7. DISCUSSION OF THE RESULTS IN RELATION TO THE *P–T* DIAGRAM

7.1. Low Temperature Structural Phase Transition at 53 kbar

In the pressure range above 35 kbar four discoveries must be explained. They are the "points of inflection" (Fig. 6), the maximum of the residual resistance at 53 kbar (Fig. 7), the kink in $T_c(P)$ at 53 kbar (Fig. 2), and the *different* pressure dependence of T_c if the pressure is applied at low tempera ture (Fig. 5) rather than at room temperature. All these features are observed irrespective of the initial phase of the La sample. Since we believe that the "points of inflection" have no direct relationship to the other anomalies (cf. Fig. 10) and do not indicate a first-order phase transformation, at least not with a change of symmetry, we discuss them further below.

The most probable reason for the maximum of the residual resistance and the kink in T_c is the occurrence of a pressure-induced, low-temperature structural phase transformation. We favor, as we will explain below, a subtle *isostructural* phase transformation between two fcc phases with a very small volume discontinuity. It is suggested that the common α/α' phase boundary terminates in a critical point. Figure 10 shows, qualitatively, the anticipated situation. A single, homogeneous fcc phase is expected to exist at the higher temperatures. This picture is simple and seems to be consistent with the available experimental information. Needless to say, further experiments are necessary in order to substantiate this concept.

The residual resistance is thought to increase toward 53 kbar because of the additional defect scattering due to a growing concentration of α'-phase "droplets" (of a slightly higher density) in the α-phase matrix. At pressures above the equilibrium pressure of 53 kbar it is useful perhaps to think in terms of residual (less dense) α-phase "droplets," imbedded in an α'-phase matrix whose concentration decreases gradually with increasing pressure. Boundary scattering between grains of α and α' phase thus takes on a maximum at 53 kbar. Note, however, that the bulk of the sample must undergo a surprisingly *sharp* transition from α to α' (and back again) at 53 kbar. Otherwise, the kink of T_c vs. P should be more strongly rounded by the superconducting proximity effect.

Supposing this simple picture is correct, what might be the reason for the phenomenon's spreading over such a broad pressure interval (Fig. 7)? As mentioned before, our La samples are inevitably strongly disordered, strained samples above 35 kbar. It seems quite conceivable, therefore, that α'-phase droplets may nucleate in areas of compressional eigenstrain at a superimposed external pressure which still is considerably below the

true equilibrium pressure of 53 kbar. Also, α-phase droplets may persist well above an average external pressure of 53 kbar if they reside in an area of dilatational eigenstrain. In case this is the proper approach, one should expect that the smearing of the residual resistance maximum will diminish if the samples could be subjected to a thorough anneal while under pressure. On the other hand, annealing will have little effect in this respect if the microscopic strain fields around single lattice defects are the actual scatterers.

The sudden change of the slope of the T_c–P dependence at 53 kbar is the most interesting feature. The pressure dependence of T_c of the α' phase is (roughly) a factor of four smaller than for the α phase. In our model, with two different fcc phases at liquid helium temperature, one certainly immediately starts wondering why this might be so. It does not seem rather likely that two phases of the same substance with the same lattice symmetry and, probably, almost the same densities, stemming from a common fcc parent phase at temperatures above the critical point, are capable of such a radically different pressure dependence of T_c. The phonon spectra as well as the electronic properties and, hence, the pressure dependence of T_c should be very similar. The abrupt change of the slope dT_c/dP is all the more surprising since $T_c(P)$ *itself* shows *no* discontinuity at the phase change. Obviously, the latter fact nicely fits into our picture with two almost identical fcc phases.

We would like to suggest the following, somewhat more elaborate interpretation, which circumvents this difficulty and sketches a vivid picture of the physics, which, in our view, lies behind the plain data of Fig. 2. In Fig. 12, we have drawn a hypothetical, smooth curve for T_c (dashed line) between 35 and 80 kbar, whose extrapolation to higher pressures smoothly fits into the existing data from Fig. 1 (solid curve). On the low pressure side, the hypothetical curve touches the actual T_c–P curve at $\sim$35 kbar. The dashed curve represents a hypothetical pressure dependence of T_c for fcc La, if the 53-kbar structural transformation does *not* occur. We believe that the kink of T_c at 53 kbar comes about in the following way. The pressure-induced transformation is driven by the softening of phonon modes. This leads to a special *enhancement* of the electron–phonon coupling parameter λ and, consequently, of T_c. The enhancement increases toward the equilibrium pressure of the α and α' phases. Thus, the kink probably reflects the phonon softening near the 53-kbar phase boundary, superimposed onto a smooth general increase of λ or, equivalently, of T_c with pressure (Fig. 12, dashed line), whose origin need not concern us here. The enhancement of T_c, symmetric around 53 kbar, amounts to almost half a degree K for the "model case" sketched in Fig. 12. It is amazing that the phenomenon spreads over such a broad pressure range. Schrieffer[30] and subsequently others have discussed such a soft-mode enhancement of λ near a phase boundary. The behavior of fcc La under pressure may well be an almost perfect example in support of this point.