The Young's moduli in the three principal directions,

$$E_{100} = 1/s_{11},\ E_{010} = 1/s_{22},\ E_{001} = 1/s_{33} \qquad (3)$$

are also given in table 4 and are plotted in fig. 7 only for the 300° to 923° K range. The differences between the c_{22} and c_{33} curves and those for the corresponding E, i.e., E_{010} and E_{001} respectively, are quite pronounced, whereas, the E_{100} curve closely follows that for c_{11}. The E_{010} and E_{001} curves are, within the error of computation, straight lines in the 200° to 575° K range. Above 575° K both curves begin to decrease in slope, with very evident curvature changes.

The direction of maximum Young's modulus, E_{max}, for all temperatures above 44° K is in the (100) plane, inclined approximately 37° to the [001] direction (about 10° inclined to the nearest neighbor direction). The direction of minimum E varies with temperature, E_{010} being the smallest up to 575° K. Above 575° K the direction 45° to [001] in the (010) plane attains the minimum E value, as shown in fig. 7. The slope of the curve for the latter modulus is remarkably coincident with that for E_{max} at all temperatures above 100° K. The overall decrease from 50° to 923° K is, however, 68 % for E_{45}, in contrast to 42 % for E_{max}, E_{010} and E_{001}.

The temperature dependence of the Poisson's ratios, σ_{ij}, are shown in fig. 8. The first subscript, i, denotes the direction of the unaxial stress and the second subscript, j, denotes the direction of the coupled strain, i.e. σ_{12} is the ratio of $e_{[010]}/e_{[100]}$ for $T_{[100]}$ where e and T are the directional strain and stress, respectively. These ratios are extremely anisotropic over the range of 50° to 923° K. σ_{13} and σ_{31} are very near zero throughout the temperature range, whereas the ratios that involve the [010] direction are in the range of 0.2 to 0.5 at low temperature, increase linearly with temperature between 50° and 400° K and increase with significant positive curvature above 400° K.

4. Correlation with other physical properties

The initial objectives of this study were to obtain information that would lead to an understanding of the negative linear thermal expansion coefficient, $\alpha_{[010]}$ [5]) and the anomalous specific heat at temperatures above 350° K [7]). During the course of these measurements the existence of the transition at 41° K was established, revealing several new anomalies that also require explanation. We will attempt here to associate the elastic moduli data with the anomalies in thermal expansion and specific heat and to point out a possible relationship between the low temperature and high temperature anomalies.

4.1. The thermal expansion anomalies

Between 50° K and the temperature of the $\alpha \rightarrow \beta$ phase transformation (935° K) the three linear expansion coefficients α_1, α_2 and α_3 (subscripts 1, 2 and 3 refer to the [100], [010] and [001], respectively) are all abnormally affected by temperature changes [13]). α_1 decreases with increasing temperature to a minimum in the 100° K range and then increases continuously by a factor of two between 100° and 935° K. α_2 has a small positive value at 50° K, decreases continuously to zero at approximately 350° K and has an increasingly negative temperature dependence at higher temperatures. α_3 has a very large positive temperature dependence, increasing by a factor of almost five between 50° and 923° K.

The influence of the elastic moduli on the thermal expansion coefficients can be illustrated through the Grüneisen relation:

$$\alpha_V = \frac{C_P \beta_V \Gamma_V}{V}, \qquad (4)$$

where α_V is the volume expansion coefficient. C_P is the specific heat at constant pressure, V is the specific volume, β_V is the adiabatic compressibility [eq. (2)] and Γ_V is the Grüneisen coefficient, which for the present case, may arise from the changes with volume of 1. the average frequency of the normal modes of the lattice vibrations, 2. the density of electronic states of the Fermi surface and 3. the energy of magnetic interaction. These contributions are related to the total Γ_V on the basis of the weighted specific heat contributions: