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Positron lifetime analysis of dislocations arising from tensile strain

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Abstract. Aluminium samples in the form of single crystals were treated by uniaxial tensile strain, so that dislocations were practically the sole type of defect produced. A positron lifetime study of these samples, carried out at different dislocation densities, and in a wide temperature range, gives information about the mechanism of positron trapping, including trapping rates, binding energy and the development of defect density with deformation and applied stress.

1. Introduction

For more than 25 years the positron annihilation method has been applied to study the creation and presence of defects in metals. However, this promising and often useful method has scarcely reached the stage where the positron observations can be interpreted unambiguously in terms of a spectrum of defects. In particular, it appears difficult to clarify the role of the most enigmatic defect, the dislocation, which in the literature is described some times as a deep, and at other times as a shallow positron trap. In the present work we attempt to obtain improved information about the dislocation, by producing and studying metal samples containing as little as possible of other defect types.

The original samples were single-crystal strips of pure aluminium, which were subjected to uniaxial tensile stress in steps of increasing magnitude, providing samples with different degrees of strain. After such a treatment the content of defects was expected to consist almost exclusively of dislocations, free from interference caused by vacancy-type defects, grain boundaries or impurities. Positron lifetime spectra were recorded at a range of temperatures. We propose, and apply, a model which appears to be suitable for the analysis of the data in terms of the positron trapping mechanism, binding energy and defect density.

2. Experimental method

The aluminium samples consisted of two rectangular strips, measuring $26 \times 4.6 \times 0.65$ mm^3, which were cut from a single crystal of purity 99.9999%, annealed at 620 °C, and thereafter electropolished. In a number of stages each strip was subjected to an uniaxial elongation along the longest edge, at room temperature, to produce samples with the values of strain $\epsilon = \Delta l/l = 0.8$, 2, 4, 7, 11, 16 and 28%. The positron lifetime equipment was of a

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conventional type. A ^{22}NaCl positron source wrapped in thin nickel foil was sandwiched between two sample strips, and positioned in a closed circuit cryostat. Positron decay spectra were observed by a pair of NE102A scintillators, being part of a fast–slow lifetime spectrometer, having a time resolution corresponding to 280 ps FWHM. For each set of samples, including the undeformed one, positron lifetime spectra were obtained at a series of temperatures between 16 and 292 K.

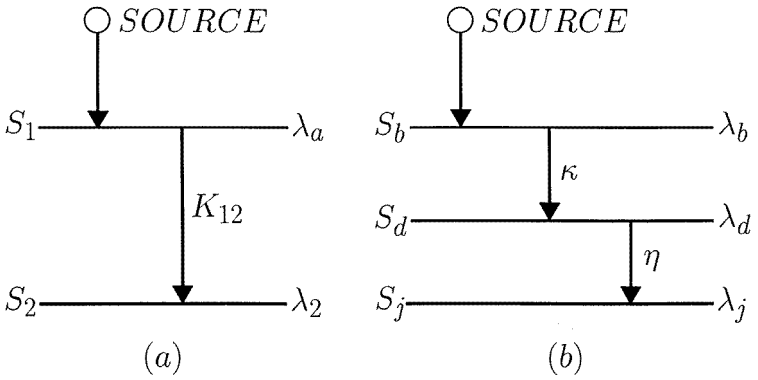

Figure 1. (*a*) The two-state and (*b*) the three-state positron trapping model. S_x represents occupation of state x. Other symbols are explained in the text.

The raw experimental data were treated with the computer program PATFIT-88 (Kirkegaard *et al* 1989). For the resolution function it was found satisfactory to employ a single Gaussian with FWHM about 292 ps. However, in order to obtain the statistically most trustworthy results, it appeared necessary to establish a specific resolution width for each new mounting of a set of samples. The best choice of FWHM could vary within about 5 ps. One reason for these variations could be the difficulty of ensuring that the mountings of source, sample and scintillators are exactly identical in every case. Clearly, a change in the geometrical setup of the order of 1 mm could give rise to timing differences of about 3 ps, due to a change in the distribution of path lengths for gamma rays and light phonons.

A source correction of 7.2% was subtracted before further data treatment.

