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Low-temperature instability of intermetallic phases.

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The thermodynamic criterion for the stability of an intermetallic phase or compound A_mB_n with respect to the components A and B at a given temperature and pressure is well known to be

$$A_mB_n \rightleftharpoons mA+nB \qquad \Delta F>0,$$
$$\Delta F=\Delta H-T\Delta S.$$

The possibility thus exists that some intermetallic phases may be formed from the elements with the absorption of heat ($\Delta H>0$), and still be stable at elevated temperatures because of the term $-T\Delta S$. Assuming no change with temperature of ΔH and ΔS, we should expect that such compounds become unstable with respect to the free elements at lower temperatures.

A survey of the literature shows that endothermic intermetallic 'compounds', resulting from combinations among the elements gold, mercury, thallium and lead, are sometimes found (Weibke & Kubaschewski, 1943).

Recent thermodynamic investigations by one of the authors (Kleppa, 1949) indicate an endothermic process for the phase Au_2Pb which is formed peritectically from practically pure gold and the liquid solution at 418° C. (Hansen, 1936). For the formation of one gram molecule of this phase from the pure liquid elements at 400° C. calculation gave $\Delta H=-2{\cdot}0\pm0{\cdot}1$ kcal. By combination with the accepted values for the heats of fusion for gold and lead, and making the additional assumption that there is no change in specific heat on fusion for these two elements, we find that the ΔH of formation for Au_2Pb is $\sim +0{\cdot}5$ kcal./g. molecule at 400° C.

One would expect that at lower temperatures this compound would break down to give free gold and free lead, or some other intermetallic phase, by a diffusion transformation which would be very slow. It was hoped, however, that a suitable combination of cold work and correct temperature would speed the decomposition.

The compound Au_2Pb was prepared by melting 99·9 % pure gold with 99·98 % pure lead 0·1 % in excess of the stoichiometric proportion, and annealing the ingot in vacuum 100 hr. at 400° C. to eliminate segregation. The diffraction pattern of the annealed material showed only the lines of Au_2Pb (Perlitz, 1934).

All analysis for phases present was done by X-ray diffraction, using the General Electric XRD-3 X-ray spectrometer.

The Au_2Pb phase is very brittle, so cold working was done by crushing in a 'diamond' mortar. It was found that as the material was reduced to a powder small plates formed indicative of some ductile material present as a binder. These plates were brittle and readily reduced to a powder in an agate mortar. Both the plates and the powder gave diffraction patterns of Au_2Pb plus gold. An estimated maximum of 30–50 % transformation was obtained.

In the as-worked condition the lines are quite broad, owing to strain and probably to small particle size, but annealing in vacuum for 1–2 hr. at 300° C. sharpens the lines with no detectable change in the amounts of the two phases present.

The other decomposition product almost certainly is $AuPb_2$, though it was found only in two specimens that had been crushed in oil and annealed in vacuum at 200° C. The strongest $AuPb_2$ lines lie close to strong Au_2Pb lines and may be present but unresolved in other specimens.

Lattice-parameter determinations gave for the Au_2Pb both in the pure and partially transformed material $7{\cdot}93\pm0{\cdot}01$ A. and for the gold in the transformed material $4{\cdot}078\pm0{\cdot}003$ A., the same as pure gold within the limits of error.

Annealing the transformed material 48 hr. at 400° C. returned it to the single phase, Au_2Pb.

Work is being continued to determine the decomposition products and the equilibrium temperatures.

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The one-dimensional crystal. III. A punched-card method for computing structure factors.

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Two methods for calculating structure factors on International Business Machines have already appeared in this *Journal* (Donohue & Schomaker, 1949; Grems & Kasper, 1949). The present method, however, may still be of interest because it is straightforward and particularly rapid for crystals of low symmetry.

The position of each atom is determined by only one co-ordinate, X; the reflection hkl is designated by only one index, H; the angle HX is expressed in cycles:

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