Chapter 7

SUMMARY AND CONCLUSION

The interlattice displacements, the second-order elastic constants, the third-order elastic constants and the anisotropic low temperature thermal expansion of the high-$T_c$ superconducting compounds $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ are studied in this thesis.

General expressions for the interlattice displacements of the atoms in the unit cells of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ in terms of the strain parameters on the basis of deformation theory have been derived. Interactions up to nine nearest-neighbours have been included, while calculating the interlattice displacements. It is found that the interlattice displacements in these compounds take place in such a way that the horizontal CuO planes do not change the centre of mass of the system.

General expressions for the strain energy of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ have also been derived using the deformation theory. This has been compared with the lattice energy density obtained from the continuum model theory to obtain the second- and third-order elastic constants of these compounds. The complete sets of second- and third-order elastic constants of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ have been determined and are compared with the available experimental results.
The second-order constants obtained in the present work for these compounds show that the elastic stiffness coefficients of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ are smaller than those of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ in agreement with the experimental observations. Even though the values of $C_{11}$ for both $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ are nearly same, $C_{33}$ differs substantially. This is ascribed to the difference in co-ordination of copper in these two materials. The results of second-order elastic constants of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ conform with that expected of a layer-like material where the longitudinal elastic stiffness within the layers being substantially larger than those normal to the layers.

The third-order elastic constants which quantify the coefficients of the cubic term in the expansion of strain energy density of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ are all negative. In all the three compounds, it is found that the absolute value of $C_{333}$ is much larger than that of $C_{111}$.

The effect of pressure upon the second-order elastic constants of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ has also been studied. The pressure derivatives of the second-order elastic constants of $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ are similar to those in layered cuprates like $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. In all these compounds, the pressure derivative $(dC_{33}/dp)$ of the longitudinal elastic stiffness along the c-axis is larger than $(dC_{11}/dp)$ in the ab-plane, as would be expected in layer-like materials with weak inter-layer binding forces, where the effect of pressure causes the layers to close up substantially while decreasing the in-plane distance to a much lesser extent.

The low temperature thermal expansion of the compounds $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ is calculated using the generalised Grüneisen functions. The low temperature behaviour of thermal expansion coefficients is governed by the generalised Grüneisen functions $\gamma_1'(\theta, \phi)$ and $\gamma_2''(\theta, \phi)$ for the
acoustic modes propagating in the crystal. These generalised Grüneisen functions have been evaluated from the knowledge of second- and third-order elastic constants of these compounds. The procedure for evaluation is given. The low temperature limits of the effective Grüneisen functions $\gamma_\perp(0)$ and $\gamma_\parallel(0)$ for all the three compounds $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ are determined. The variation of mode gammas $\gamma'_\perp(\theta)$ and $\gamma''_\perp(\theta)$ as a function of $\theta$ are also studied. The values of $\gamma'_\perp(\theta)$ and $\gamma''_\perp(\theta)$ exhibit pronounced anisotropy in these systems. The low temperature limits of the volume Grüneisen functions $\gamma_v$ obtained in the present work for $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ are compared with available experimental mean acoustic mode Grüneisen $\gamma$ values.

The scheme worked out in the thesis can be extended to other superconducting compounds. The underlying physics and chemistry of these superconducting ceramic materials are manifestly quite rich and complex. The vast majority of ultrasonic and other measurements reported on these materials have been on polycrystalline ceramics. Further high resolution work on high quality single crystalline samples is needed to accurately determine the higher order elastic constants in these compounds. Nonetheless, working out the implications of the new regimes that arise with the new results reported in this thesis will help guide the experimental worker and will present interesting challenges for future research.