3. The two state trapping model

In a numerical analysis of the experimental data for deformed aluminium it was found sufficient to employ the two-state trapping model (Brandt 1967), since in the present case this gives a very satisfactory fit to the observations at all deformations and temperatures. The notation of the model is given in figure 1(*a*). For the final state (S_2) we find the mean lifetime $\tau_2 = \lambda_2^{-1} = 220 \pm 2$ ps, which is valid for all values of ϵ, but most reliably determined in the case of largest deformation, $\epsilon = 28\%$. τ_2 was constrained to this value for the final analysis. Results from the undeformed and annealed single-crystal sample provide essentially only one lifetime component, representing annihilation in bulk metal. Its average value is $\tau_b = \lambda_b^{-1} = 153 \pm 1$ ps, increasing slightly with temperature. For the deformed samples, the analysis provides the quantities $\tau_1 = \lambda_1^{-1}$, I_1 and $I_2 = 1 - I_1$. In computing $\lambda_a = I_1\lambda_1 + I_2\lambda_2$ one generally finds that λ_a^{-1} is slightly higher than τ_b by a couple of picoseconds. The two-state positron trapping rates $K_{12} = (\lambda_a - \lambda_2)I_2/I_1$ have been plotted in figure 2 for some of the observed deformations and temperatures.

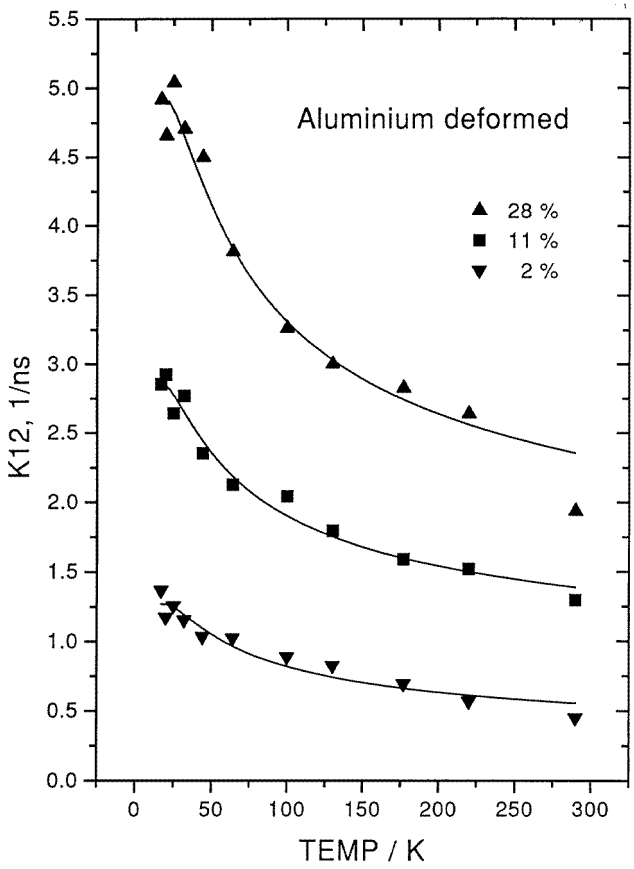

Figure 2. Experimental results expressed in terms of positron trapping rate K_{12}, as a function of sample temperature, for three different degrees of deformation.

4. The three-state trapping model

A physical interpretation of the experimental data has been based of the following assumptions.

(i) The defect content of the aluminium samples, deformed by uniaxial stress, consists mainly of dislocations, with very little, if any, admixture of free point defects. Dislocation jogs will appear increasingly as deformation is increased.

(ii) Positrons can be trapped to dislocations (trapping rate, κ), where they are weakly bound, with binding energy E_b, of the order of 0.05 eV (Martin and Paetsch 1972). In the narrow free space of a dislocation the positron lifetime is short, $\lambda_d \approx \lambda_b$.

(iii) The wavefunction of the trapped positron expands along the axis of the dislocation, causing interaction with other defects, such as jogs (Doyama and Cotterill 1979). The trapping rate η into jogs is fast, depending upon jog density, but not greatly influenced by temperature.

(iv) For a positron trapped into a jog, the annihilation rate, λ_j, is expected to be similar to, but somewhat faster, than the annihilation rate in a vacancy.

The trapping model resulting from these considerations is illustrated in figure 1(*b*), where

positron transition rates from bulk metal to dislocations and from dislocations to jogs are indicated, while, for the present purpose, we shall neglect detrapping from the dislocation-bound state to bulk metal. This model is quite analogous to the scheme proposed by Smedskjaer *et al* (1980), but here, in order to seek a connection between experiment and theory, with a possibility of deriving numerical results, we employ a coarser, although more concretely applicable model.

