PHYSICAL REVIEW B VOLUME 16, NUMBER 10 15 NOVEMBER 1977

Comment on "Evidence for temperature dependence of positron trapping rate in plastically deformed copper" by P. Rice-Evans, T. Hlaing, and I. Chaglar

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(Received 16 December 1976)

Temperature-dependent changes near liquid He temperatures in the Doppler-broadened line from positron annihilation in deformed Cu are attributed to thermally activated detrapping from grain boundaries.

Almost all of the early publications on the temperature dependence of positron-annihilation energy spectra in metals have ignored the range $4.2 < T < 77$ K, but three papers presented at the latest conference on positron annihilation revealed evidence of surprisingly strong temperature dependence in this interval. An incomplete summary of the results is that (i) line broadening for $T \rightarrow 4.2$ K was observed[1] for deformed Cu but no temperature dependence for annealed Cu; (ii) line broadening for $T \rightarrow 4.2$ K was observed[2] for Cu specimens containing voids and for Cu specimens containing dislocation loops but no temperature dependence for annealed or electron irradiated Cu; (iii) line narrowing for $T \rightarrow 4.2$ K was observed[3] in annealed Cd and Au and in quenched Au but not in electron-irradiated Au nor in annealed Cu. Two of these papers have been published subsequently[4,5] and in the former an explanation of the anomalous temperature dependence was proposed in terms of a varying trapping cross section. While such a phenomenon is not impossible, nor even unlikely, it does not suffice to explain the line narrowing in the annealed specimens[3] and seems to be in conflict (perhaps only superficially) with the temperature independence for the electron-irradiated Au,[3] or Cu.[2] We propose an alternative explanation based on thermally activated positron detrapping from shallow traps.

There is no consensus on the types of positron traps generated by room-temperature deformation in Cu but it seems clear that two or more types result. We will make the nonessential but simplifying assumption that only two types of traps are present, dislocations and grain boundaries. Each annihilation event will then belong to one of three classes: (a) free positrons, (b) positrons trapped in dislocations, or (c) positrons trapped in grain boundaries. If the defect density is very high there will be almost no free annihilations at $T = 0$ and the events will be distributed between the last two classes, the proportions being determined primarily by the defect densities and trapping efficiencies. Suppose that one of the traps is deep enough to localize the positrons at very low temperature but not under the influence of a flux of phonons. The effect of an increase of temperature would be to change the balance so that more annihilations would occur in the deeper traps. The overall result would then be line broadening for $T \rightarrow 4.2$ K from above as observed in Ref. 4. Annealing studies of deformed metals show very large line-shape changes when dislocations are swept out by recrystallization but little if any detectable change at the higher temperatures where grain growth reduces grain-boundary volume.[6] We conclude, therefore, that the deep traps are dislocations and the shallow traps are grain boundaries. We now consider the possibility that grain boundaries or other very shallow traps can also account for the line narrowing observed in Au and Cd. In this case we assume that annealing succeeds in removing a very high proportion of deep traps—an assumption which is implicit to many studies in this field and is reinforced by the lack of long-lifetime components in the time spectra of annealed metals.[7] It is not, however, possible to remove all nonequilibrium defects in a metal and hence we can be sure that some potential positron traps are present in even the most carefully annealed specimens. At $T = 0$, the fate of each positron is to annihilate in a free state or in a shallow trap. Detrapping at higher temperature causes an increased fraction of free annihilations and thus we are led to expect line narrowing as $T \rightarrow 4.2$ K from above. This is, of course, consistent with the observations in annealed Au and Cd. The absence of such an effect in annealed Cu is surprising but, considering that the traps in Au and Cd are so shallow that detrapping is complete at 100 K, it is conceivable that the equivalent traps in Cu are too shallow to cause an observable effect.

We have not dealt with the unpublished data of Ref. 2 which presents additional uncertainties because of the temperature dependence of the specific trapping rate with these extended defects.

The postulate that detrapping from shallow traps can account for the low-temperature anomalies in Refs. 4 and 5 can be put to a simple test. Severe deformation followed by annealing at a temperature slightly above the recrystallization stage should produce a specimen with a large grain-boundary volume but very low dislocation density within the grains. We would anticipate that such a specimen would show an exaggerated version of the low-temperature behavior seen in annealed Au and Cd, i.e., heavy deformation plus recrystallization should show a reverse of the behavior seen for deformation alone. The test should be done in either Au or Cd since we know of no conclusive evidence of grain-boundary trapping in Cu.

One final point is that shallow traps may introduce confusion and fundamental limitations on the resolution when studying Fermi surfaces at very high resolution. Experiment may well show that in Au, Cd, and possibly many other metals it will not be possible to take full advantage of the complete thermalization[8] at 4.2 K which has been demonstrated in Mg and Al.

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