear decrease in the thermal expansion coefficient  $\alpha = (1/a_0)(da_T/dT)_p$ , with increase in temperature (from  $\sim 25$  to  $\sim 17 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ ). For Cu-Ge alloys (Fig. 3), the expansion coefficient  $\alpha$  for the initial composition (Cu-3.05 at.% Ge) is also found to decrease linearly from  $\sim 22 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$  to  $\sim 17 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ , but for the higher 9.25 at.% Ge sample the tendency is reversed and  $\alpha$  increases rather rapidly from  $\sim 15 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$  to  $\sim 32 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ . This is, however, depicted from the nature of the slopes in the  $a$ - $T$  plot (Fig. 2) and also from the coefficients in the analytical expressions for the Cu-Ge samples (i) and (ii).

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**Comments on X-ray linear absorption coefficient of silicon for Cu  $K\alpha$  and Mo  $K\alpha$  radiations by J. L. Lawrence.** By P. SUORTTI, *Department of Physics, University of Helsinki, Siltavuorenpenger 20 D, SF-00170 Helsinki 17, Finland*

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The reported large discrepancies between the measured and the tabulated absorption coefficients of silicon [Lawrence, *Acta Cryst.* (1977), **A33**, 343] are shown to arise from the neglect of the scattering contribution and probably from contamination of the incident beam by harmonic wavelengths.

The measured values of the absorption coefficient for single-crystal silicon are 12.9 and 6.8% lower than those quoted in *International Tables for X-ray Crystallography* (1974) (*ITXC*) for Cu  $K\alpha$  and Mo  $K\alpha$  radiations, respectively. However, the measured value does not include the contribution of the Bragg scattering to the attenuation, while it is accounted for in the tabulated values. According to DeMarco & Suortti (1971) this amounts in Si to 1.0% for Cu  $K\alpha$  and 3.1% for Mo  $K\alpha$ . Moreover, the tabulated values are for the weighted means of  $\alpha_1$  and  $\alpha_2$ , whereas the experimental set-up of a perfect crystal monochromator and very small apertures suggests that only one component was selected from the X-ray beam, and presumably this was the more intense  $\alpha_1$  component. This would affect the attenuation coefficients by 0.2% for Cu  $K\alpha$  and 0.6% for Mo  $K\alpha$ . Thus the difference for Mo  $K\alpha$  is reduced to 3.1%, while the value for Cu  $K\alpha$  is still 11.7%, low in comparison with the tabulated value. Recent measurements, as quoted by Inkinen, Pesonen & Paakkari (1970), for the neighboring element, Al, suggest that the value in *ITXC* (1974) for Cu  $K\alpha$  may be too high by 1 to 2%.

The reported low value for Cu  $K\alpha$  radiation probably arises from beam hardening. The attenuation of Cu  $K\alpha$  in the 0.5 mm thick slab of Si crystal varies from  $10^3$  to  $10^6$  with  $\varphi = 0$  to  $\varphi = 60^\circ$ , while the crystal is almost transparent for  $\lambda/2$  and higher harmonics. Even a minute harmonic contamination of the order of  $10^{-5}$  in the incident beam reduces the attenuation coefficient by several percent. This amount of  $\lambda/2$  is almost unavoidable in the beam reflected from a perfect Si(111) monochromator, if the X-ray tube is run above the excitation voltage of about 16 kV. The actual amount depends on the operation conditions of the X-ray tube and on the width of the reflected  $\lambda/2$  wavelength

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band, which is in turn determined by the beam divergences. The power in the  $\lambda/2$  band is typically of the order of 1% of the characteristic radiation [see, for example, *ITXC* (1962) p. 151]. For a perfect Si crystal, the reflecting power of 222 is about 1% of that of 111 (Aldred & Hart, 1973), and a PHA (pulse-height analyzer) may reduce the  $\lambda/2$  contamination by an additional factor of 10. The author implies that no curvature due to beam hardening was found in the graph of  $\log I$  against  $1/\cos \varphi$ , but it may have been concealed by other difficulties in measuring very small count rates (a few counts per second) when approaching  $\varphi = 60^\circ$ .

It may be useful to note in this context that  $\lambda/3$  and higher harmonics also cause subtle difficulties in absorption measurements. Although not counted in the PHA window set for the characteristic radiation they increase drastically the dead time of the counting sequence, as demonstrated by Suortti & Jennings (1977).

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