When solving the set of differential equations describing this system (in a manner analogous to the discussion by Pagh *et al* (1984)), one finds that the positron decays with a time dependence consisting of three exponential terms, having rates $\alpha = \lambda_b + \kappa$, $\beta = \lambda_d + \eta$ and λ_j, with the apparent intensities (as extrapolated to $t = 0$)

$$\begin{aligned} I_\alpha &= 1 - [\kappa/(\alpha - \beta)][1 - \eta/(\alpha - \lambda_j)] \\ I_\beta &= [\kappa/(\alpha - \beta)][1 - \eta/(\beta - \lambda_j)] \\ I_j &= \kappa\eta/[(\alpha - \lambda_j)(\beta - \lambda_j)] \end{aligned} \tag{1}$$

respectively, where $I_\alpha + I_\beta + I_j = 1$.

In order to interpret the observed two-state-analysis data in terms of the three-state model, we note, as mentioned above, that $\lambda_d \approx \lambda_b > \lambda_j = \lambda_2$. The decay rates α and β are faster than λ_d, and cannot be resolved in the detecting process. Therefore, in the two-state analysis the observed fast decay rate must be a combination of α and β,

$$\lambda_1 = \tau_1^{-1} = (I_\alpha\alpha + I_\beta\beta)/(I_\alpha + I_\beta) \tag{2}$$

with $I_1 = I_\alpha + I_\beta$. Setting $\lambda_b - \lambda_j \approx \lambda_d - \lambda_j = \Delta\lambda$, we obtain the intensity of the longer-lifetime component

$$I_2 = [(1 + \Delta\lambda/\kappa)(1 + \Delta\lambda/\eta)]^{-1} \tag{3}$$

which in terms of the observed trapping rate is

$$I_2 = (1 + \Delta\lambda/K_{12})^{-1}. \tag{4}$$

Comparison between the observed and the real trapping rate to dislocations gives

$$\kappa = K_{12}(1 + \Delta\lambda/\eta + \kappa/\eta) \tag{5}$$

showing that the calculated K_{12} is a lower limit of κ, valid in the case where $\eta \gg \Delta\lambda$.

5. The temperature dependence of the trapping rate

Provided that it is justified to neglect detrapping of positrons from dislocations, and under the condition that η is basically a constant, the temperature dependence of K_{12} must be ascribed to the trapping rate $\kappa(T) = D\nu(T)$. Here, we introduce the specific trapping rate ν into a unit length of dislocation, and D, the density of dislocations. In order to discuss $\nu(T)$ we again use the same arguments as Smedskjaer *et al* (1980), but here with less detail. However, we try to be more specific with respect to possible comparisons with experiments.

As the binding energy for positron trapping in dislocations is expected to be very low, the dominant trapping mechanism will be the emission of an acoustic phonon (Bergersen and McMullen 1977, Smedskjaer *et al* 1980). With E_+, E_b and E_p being the energies of the free positron, of its binding in the dislocation, and of the emitted phonon, respectively, the energy balance becomes

$$E_+ = E_p - E_b. \tag{6}$$

Assuming the Debye approximation, we have a maximum for the phonon energy, $E_D = k\Theta$, where Θ is the Debye temperature, and k is the Boltzmann constant. This means that there is a maximum energy for the positrons that can be trapped,

$$E_{+,max} = E_D - E_b. \tag{7}$$

In terms of the golden rule, the specific positron trapping rate at temperature T can be written as

$$\nu(E_+, T) = 2\pi\bar{h}^{-1}|M_{if}|^2 n_+(E_+, T) n_p(E_p, T) \tag{8}$$

where M_{if} is the positron trapping matrix element, $n_+(E_+, T)$ is the density of positrons and $n_p(E_p, T)$ is the density of final states, expressed in terms of phonon energy. We denote $2\pi\bar{h}^{-1}|M_{if}|^2 = \nu_1(T)$, being the basic trapping rate into a dislocation, here not necessarily considered to be temperature independent.

It can be expected that the range of emitted phonon energies, $[E_b;\ E_D]$, is considerably smaller than E_D itself, so, for a given T, the quantities ν_1 and n_p will be nearly constant in that interval. This assumption is supported by the final results obtained for E_b. At high temperatures, $T \geqslant \Theta$, the phonon occupation number is expected to be proportional to T, while the temperature dependence of n_p is less well known in the region between about 0.1Θ and Θ. Since also ν_1 may be temperature dependent, we introduce an adjustable exponent μ, so that $\nu_1(T)n_p(T) \approx \nu_0 n_0 T^\mu$ with ν_0 and n_0 being constants.

The thermalized positrons obey the Boltzmann distribution,

$$n_+(E_+, T) = 2\pi^{-1/2} E_+^{1/2} (kT)^{-3/2} \exp(-E_+/kT). \tag{9}$$

Integration over positron energies is now expressed as

$$\nu(T) = \nu_0 n_0 T^\mu \int_0^{k\Theta - E_b} n_+(E_+, T)\, \mathrm{d}E_+ \tag{10}$$

where the integral has no analytic solution. For the purpose of fitting a function to the experimental data, we replace the integral in (10) by

$$A[1 - (1+s)^{2/3} \mathrm{e}^{-s}] \tag{11}$$

where $s = (\Theta - E_b/k)/T$. Expression (11) differs from (10) by not more than 3% in the region $0.3 \leqslant s \leqslant 5$, when $A = 1.02$†.

6. Results and discussion

Of the two lifetimes emerging from the application of the two-state trapping model, the longer one is consistently found to have the value $\tau_2 = 220 \pm 2$ ps, interpreted as the positron lifetime in a typical dislocation jog. This is, as expected, slightly lower than the positron lifetime in a vacancy, known to be about 245 ps. The shorter lifetime, λ_a^{-1}, is found to have values slightly higher than, on average by about 2 ps, the bulk metal value, $\tau_b = 153$ ps, but this difference has only been determined with a poor accuracy. Recalling that λ_a is expected to be the unresolved average between the decay rates λ_b in bulk and λ_d in a dislocation line, we conclude that the magnitude of λ_d^{-1} must be in the region of 155–160 ps.

By use of the expression

$$K_{12} \approx \kappa = cT^\mu [1 - (1+s)^{2/3} \mathrm{e}^{-s}] \tag{12}$$

† Another analytic expression, also providing a reasonable approximation to (a), has been given as $\nu_s(T) = \nu_0[1 + \rho \exp(-\gamma T)]$, in which case $\gamma^{-1} \approx 2(\Theta - E_b/k)$ (Trumpy 1994).

curves have been fitted to the experimentally obtained values $K_{12}(T)$ in order to determine the best values for the parameters c, μ and s, where $c = D\nu_0 n_0 A$. We may expect that the exponents μ and s are largely independent of the degree of deformation. Applying this condition in the curve-fitting process, we first found the statistically best value for μ, common for all strains. Thereupon, with this value used as a constraint, the best value for sT was found, and finally, when also sT had been constrained, we obtained c as a function of the strain ϵ. The results are $\mu = 0.76 \pm 0.04$ and $sT = 28.7 \pm 4.7$ K, and the results for $c(\epsilon)$ are plotted in figure 3. These final results were used to draw the continuous lines in figure 2, showing the best fit of the model for some of the experimental data.

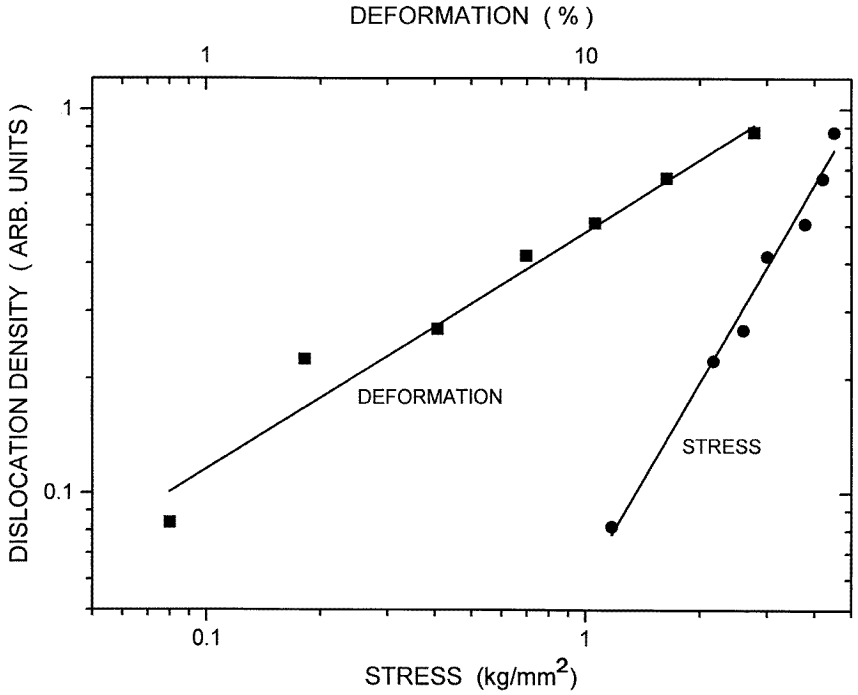

Figure 3. Observed relative variations of the dislocation density, expressed in terms of the factor c, as a function of longitudinal deformation (squares) and applied stress (circles).

With $\Theta(\mathrm{Al}) = 394$ K, and the value for sT, one obtains the binding energy for positrons in a dislocation line, $E_b = 31.0 \pm 0.4$ eV. This appears to be consistent with previous dislocation-related results for E_b in nickel (38 ± 10 meV) (Trumpy 1994) and in zinc (40 ± 20 meV) (Hidalgo *et al* 1987). Since $E_b/k = 365$ K, it is seen that the assumption of a small detrapping rate has been justified for observations below room temperature. However, it is apparent from figure 2 that the observed values for K_{12} at room temperature fall somewhat below the calculated curves, as must be expected when the detrapping effect is neglected in the curve fitting.

The value obtained for μ is related to two different physical properties. For the applied range of temperatures, it may be reasonable to set $n_p = n_0 T^{(1+\gamma)}$, where γ is expected to be a small positive number. In this case we have $\nu_1 = \nu_0 T^{-(0.24+\gamma)}$. The negative T dependence of ν_1 has a parallel in the behaviour of positron trapping rates K_v into vacancy-like defects, which were shown to obey the relation $K_v = a + bT^{-1/2}$ (Trumpy

and Petersen 1994). These results are at variance with a long-standing theoretical statement that the trapping rate matrix element M_{if} is independent of T, in analogy with slow neutron absorption in nuclei (Hodges 1970, 1974, Brandt 1974). The derivation of this result hinges on the condition that the penetration factor $\mathcal{T}$ for entering the potential well is proportional to the particle velocity v. This requires that the potential has a steep edge, and is deep compared with the energy of the incoming particle. Neutrons interacting with nuclei are clearly obeying this rule, but its applicability to positrons and dislocations (or vacancies) is not quite evident. One can also consider the phase shift of the particle wave as it passes through, and is emitted from the other side of the potential well. In the case of a very small phase shift, the factor $\mathcal{T}$ is almost independent of v. For neutrons on nuclei the phase shift is many radians, but for positrons on dislocations it amounts to about 0.2 rad. As a consequence of these considerations we believe that the theory for the matrix element for positron trapping at dislocations (and at vacancies) would not necessarily predict temperature independence, indeed, a resulting negative temperature coefficient should be expected.

Figure 3 shows the value of c, which is proportional to dislocation density D, as a function of strain, and, on the right, as a function of stress. In both cases one obtains roughly a linear dependence for the data when they are presented in a log–log diagram. The straight lines in the figure represent the relationships

$$D = C_\epsilon \epsilon^{0.62} = C_\sigma \sigma^2 \tag{13}$$

where C_ϵ and C_σ are constants. We note with interest the parallel between our result and the old observation that the dislocation density D is proportional to the square of the applied shear stress (Hayden *et al* 1965). In view of the assumptions that the defects are dislocations, and that our model is applicable, this is a reassuring information.

7. Conclusion

We have presented a method which can be used to study the positron trapping mechanism in dislocations, and to investigate changes in the dislocation network as a function of deformation. Numerical data have been given for positron lifetimes, for the binding energy in a dislocation and for the variation of dislocation density with tensile stress and strain, in the case of pure aluminium. In view of the obtained results, we believe that the model is basically sound, and can be used for a consistent analysis of positron annihilation data in the presence of dislocations, even when other defect types, such as vacancies and grain boundaries, complicate the observation. In the form presented here, the method is rather coarse, although reasonably reliable for the range of data studied. As possible extensions, in a data analysis covering higher and lower temperatures, one could include detrapping of positrons from the dislocation line, and the analytic expression representing the integral in equation (10) could be extended, for instance by introduction of additional terms. Further, instead of using the Debye approximation, one could try the quite elaborate process of employing a more realistic spectrum for available phonon states.

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